

Article

Conformational states of the CXCR4 inhibitor peptide EPI-X4 - a theoretical analysis

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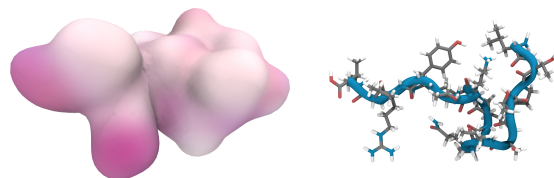
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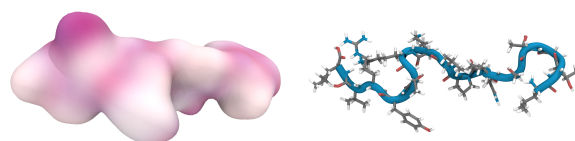
1. SI

Here, the distance between all possible amino acid residue pairs of the three-dimensional peptide structure is represented using a two-dimensional matrix. The ij element of the matrix is colored darker, depending on how close the two residues are. The distance between atoms i and j (*i.e.* the bond C_i-C_j) atom has been established at the threshold of 11 Å. Figure (see SI (f)) also shows the contact map for the published EPI-X4 structure (N1).

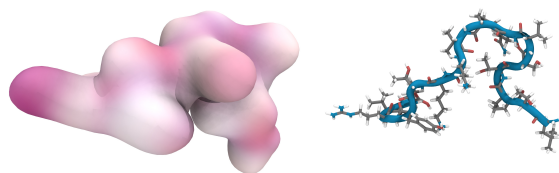
(a) Conformer C001



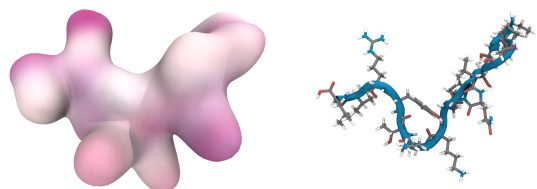
(b) Conformer C026



(c) Conformer C054



(d) Conformer C090



(e) Conformer C125

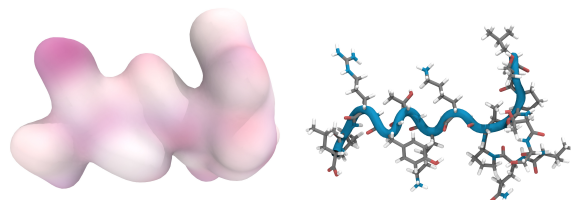


Figure S1. Charge distribution of selected conformers gained from ReaxFF structure optimizations.(a) Conformer 001 as the energetically favored conformer, (b)-(e) conformers C026, C054, C090 and C125. Red color refers to negatively charged areas, white represents charge neutrality and blue would refer to positively charged areas of the structures. On the right side are schematics of the conformers shown.

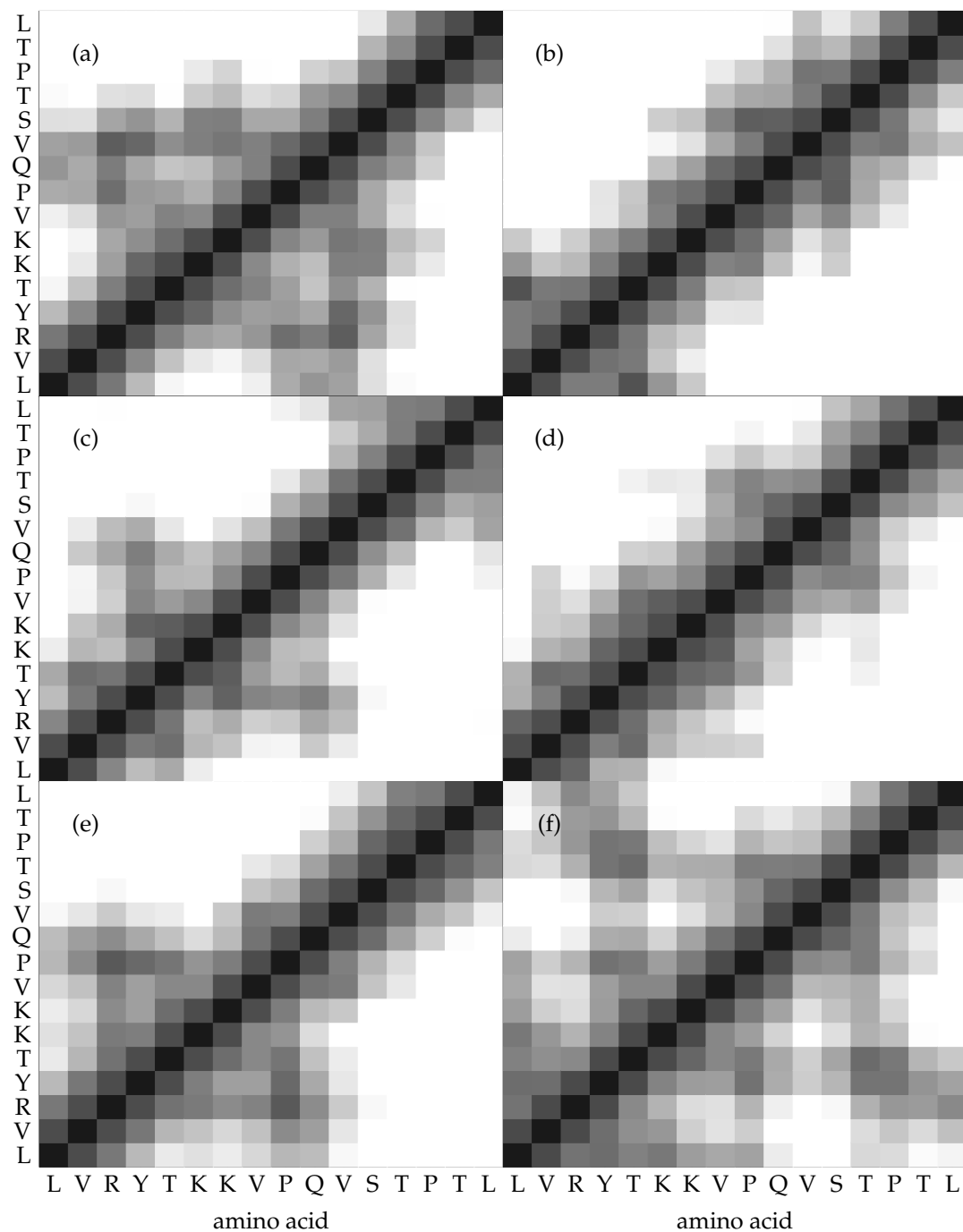


Figure S2. Contact maps of certain conformers: (a) Conformer 1 as the energetically favoured structure (b)-(e) conformers C026, C054, C090 and C125 (f) NMR conformer N1. White stands both for a distance of 11 Å and more, black for 0 Å. The gray tones are linearly interpolated between white and black.

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1 EPI-X4 xyz structures

The stable structures in comparison with the NMR structure (and this one).

Listing 1: C00001.xmolout

1	276								
2	150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	1.7765	7106	
	0.2500	300.00	0.00	0.00	0.00	-1295.6273	0.0000	300.0000	
3	H	67.50467	66.03206	73.75534	-2043.14101	-1757.64893	399.89339	1	
4	N	67.90687	66.60675	74.49259	426.75047	490.45733	-334.42467	1	
5	H	67.09319	66.85163	75.05133	442.25559	-1110.30854	-2448.52907	1	
6	C	68.70489	67.69291	74.07796	415.32972	-666.39213	83.73172	1	
7	H	69.30200	67.30130	73.22781	879.32219	2491.00447	667.35213	1	
8	C	67.74093	68.92001	73.68223	31.35357	477.41777	628.23362	1	
9	H	67.18670	69.25304	74.59262	1168.38489	2240.25337	-1019.71136	1	
10	H	68.35145	69.79807	73.36012	-360.43770	2534.90498	931.67112	1	
11	C	66.77373	68.51515	72.59811	463.18208	512.70242	-382.34388	1	
12	H	66.25868	67.57969	72.91111	1725.29117	1863.52247	-987.07854	1	
13	C	65.71525	69.59270	72.39998	710.42801	-144.27427	-313.15367	1	
14	H	64.97212	69.30247	71.61282	364.20195	-1033.13725	2494.72524	1	
15	H	65.14128	69.78840	73.34251	2567.61904	335.80679	847.48802	1	
16	H	66.17203	70.56514	72.08157	-2587.99029	680.92867	-512.16411	1	
17	C	67.49361	68.25718	71.28184	268.17616	741.64379	-40.42634	1	
18	H	66.77736	67.97373	70.46770	1283.54314	-1945.37420	-1411.27812	1	
19	H	68.05007	69.16522	70.93229	-1258.57796	1317.15249	-2026.02085	1	
20	H	68.23920	67.42568	71.37139	-2502.84526	909.80597	575.92391	1	
21	C	69.58912	68.12512	75.37727	619.36578	-458.64843	-172.09273	1	
22	O	69.10705	68.76066	76.29653	-81.40433	433.87611	522.34594	1	
23	N	70.85223	67.72967	75.22088	175.23996	-622.20190	341.55523	1	
24	H	71.07607	67.17914	74.39208	-876.57256	-303.22879	-2561.90213	1	
25	C	71.59349	67.54527	76.43883	-571.88214	-534.10783	-106.15033	1	
26	H	70.79727	67.52437	77.21635	-2713.20841	-16.25800	-248.80809	1	
27	C	72.44684	66.19917	76.31609	166.60354	288.16399	-716.09568	1	
28	H	73.18667	66.31682	75.47840	-2097.85574	1636.78449	-586.18044	1	
29	O	71.69000	65.01068	76.03298	-317.80580	-363.38227	484.43082	1	
30	H	72.09925	64.71701	75.19455	1863.74748	-1451.84923	1357.29467	1	
31	C	73.21840	66.20910	77.68776	503.80731	517.99032	318.51606	1	
32	H	73.94022	65.36244	77.75566	640.61020	-2157.10410	-1536.29104	1	
33	H	73.80150	67.15012	77.83254	1687.88455	465.60692	2087.56452	1	
34	H	72.51756	66.11527	78.54959	-1293.07895	-1899.88581	-1463.57452	1	
35	C	72.63430	68.78404	76.59303	-153.07550	-733.68902	248.70981	1	
36	O	73.61624	68.87146	75.87299	186.15459	-480.78787	-449.34387	1	
37	N	72.27568	69.56283	77.61520	-487.53139	543.18517	42.03850	1	
38	C	73.04234	70.72584	77.95789	-699.35871	69.34393	360.10701	1	
39	H	73.39053	71.14887	76.98966	2.81126	-221.99807	-2715.58072	1	
40	C	71.98395	71.60116	78.74255	-507.46439	-592.59194	122.07761	1	
41	H	72.46211	72.36385	79.39667	-1975.08116	525.87560	-1801.71556	1	
42	H	71.32949	72.15301	78.03221	1588.27743	-1913.22100	1113.83566	1	
43	C	71.18086	70.51101	79.52250	-613.62442	-457.55993	-194.14490	1	
44	H	71.73160	70.19682	80.43719	1707.54637	-721.27992	1996.92523	1	
45	H	70.17672	70.85174	79.86106	758.23357	2100.81767	1560.55011	1	
46	C	71.11360	69.33173	78.46295	-352.41524	704.96076	49.21465	1	

47	H	71.20805	68.30973	78.90104	1714.76886	-2070.42778	443.35792	1
48	H	70.22412	69.35705	77.75695	1224.15040	1801.50881	1636.97633	1
49	C	74.29204	70.20397	78.88857	566.85117	537.05831	117.62814	1
50	O	74.35944	70.43024	80.06883	-550.26779	-406.08867	4.21666	1
51	N	75.10344	69.50789	78.09856	566.34832	-425.77725	180.18749	1
52	H	74.85432	69.37418	77.09582	644.44502	2646.80550	-52.73430	1
53	C	76.43380	69.26456	78.58789	612.34801	-281.48662	411.56221	1
54	H	76.31023	68.72733	79.55389	1667.23498	-1490.75142	1556.16753	1
55	C	77.13853	68.41691	77.43634	-714.45746	-175.43074	286.98927	1
56	H	77.02126	68.98044	76.47076	-787.09484	1763.03619	-1922.46060	1
57	O	76.57272	67.11432	77.18389	-429.46514	516.51932	-128.40526	1
58	H	76.19034	67.24455	76.29290	1981.82785	436.16847	-1818.18182	1
59	C	78.64606	68.45608	77.88369	630.79189	-468.94448	76.03230	1
60	H	79.30769	67.97335	77.12756	-1775.71861	2062.30353	131.89849	1
61	H	79.00909	69.50177	78.02321	-1855.14608	88.94118	1993.53760	1
62	H	78.79966	67.91953	78.84847	-1504.82350	-780.94249	-2132.90992	1
63	C	77.11921	70.72276	78.76248	288.57638	618.62814	-397.00270	1
64	O	77.24881	71.48979	77.81134	321.70495	-185.26452	574.37218	1
65	N	77.55870	70.92090	80.03762	-447.05792	-446.53431	367.76425	1
66	H	77.33186	70.00450	80.45788	350.31316	1975.63644	-1843.31522	1
67	C	76.90830	72.03780	80.72782	-511.23061	374.03917	-471.51480	1
68	H	75.91038	72.10271	80.23481	2234.79579	-898.70890	-1273.45190	1
69	C	76.81895	71.56396	82.24587	529.53781	-159.34528	563.72604	1
70	H	76.32568	72.37159	82.84977	654.59388	2347.94251	1217.51488	1
71	H	76.12195	70.68409	82.26225	-1526.55661	2103.42026	817.87394	1
72	O	78.07639	71.21624	82.89776	-554.84278	14.12789	399.58769	1
73	H	78.36291	70.49401	82.31243	1297.06236	2061.84854	1220.68812	1
74	C	77.72757	73.39128	80.58280	-662.15484	-412.13544	123.62687	1
75	O	77.74185	74.22915	81.46761	-540.01537	-317.05804	274.91456	1
76	N	78.28211	73.47425	79.37147	-202.76299	-690.00100	-131.49145	1
77	H	78.04981	72.74780	78.64765	-702.62132	-2617.37191	281.70413	1
78	C	79.12342	74.62070	79.00829	-491.73914	576.34187	222.73509	1
79	H	79.66224	74.85073	79.95846	1977.17978	-1823.58850	-434.68928	1
80	C	80.00058	74.19279	77.84728	-649.50797	-328.66843	306.11224	1
81	H	79.33352	73.98493	76.97809	2075.07803	1452.16490	-1004.45904	1
82	C	80.95990	75.29693	77.44242	-615.18735	-489.99689	-70.96352	1
83	H	81.58311	75.00140	76.55391	-1226.32661	-1724.38906	-1716.47170	1
84	H	80.40194	76.23622	77.16543	2381.64273	-969.84735	900.46860	1
85	H	81.66821	75.55903	78.27621	2122.74991	1702.23946	-141.36228	1
86	C	80.76566	72.91784	78.15280	-501.86074	-479.61276	-376.42482	1
87	H	81.37147	72.57291	77.27062	993.79261	-2246.95401	-1177.81305	1
88	H	81.47600	73.05941	79.01298	42.71279	-626.15391	-2651.37258	1
89	H	80.07215	72.07731	78.43359	-2026.39012	-1590.33709	-887.82922	1
90	C	78.08471	75.83580	78.55982	-672.89153	382.57394	-156.34072	1
91	O	78.13286	76.27196	77.44050	410.04627	221.86223	500.35950	1
92	N	77.40525	76.24963	79.61603	-378.11782	-443.79414	-441.10984	1
93	H	77.57352	75.73793	80.51208	2404.15973	-568.14894	1149.30085	1
94	C	76.09132	76.81654	79.46788	-544.54484	466.16019	331.29119	1
95	H	76.02455	77.51722	80.32982	-1409.80988	-170.17955	2325.32679	1
96	C	75.97848	77.53701	78.07071	-184.48284	116.78282	-758.89137	1
97	H	76.90538	78.12634	77.87134	1893.78641	1861.14652	611.04528	1
98	H	75.92327	76.77468	77.25295	-2170.79665	-974.19311	1327.50117	1
99	C	74.73279	78.47818	78.01747	389.51668	672.81878	-138.49152	1
100	H	73.79768	77.87495	78.05768	510.64577	1933.03327	1851.02484	1
101	H	74.70548	79.17087	78.88572	-2302.30869	-1105.72939	-948.89774	1
102	C	74.85818	79.29245	76.64731	-559.93427	-126.34590	542.30857	1
103	O	75.09032	80.47114	76.58906	-670.36003	-111.83166	76.36448	1
104	N	74.72309	78.43315	75.62859	-216.06729	-537.07037	446.51379	1
105	H	74.58869	77.38111	75.74746	-1251.96487	1074.12894	-2168.52500	1
106	H	74.87042	78.62655	74.61232	-2451.83023	-720.73851	944.84612	1
107	C	75.01965	75.59585	79.61113	546.24052	-563.88337	-85.11809	1
108	O	75.11550	74.58121	78.97234	71.70702	-307.40463	606.69673	1

109	N	74.06823	75.94915	80.50356	479.90863	-504.50129	222.86849	1
110	C	73.04390	75.04331	80.87025	75.51268	-600.91904	506.73700	1
111	H	73.40228	74.02297	80.60523	-2033.61562	1795.30103	254.89480	1
112	C	72.87521	75.35797	82.41300	523.79067	517.99274	284.45581	1
113	H	71.90545	74.99835	82.82498	1599.61665	-1127.00911	1895.98173	1
114	H	73.67974	74.88336	83.01810	-1881.83093	1275.82488	-1501.55016	1
115	C	73.00690	76.91416	82.41380	-600.05639	-404.05026	316.64485	1
116	H	72.05545	77.39463	82.08536	-2597.05260	496.36221	657.73249	1
117	H	73.24746	77.34118	83.41351	-1666.24518	1294.38985	-1723.90591	1
118	C	74.15852	77.13912	81.34547	493.57570	-129.95376	-602.56394	1
119	H	74.01637	78.03004	80.68963	-1469.08415	-637.84797	2204.22581	1
120	H	75.19365	77.14515	81.76535	-1038.97840	1068.88701	-2280.71789	1
121	C	71.60616	75.44552	80.11771	188.88100	241.05089	-727.87821	1
122	O	71.10559	76.54103	80.22188	531.88613	-49.19943	427.07960	1
123	N	70.81306	74.24628	80.40650	708.14833	26.93417	-179.73509	1
124	H	71.36353	73.42484	80.65918	-2232.69501	-1179.09831	1023.94816	1
125	C	69.81847	73.97521	79.35940	-738.32412	259.92548	104.42456	1
126	H	69.55203	72.89351	79.41996	2028.89123	1260.02983	1311.33324	1
127	C	68.63477	74.91059	79.56705	-258.65678	-345.52513	661.28459	1
128	H	69.02888	75.95434	79.55278	-1826.06090	-1801.46097	-918.64554	1
129	C	67.60443	74.76279	78.46439	-541.23400	531.92970	-218.41428	1
130	H	66.72750	75.44939	78.62063	1311.73218	-2219.18200	882.19023	1
131	H	68.03982	75.00195	77.45500	-1048.71298	1223.58118	-2196.97971	1
132	H	67.20007	73.71433	78.41360	419.06414	1903.92898	1903.44670	1
133	C	67.99175	74.68767	80.92360	-423.86431	152.66566	-648.55262	1
134	H	67.14663	75.40575	81.10973	105.68386	-2342.50080	1387.51238	1
135	H	67.57499	73.64762	81.01940	-1695.63603	-1484.73621	-1531.02793	1
136	H	68.73971	74.82477	81.75275	-1853.57121	-487.39031	1936.59343	1
137	C	70.72318	74.37030	78.04811	539.71428	-510.58232	267.58633	1
138	O	71.75078	75.13817	78.26745	-15.93758	-278.34085	-624.49402	1
139	N	70.31587	73.90371	76.93477	-676.81886	12.05292	276.17960	1
140	H	69.47463	73.35074	77.14182	-1694.44250	-373.84189	-2100.66098	1
141	C	70.88770	74.15421	75.65605	412.33078	-664.70360	108.35451	1
142	H	70.05658	73.92956	74.95122	1765.77476	1294.44366	1621.76594	1
143	C	71.37992	75.65935	75.64111	-179.66635	-721.95667	-264.73915	1
144	H	70.79220	76.28138	76.35430	-607.34922	2587.87032	-598.10018	1
145	H	72.44011	75.72323	75.99688	-359.69332	-1479.13954	-2259.74260	1
146	C	71.26055	76.19784	74.17569	-240.01076	616.02425	431.85322	1
147	H	71.50853	75.40415	73.43528	-1359.17131	782.54425	2227.99181	1
148	H	70.21480	76.50752	73.95427	-820.36667	85.81767	-2596.78715	1
149	C	72.26134	77.41004	74.03350	-513.07015	236.18570	-551.87280	1
150	H	72.20703	78.07682	74.92474	1816.11944	-1183.11722	-1650.94321	1
151	H	73.31584	77.03947	74.00514	-1800.04429	-1361.53473	1526.34643	1
152	C	71.91881	78.20583	72.74431	726.08972	-253.19732	-179.64713	1
153	H	71.80074	77.57268	71.84148	1224.27271	-456.51798	-2390.90304	1
154	H	71.04969	78.88987	72.83150	1206.40339	-1150.93514	-2154.90344	1
155	N	73.13772	79.10526	72.44847	329.70796	-633.68968	-155.67358	1
156	H	73.31814	79.35717	71.39023	1348.31305	1938.76845	1359.00643	1
157	H	73.12503	80.05203	72.93782	2096.92035	1446.54551	-966.48890	1
158	H	74.09871	78.66677	72.76654	-1197.07217	-2303.53719	827.28733	1
159	C	72.18323	73.18300	75.40797	-378.01186	-556.17301	-413.96481	1
160	O	72.14571	72.41107	74.47659	-409.44433	-307.55053	-453.30833	1
161	N	73.14198	73.34845	76.31640	-429.02477	524.70884	274.08502	1
162	H	72.94972	74.04291	77.04966	1706.34263	-1425.96036	1574.38926	1
163	C	74.51473	73.25145	75.87094	-45.25864	-626.22952	478.93267	1
164	H	75.01963	73.12711	76.85761	1988.63164	570.90773	1772.87287	1
165	C	74.65264	71.99291	74.92501	551.77128	-20.49526	-564.54996	1
166	H	73.93594	71.19325	75.23223	1434.61535	-1753.10253	1513.99471	1
167	H	74.34778	72.25075	73.88459	-714.67738	1819.09770	1898.36494	1
168	C	76.12781	71.47209	74.96882	446.99263	-555.77305	338.97221	1
169	H	76.83440	72.20421	74.51178	1953.68466	1892.25957	-161.67766	1
170	H	76.48100	71.33424	76.03370	-403.03785	2688.07032	-188.43591	1

171	C	76.11684	70.10250	74.18033	567.86262	335.74681	434.04421	1
172	H	75.51781	69.33497	74.73000	-1080.02275	1568.26081	-1948.78900	1
173	H	75.61272	70.22116	73.19357	-919.54108	2111.34692	1456.13463	1
174	C	77.58303	69.65084	73.98318	195.81897	173.33862	-745.11536	1
175	H	78.18725	70.32227	73.34118	1405.67949	-2301.21089	-390.08113	1
176	H	78.13701	69.42822	74.91670	-940.37328	-1118.32446	2299.72133	1
177	N	77.54327	68.29176	73.20690	319.26422	656.36007	-42.02424	1
178	H	78.48794	67.87119	72.97075	1961.03633	619.91968	1787.09422	1
179	H	77.06596	67.47360	73.68592	854.14343	-2156.80752	1429.08711	1
180	H	77.07290	68.29418	72.25497	1237.02905	-1378.50857	-1998.28500	1
181	C	74.89673	74.67619	75.21959	532.53319	-268.57236	517.55729	1
182	O	74.53502	75.71279	75.78518	266.16714	-290.73804	-558.88002	1
183	N	75.60224	74.59206	74.10686	-226.25352	640.49678	-270.32839	1
184	H	75.82237	73.65102	73.78665	2007.69063	-1035.27229	1523.50231	1
185	C	76.56641	75.63785	73.86930	-540.76542	-573.33303	49.50000	1
186	H	76.63032	76.12822	74.86900	-2374.20950	-1036.76023	843.75774	1
187	C	77.91204	74.91408	73.40951	-77.09082	666.87422	-415.84136	1
188	H	77.76623	74.41621	72.40976	-985.81834	617.19825	2463.91927	1
189	O	78.39053	73.84684	74.25592	293.29899	-391.65602	-477.80926	1
190	H	78.48742	73.12263	73.60614	2528.72714	-681.76262	-751.27122	1
191	C	78.85893	76.15837	73.24696	252.47363	-605.14473	440.05134	1
192	H	79.84528	75.86684	72.81739	-2052.65063	1456.49051	-1043.51830	1
193	H	78.41763	76.93173	72.57468	-2152.98800	-1661.97574	-161.70652	1
194	H	79.05683	76.64523	74.23039	-473.12726	-1584.27339	2165.61725	1
195	C	75.94142	76.64861	72.76363	360.36307	488.46713	505.10056	1
196	O	75.34729	77.66640	73.17503	-200.08817	-528.03552	-385.82850	1
197	N	76.15797	76.27967	71.53397	-597.54095	-226.44775	355.20479	1
198	H	76.66025	75.39975	71.42034	2179.23655	-1300.70981	-991.33835	1
199	C	75.42998	76.81408	70.43759	-687.68921	297.39807	-249.45179	1
200	H	75.79384	76.24222	69.55428	-349.16256	-2467.37713	-1101.72831	1
201	C	73.86611	76.63250	70.74662	672.47345	361.54328	-201.62880	1
202	H	73.67030	76.97502	71.78822	1541.41502	582.18425	2169.97026	1
203	H	73.27228	77.27845	70.05690	-2534.67717	60.25153	997.72295	1
204	C	73.47500	75.15803	70.58690	574.26774	-389.43119	-377.02542	1
205	C	73.25559	74.62065	69.28259	688.82679	-287.33580	-257.96133	1
206	H	73.37869	75.25160	68.38369	331.14182	1470.38163	2269.80013	1
207	C	73.33317	74.33863	71.74701	-383.52382	-675.04808	144.24917	1
208	H	73.52874	74.74663	72.75619	4.09847	1517.59662	2262.86397	1
209	C	72.87661	73.28352	69.16874	-134.76730	428.45285	-649.50303	1
210	H	72.70250	72.86648	68.16148	-903.23433	1600.49020	2011.53387	1
211	C	72.93596	73.01034	71.57804	-335.53281	-615.00040	-364.39058	1
212	H	72.78930	72.38465	72.48260	1596.45398	-1369.33862	1732.02659	1
213	C	72.69529	72.43266	70.29780	585.48547	-340.24194	-406.23938	1
214	O	72.29911	71.08000	70.13044	-419.15649	-173.04408	-511.94141	1
215	H	72.23047	70.80930	71.07714	-1071.84350	1559.71507	-1960.13012	1
216	C	75.58173	78.42432	70.30475	291.41878	-183.13091	710.72246	1
217	O	74.57051	79.14052	70.32009	379.87695	523.47396	-222.23622	1
218	N	76.83314	78.76757	70.12642	564.30591	373.09380	277.24371	1
219	H	77.53344	78.02609	70.14890	-120.59931	-2436.07824	-1214.35098	1
220	C	77.18044	80.14755	70.27782	404.07514	-299.37480	608.84009	1
221	H	76.24760	80.63642	69.91123	-1071.07882	-841.69025	2359.66467	1
222	C	77.38273	80.39032	71.83507	-683.12807	68.71770	-390.13096	1
223	H	76.65445	79.78476	72.42215	2068.88918	1596.58590	770.89603	1
224	H	78.38702	80.02666	72.14829	1379.86429	2342.49779	-179.85638	1
225	C	77.21642	81.90638	72.14717	-176.39967	537.49466	550.97268	1
226	H	77.63046	82.53943	71.33246	-396.28051	1942.22168	1869.33314	1
227	H	76.14498	82.19358	72.22446	-94.44700	586.00678	-2659.20016	1
228	C	77.99881	82.16023	73.52912	-291.69381	-718.18079	-150.72929	1
229	H	77.47587	81.81165	74.45510	-2303.38776	1089.76242	964.62032	1
230	H	79.04778	81.77044	73.48823	884.16729	2568.80533	-207.74283	1
231	N	78.08455	83.55033	73.51091	-594.49522	-252.81478	342.29276	1
232	H	78.51235	83.95122	72.68696	-1735.17426	2084.05705	-263.71605	1

233	C	77.72203	84.34529	74.44212	595.23177	-271.52487	442.22352	1
234	N	77.15331	83.80832	75.59728	585.53813	-424.79750	-105.81303	1
235	H	76.94115	82.83854	75.83128	959.88797	1327.56823	-2177.11905	1
236	H	76.83289	84.35161	76.40007	1578.48647	16.27378	-2220.76233	1
237	N	78.00395	85.66779	74.08131	-452.17763	-390.33541	-421.51853	1
238	H	78.43013	86.05368	73.23970	470.26107	1974.25629	-1817.92087	1
239	H	77.81292	86.46775	74.68593	1856.67307	-1573.97321	-1224.35416	1
240	C	78.48465	80.41131	69.34286	-531.47271	-581.45780	-55.06206	1
241	O	78.54742	79.92761	68.21156	-243.00837	192.73507	609.52485	1
242	N	79.33313	81.24267	69.91093	343.49288	-644.25607	38.09164	1
243	H	79.07475	81.53375	70.85040	-1691.16043	-1535.97525	-1484.73099	1
244	C	80.61777	81.62827	69.35460	542.66492	350.14337	454.42563	1
245	H	81.11771	82.17100	70.19253	1209.57979	-2396.95920	463.86744	1
246	C	81.36842	80.37797	68.91061	-737.14309	145.93010	242.71942	1
247	H	80.71213	79.81671	68.20339	-1050.18303	159.36419	-2509.06125	1
248	C	82.65333	80.73495	68.18866	-706.77696	-252.88343	-245.16230	1
249	H	83.18063	79.82082	67.79884	-1624.64039	-1665.49085	1417.86935	1
250	H	82.46040	81.41104	67.30955	2566.10521	598.51109	693.22305	1
251	H	83.37338	81.27215	68.86589	-1972.69758	107.10018	-1876.34312	1
252	C	81.65749	79.45539	70.07965	412.85148	672.58832	-27.69222	1
253	H	82.16212	78.50680	69.74664	1447.02277	1762.76533	-1490.78944	1
254	H	82.33114	79.94408	70.83634	1320.77379	-145.20455	2378.68491	1
255	H	80.71107	79.16374	70.61396	-1512.10848	1470.52031	1724.75147	1
256	C	80.31721	82.65121	68.06809	-607.11113	499.56689	73.73769	1
257	O	80.66855	83.79339	68.17254	357.97126	460.81534	356.68785	1
258	N	79.76503	82.01138	67.04597	536.55407	-368.62270	332.76306	1
259	H	79.49418	81.00967	67.19625	524.38866	2297.69985	1367.20941	1
260	C	78.94277	82.76052	66.14819	46.50277	-774.29190	-147.97904	1
261	H	78.38937	81.95505	65.61643	1676.51875	1883.29066	1032.55549	1
262	C	77.95706	83.73147	66.97650	-559.41456	-34.19198	-556.30433	1
263	H	78.56704	84.45839	67.56767	-64.66664	395.18769	2695.05373	1
264	H	77.33321	84.34581	66.28359	-2703.44278	-60.40056	333.79418	1
265	C	77.10355	82.88559	67.88273	-519.76435	377.31045	459.42366	1
266	H	77.73907	82.06091	68.29506	-1746.74323	1667.50644	-1261.73691	1
267	C	76.57511	83.71218	69.04813	570.95554	16.46261	-545.27700	1
268	H	75.93722	83.09873	69.73525	2391.58273	28.05277	-1305.07271	1
269	H	77.40960	84.14057	69.66123	175.75588	917.63458	2559.43867	1
270	H	75.94936	84.57090	68.69299	-1063.97851	-2155.34650	1283.00462	1
271	C	75.94121	82.26462	67.11962	193.76014	2.62946	-765.53141	1
272	H	75.30876	81.61981	67.78309	507.39394	-846.55087	2539.60089	1
273	H	75.27094	83.04728	66.67941	1337.57841	1818.19054	1526.01994	1
274	H	76.29787	81.61956	66.27595	1100.88635	-1172.91350	-2199.08909	1
275	C	79.86837	83.61667	65.15852	-549.21115	475.64486	-309.38218	1
276	O	79.47313	84.62083	64.62520	556.06106	-390.37755	-78.24250	1
277	O	81.10253	83.03341	64.77164	-572.27940	-310.19032	-209.75862	1
278	H	81.13914	82.29878	65.44502	-1380.08193	2212.14486	790.85944	1

Listing 2: C00002.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	1.1710	4684
		0.2500	300.00	0.00	0.00	0.00	-1294.9636	0.0000	300.0000
3	H	61.22334	76.68362	69.85415	-2043.14101	-1757.64893	399.89339		1
4	N	61.61283	77.38906	70.47541	426.75047	490.45733	-334.42467		1
5	H	60.77473	77.83945	70.83632	442.25559	-1110.30854	-2448.52907		1
6	C	62.55780	78.25394	69.88593	415.32972	-666.39213	83.73172		1
7	H	63.20906	77.56971	69.30234	879.32219	2491.00447	667.35213		1
8	C	61.83823	79.35068	68.95132	31.35357	477.41777	628.23362		1
9	H	61.01258	79.85053	69.51305	1168.38489	2240.25337	-1019.71136		1
10	H	62.57375	80.15579	68.70867	-360.43770	2534.90498	931.67112		1
11	C	61.31679	78.71576	67.68877	463.18208	512.70242	-382.34388		1
12	H	60.57655	77.93104	67.96201	1725.29117	1863.52247	-987.07854		1

13	C	60.62069	79.76244	66.82667	710.42801	-144.27427	-313.15367	1
14	H	60.20629	79.31523	65.88648	364.20195	-1033.13725	2494.72524	1
15	H	59.76885	80.24793	67.36891	2567.61904	335.80679	847.48802	1
16	H	61.32650	80.57769	66.52137	-2587.99029	680.92867	-512.16411	1
17	C	62.43470	78.07005	66.88100	268.17616	741.64379	-40.42634	1
18	H	62.06577	77.69610	65.89125	1283.54314	-1945.37420	-1411.27812	1
19	H	63.26358	78.79522	66.67346	-1258.57796	1317.15249	-2026.02085	1
20	H	62.88526	77.19425	67.41433	-2502.84526	909.80597	575.92391	1
21	C	63.36044	79.04730	71.04790	619.36578	-458.64843	-172.09273	1
22	O	63.85778	80.13073	70.81440	-81.40433	433.87611	522.34594	1
23	N	63.47869	78.30939	72.15171	175.23996	-622.20190	341.55523	1
24	H	63.00235	77.40806	72.16680	-876.57256	-303.22879	-2561.90213	1
25	C	64.27440	78.79927	73.21833	-571.88214	-534.10783	-106.15033	1
26	H	64.55346	79.83097	72.89583	-2713.20841	-16.25800	-248.80809	1
27	C	63.41964	78.69872	74.57272	166.60354	288.16399	-716.09568	1
28	H	63.31345	77.60945	74.83950	-2097.85574	1636.78449	-586.18044	1
29	O	62.08672	79.23331	74.51794	-317.80580	-363.38227	484.43082	1
30	H	61.55186	78.42999	74.68197	1863.74748	-1451.84923	1357.29467	1
31	C	64.38005	79.39487	75.60595	503.80731	517.99032	318.51606	1
32	H	63.98128	79.32105	76.64430	640.61020	-2157.10410	-1536.29104	1
33	H	65.39626	78.93134	75.60677	1687.88455	465.60692	2087.56452	1
34	H	64.50664	80.47874	75.37788	-1293.07895	-1899.88581	-1463.57452	1
35	C	65.53302	77.77394	73.43731	-153.07550	-733.68902	248.70981	1
36	O	65.46514	77.01201	74.36667	186.15459	-480.78787	-449.34387	1
37	N	66.48937	77.88136	72.49857	-487.53139	543.18517	42.03850	1
38	C	67.78042	77.31179	72.70104	-699.35871	69.34393	360.10701	1
39	H	67.67921	76.53089	73.48957	2.81126	-221.99807	-2715.58072	1
40	C	68.14202	76.79405	71.24356	-507.46439	-592.59194	122.07761	1
41	H	69.23345	76.62541	71.10277	-1975.08116	525.87560	-1801.71556	1
42	H	67.63713	75.82900	71.01443	1588.27743	-1913.22100	1113.83566	1
43	C	67.57218	77.95530	70.36977	-613.62442	-457.55993	-194.14490	1
44	H	68.25319	78.85074	70.39032	1707.54637	-721.27992	1996.92523	1
45	H	67.43554	77.68392	69.29825	758.23357	2100.81767	1560.55011	1
46	C	66.20390	78.25352	71.11510	-352.41524	704.96076	49.21465	1
47	H	65.87998	79.32355	71.09825	1714.76886	-2070.42778	443.35792	1
48	H	65.34823	77.60855	70.80571	1224.15040	1801.50881	1636.97633	1
49	C	68.88370	78.47902	73.07452	566.85117	537.05831	117.62814	1
50	O	70.00329	78.14808	73.38001	-550.26779	-406.08867	4.21666	1
51	N	68.36295	79.69317	72.95767	566.34832	-425.77725	180.18749	1
52	H	67.37962	79.71306	72.69380	644.44502	2646.80550	-52.73430	1
53	C	69.16173	80.86973	72.84625	612.34801	-281.48662	411.56221	1
54	H	68.37081	81.64380	72.72645	1667.23498	-1490.75142	1556.16753	1
55	C	69.98475	81.05054	74.20373	-714.45746	-175.43074	286.98927	1
56	H	70.82589	80.30139	74.20748	-787.09484	1763.03619	-1922.46060	1
57	O	69.26810	80.81854	75.43197	-429.46514	516.51932	-128.40526	1
58	H	69.70037	79.99733	75.74220	1981.82785	436.16847	-1818.18182	1
59	C	70.52674	82.51985	74.04425	630.79189	-468.94448	76.03230	1
60	H	71.27368	82.76759	74.83258	-1775.71861	2062.30353	131.89849	1
61	H	71.01363	82.69768	73.05775	-1855.14608	88.94118	1993.53760	1
62	H	69.70020	83.26154	74.13368	-1504.82350	-780.94249	-2132.90992	1
63	C	70.03949	80.70139	71.48813	288.57638	618.62814	-397.00270	1
64	O	69.49100	80.46298	70.43630	321.70495	-185.26452	574.37218	1
65	N	71.33083	80.97352	71.68846	-447.05792	-446.53431	367.76425	1
66	H	71.71345	81.06685	72.64906	350.31316	1975.63644	-1843.31522	1
67	C	72.25035	80.34538	70.77862	-511.23061	374.03917	-471.51480	1
68	H	71.65858	79.64695	70.14272	2234.79579	-898.70890	-1273.45190	1
69	C	72.95581	81.52700	69.95325	529.53781	-159.34528	563.72604	1
70	H	73.48566	81.06157	69.07791	654.59388	2347.94251	1217.51488	1
71	H	72.12590	82.15553	69.53663	-1526.55661	2103.42026	817.87394	1
72	O	73.93473	82.32310	70.66847	-554.84278	14.12789	399.58769	1
73	H	73.32749	82.90652	71.16291	1297.06236	2061.84854	1220.68812	1
74	C	73.28505	79.68447	71.82481	-662.15484	-412.13544	123.62687	1

75	O	73.15684	79.98381	73.02628	-540.01537	-317.05804	274.91456	1
76	N	74.17687	78.90739	71.26565	-202.76299	-690.00100	-131.49145	1
77	H	74.09671	78.82558	70.25172	-702.62132	-2617.37191	281.70413	1
78	C	75.21957	78.22650	71.99872	-491.73914	576.34187	222.73509	1
79	H	75.79294	77.69588	71.20091	1977.17978	-1823.58850	-434.68928	1
80	C	76.03897	79.23514	72.79920	-649.50797	-328.66843	306.11224	1
81	H	75.35569	79.68153	73.55991	2075.07803	1452.16490	-1004.45904	1
82	C	77.17425	78.53444	73.52021	-615.18735	-489.99689	-70.96352	1
83	H	77.70882	79.21966	74.23386	-1226.32661	-1724.38906	-1716.47170	1
84	H	76.78881	77.65568	74.11288	2381.64273	-969.84735	900.46860	1
85	H	77.94285	78.13443	72.80271	2122.74991	1702.23946	-141.36228	1
86	C	76.55501	80.36619	71.93244	-501.86074	-479.61276	-376.42482	1
87	H	77.15315	81.10964	72.52798	993.79261	-2246.95401	-1177.81305	1
88	H	77.22018	79.98596	71.10861	42.71279	-626.15391	-2651.37258	1
89	H	75.70638	80.92872	71.44479	-2026.39012	-1590.33709	-887.82922	1
90	C	74.46021	77.18880	73.08090	-672.89153	382.57394	-156.34072	1
91	O	74.53077	77.34620	74.28976	410.04627	221.86223	500.35950	1
92	N	73.82516	76.28029	72.38695	-378.11782	-443.79414	-441.10984	1
93	H	73.95864	76.37514	71.38303	2404.15973	-568.14894	1149.30085	1
94	C	73.17517	75.16851	73.00514	-544.54484	466.16019	331.29119	1
95	H	72.71310	75.56770	73.93535	-1409.80988	-170.17955	2325.32679	1
96	C	72.15620	74.64849	71.90199	-184.48284	116.78282	-758.89137	1
97	H	71.44276	75.45712	71.62486	1893.78641	1861.14652	611.04528	1
98	H	72.70364	74.39577	70.96613	-2170.79665	-974.19311	1327.50117	1
99	C	71.39358	73.39905	72.43716	389.51668	672.81878	-138.49152	1
100	H	72.11387	72.64012	72.81612	510.64577	1933.03327	1851.02484	1
101	H	70.78655	73.67215	73.32797	-2302.30869	-1105.72939	-948.89774	1
102	C	70.46223	72.74099	71.34776	-559.93427	-126.34590	542.30857	1
103	O	69.93065	71.68734	71.58510	-670.36003	-111.83166	76.36448	1
104	N	70.33309	73.46366	70.21452	-216.06729	-537.07037	446.51379	1
105	H	70.74239	74.37151	69.96499	-1251.96487	1074.12894	-2168.52500	1
106	H	69.74347	73.18586	69.42209	-2451.83023	-720.73851	944.84612	1
107	C	74.32086	74.05363	73.27751	546.24052	-563.88337	-85.11809	1
108	O	75.07989	73.72518	72.37282	71.70702	-307.40463	606.69673	1
109	N	74.22248	73.55711	74.50237	479.90863	-504.50129	222.86849	1
110	C	75.26002	72.72780	75.06974	75.51268	-600.91904	506.73700	1
111	H	76.21230	73.20582	74.74133	-2033.61562	1795.30103	254.89480	1
112	C	74.94849	72.80770	76.62778	523.79067	517.99274	284.45581	1
113	H	75.34912	71.93128	77.19145	1599.61665	-1127.00911	1895.98173	1
114	H	75.39021	73.72301	77.08890	-1881.83093	1275.82488	-1501.55016	1
115	C	73.38917	72.88021	76.62129	-600.05639	-404.05026	316.64485	1
116	H	72.94386	71.88484	76.39584	-2597.05260	496.36221	657.73249	1
117	H	72.95039	73.21840	77.58686	-1666.24518	1294.38985	-1723.90591	1
118	C	73.15606	73.90787	75.43102	493.57570	-129.95376	-602.56394	1
119	H	72.17604	73.81663	74.90757	-1469.08415	-637.84797	2204.22581	1
120	H	73.33245	74.97531	75.70713	-1038.97840	1068.88701	-2280.71789	1
121	C	75.12228	71.21298	74.52252	188.88100	241.05089	-727.87821	1
122	O	74.85960	70.29945	75.27522	531.88613	-49.19943	427.07960	1
123	N	75.40167	71.17057	73.22364	708.14833	26.93417	-179.73509	1
124	H	75.55701	72.07708	72.71655	-2232.69501	-1179.09831	1023.94816	1
125	C	75.05557	69.95327	72.46245	-738.32412	259.92548	104.42456	1
126	H	74.07894	69.65777	72.91234	2028.89123	1260.02983	1311.33324	1
127	C	74.98825	70.28982	70.99017	-258.65678	-345.52513	661.28459	1
128	H	75.96244	70.74702	70.70299	-1826.06090	-1801.46097	-918.64554	1
129	C	74.78418	69.05263	70.13295	-541.23400	531.92970	-218.41428	1
130	H	74.76394	69.30575	69.03711	1311.73218	-2219.18200	882.19023	1
131	H	75.61106	68.30287	70.28608	-1048.71298	1223.58118	-2196.97971	1
132	H	73.81457	68.53589	70.37310	419.06414	1903.92898	1903.44670	1
133	C	73.89526	71.29700	70.67943	-423.86431	152.66566	-648.55262	1
134	H	73.86281	71.55202	69.58441	105.68386	-2342.50080	1387.51238	1
135	H	72.87730	70.90710	70.95900	-1695.63603	-1484.73621	-1531.02793	1
136	H	74.05104	72.26279	71.24456	-1853.57121	-487.39031	1936.59343	1

137	C	76.24023	68.84572	72.79943	539.71428	-510.58232	267.58633	1
138	O	77.10220	68.60723	71.99177	-15.93758	-278.34085	-624.49402	1
139	N	76.03058	68.31581	73.98914	-676.81886	12.05292	276.17960	1
140	H	75.27433	68.69947	74.59607	-1694.44250	-373.84189	-2100.66098	1
141	C	76.85421	67.25384	74.45990	412.33078	-664.70360	108.35451	1
142	H	76.21835	66.77262	75.23702	1765.77476	1294.44366	1621.76594	1
143	C	77.21182	66.29866	73.24588	-179.66635	-721.95667	-264.73915	1
144	H	76.31442	66.12219	72.61077	-607.34922	2587.87032	-598.10018	1
145	H	77.96955	66.77720	72.57444	-359.69332	-1479.13954	-2259.74260	1
146	C	77.76828	64.95473	73.82435	-240.01076	616.02425	431.85322	1
147	H	78.71416	65.13920	74.38781	-1359.17131	782.54425	2227.99181	1
148	H	77.05609	64.50658	74.55281	-820.36667	85.81767	-2596.78715	1
149	C	78.01218	63.97677	72.60548	-513.07015	236.18570	-551.87280	1
150	H	77.05591	63.75509	72.07810	1816.11944	-1183.11722	-1650.94321	1
151	H	78.67384	64.45081	71.84438	-1800.04429	-1361.53473	1526.34643	1
152	C	78.65211	62.67935	73.15135	726.08972	-253.19732	-179.64713	1
153	H	79.68063	62.80373	73.54508	1224.27271	-456.51798	-2390.90304	1
154	H	78.03005	62.12920	73.88522	1206.40339	-1150.93514	-2154.90344	1
155	N	78.80500	61.68984	71.94669	329.70796	-633.68968	-155.67358	1
156	H	79.26967	60.76286	72.17018	1348.31305	1938.76845	1359.00643	1
157	H	77.91262	61.36539	71.47214	2096.92035	1446.54551	-966.48890	1
158	H	79.38479	62.02004	71.12126	-1197.07217	-2303.53719	827.28733	1
159	C	78.22700	67.86154	75.10515	-378.01186	-556.17301	-413.96481	1
160	O	79.22343	67.17648	75.16118	-409.44433	-307.55053	-453.30833	1
161	N	78.03199	69.06793	75.63941	-429.02477	524.70884	274.08502	1
162	H	77.11636	69.49370	75.48328	1706.34263	-1425.96036	1574.38926	1
163	C	79.20626	69.82188	75.96485	-45.25864	-626.22952	478.93267	1
164	H	80.02762	69.28613	75.43305	1988.63164	570.90773	1772.87287	1
165	C	78.97143	71.30876	75.47312	551.77128	-20.49526	-564.54996	1
166	H	78.59326	71.31347	74.42573	1434.61535	-1753.10253	1513.99471	1
167	H	78.18327	71.81320	76.08343	-714.67738	1819.09770	1898.36494	1
168	C	80.33443	72.07084	75.58543	446.99263	-555.77305	338.97221	1
169	H	80.58657	72.26781	76.65386	1953.68466	1892.25957	-161.67766	1
170	H	81.16502	71.44628	75.18577	-403.03785	2688.07032	-188.43591	1
171	C	80.23118	73.42317	74.77876	567.86262	335.74681	434.04421	1
172	H	80.00445	73.22461	73.70616	-1080.02275	1568.26081	-1948.78900	1
173	H	79.38785	74.05238	75.15354	-919.54108	2111.34692	1456.13463	1
174	C	81.57289	74.19023	74.92323	195.81897	173.33862	-745.11536	1
175	H	81.77296	74.57413	75.94573	1405.67949	-2301.21089	-390.08113	1
176	H	82.46592	73.65802	74.53550	-940.37328	-1118.32446	2299.72133	1
177	N	81.41702	75.45327	74.04327	319.26422	656.36007	-42.02424	1
178	H	82.17970	76.18417	74.12376	1961.03633	619.91968	1787.09422	1
179	H	81.42425	75.28819	72.99684	854.14343	-2156.80752	1429.08711	1
180	H	80.45606	76.00467	74.23665	1237.02905	-1378.50857	-1998.28500	1
181	C	79.46612	69.87102	77.57360	532.53319	-268.57236	517.55729	1
182	O	80.48276	70.44572	77.97337	266.16714	-290.73804	-558.88002	1
183	N	78.51080	69.29273	78.26038	-226.25352	640.49678	-270.32839	1
184	H	77.78280	68.88954	77.67114	2007.69063	-1035.27229	1523.50231	1
185	C	78.41220	69.24255	79.67209	-540.76542	-573.33303	49.50000	1
186	H	77.59912	68.50647	79.85655	-2374.20950	-1036.76023	843.75774	1
187	C	79.81913	68.81076	80.30081	-77.09082	666.87422	-415.84136	1
188	H	80.60442	69.54356	79.95528	-985.81834	617.19825	2463.91927	1
189	O	80.29618	67.50488	79.93243	293.29899	-391.65602	-477.80926	1
190	H	81.05466	67.73817	79.35912	2528.72714	-681.76262	-751.27122	1
191	C	79.53570	69.04071	81.83048	252.47363	-605.14473	440.05134	1
192	H	80.46504	68.95019	82.44028	-2052.65063	1456.49051	-1043.51830	1
193	H	79.10416	70.05667	82.02103	-2152.98800	-1661.97574	-161.70652	1
194	H	78.80803	68.29389	82.22522	-473.12726	-1584.27339	2165.61725	1
195	C	78.02964	70.72448	80.26663	360.36307	488.46713	505.10056	1
196	O	77.15791	70.81919	81.09589	-200.08817	-528.03552	-385.82850	1
197	N	78.87982	71.64264	79.82701	-597.54095	-226.44775	355.20479	1
198	H	79.65029	71.37654	79.16862	2179.23655	-1300.70981	-991.33835	1

199	C	78.53251	73.00653	79.99920	-687.68921	297.39807	-249.45179	1
200	H	77.70988	72.95334	80.74995	-349.16256	-2467.37713	-1101.72831	1
201	C	79.84913	73.75399	80.52252	672.47345	361.54328	-201.62880	1
202	H	80.61707	73.80749	79.71628	1541.41502	582.18425	2169.97026	1
203	H	79.61336	74.80165	80.82031	-2534.67717	60.25153	997.72295	1
204	C	80.38520	72.95807	81.72053	574.26774	-389.43119	-377.02542	1
205	C	79.76104	73.10145	82.99601	688.82679	-287.33580	-257.96133	1
206	H	78.91963	73.80382	83.13695	331.14182	1470.38163	2269.80013	1
207	C	81.46037	72.03559	81.54160	-383.52382	-675.04808	144.24917	1
208	H	81.93431	71.91066	80.55115	4.09847	1517.59662	2262.86397	1
209	C	80.22722	72.32709	84.05766	-134.76730	428.45285	-649.50303	1
210	H	79.74301	72.43697	85.04373	-903.23433	1600.49020	2011.53387	1
211	C	81.89338	71.28454	82.63687	-335.53281	-615.00040	-364.39058	1
212	H	82.72557	70.57471	82.48754	1596.45398	-1369.33862	1732.02659	1
213	C	81.30026	71.39848	83.92815	585.48547	-340.24194	-406.23938	1
214	O	81.72861	70.63629	85.04621	-419.15649	-173.04408	-511.94141	1
215	H	82.47367	70.13941	84.63321	-1071.84350	1559.71507	-1960.13012	1
216	C	78.02645	73.53448	78.53827	291.41878	-183.13091	710.72246	1
217	O	77.27561	72.88695	77.83571	379.87695	523.47396	-222.23622	1
218	N	78.51208	74.74535	78.30252	564.30591	373.09380	277.24371	1
219	H	79.10575	75.16556	79.01497	-120.59931	-2436.07824	-1214.35098	1
220	C	77.99750	75.48793	77.19713	404.07514	-299.37480	608.84009	1
221	H	77.41676	74.76387	76.57735	-1071.07882	-841.69025	2359.66467	1
222	C	77.10216	76.62200	77.86620	-683.12807	68.71770	-390.13096	1
223	H	76.41305	76.17451	78.61629	2068.88918	1596.58590	770.89603	1
224	H	77.73989	77.33354	78.43692	1379.86429	2342.49779	-179.85638	1
225	C	76.30253	77.37084	76.76008	-176.39967	537.49466	550.97268	1
226	H	76.98175	77.86720	76.03324	-396.28051	1942.22168	1869.33314	1
227	H	75.66283	76.68083	76.16032	-94.44700	586.00678	-2659.20016	1
228	C	75.42951	78.43498	77.57066	-291.69381	-718.18079	-150.72929	1
229	H	74.73014	77.99024	78.32116	-2303.38776	1089.76242	964.62032	1
230	H	76.00143	79.25273	78.07772	884.16729	2568.80533	-207.74283	1
231	N	74.62355	79.00458	76.58748	-594.49522	-252.81478	342.29276	1
232	H	74.61583	78.51486	75.68478	-1735.17426	2084.05705	-263.71605	1
233	C	73.91705	80.04325	76.81551	595.23177	-271.52487	442.22352	1
234	N	73.96270	80.63183	78.08563	585.53813	-424.79750	-105.81303	1
235	H	74.47856	80.34245	78.91534	959.88797	1327.56823	-2177.11905	1
236	H	73.42120	81.44825	78.37074	1578.48647	16.27378	-2220.76233	1
237	N	73.19624	80.40124	75.68088	-452.17763	-390.33541	-421.51853	1
238	H	73.23344	79.96570	74.72494	470.26107	1974.25629	-1817.92087	1
239	H	72.57633	81.21909	75.66629	1856.67307	-1573.97321	-1224.35416	1
240	C	79.22997	76.20786	76.42370	-531.47271	-581.45780	-55.06206	1
241	O	79.21155	76.32977	75.19046	-243.00837	192.73507	609.52485	1
242	N	80.11442	76.64855	77.26731	343.49288	-644.25607	38.09164	1
243	H	79.95585	76.45900	78.25961	-1691.16043	-1535.97525	-1484.73099	1
244	C	81.32035	77.36285	76.90022	542.66492	350.14337	454.42563	1
245	H	81.57830	77.04463	75.86365	1209.57979	-2396.95920	463.86744	1
246	C	81.04840	78.86299	77.00928	-737.14309	145.93010	242.71942	1
247	H	80.81346	79.08652	78.07338	-1050.18303	159.36419	-2509.06125	1
248	C	82.25552	79.68473	76.60814	-706.77696	-252.88343	-245.16230	1
249	H	82.04909	80.78793	76.68766	-1624.64039	-1665.49085	1417.86935	1
250	H	83.16356	79.46890	77.26762	2566.10521	598.51109	693.22305	1
251	H	82.55953	79.48129	75.54413	-1972.69758	107.10018	-1876.34312	1
252	C	79.84369	79.27022	76.18137	412.85148	672.58832	-27.69222	1
253	H	79.62561	80.37024	76.26646	1447.02277	1762.76533	-1490.78944	1
254	H	79.99776	79.04003	75.09110	1320.77379	-145.20455	2378.68491	1
255	H	78.91988	78.71654	76.50465	-1512.10848	1470.52031	1724.75147	1
256	C	82.38328	76.87131	78.09163	-607.11113	499.56689	73.73769	1
257	O	81.99301	76.47216	79.16250	357.97126	460.81534	356.68785	1
258	N	83.62145	77.01016	77.64795	536.55407	-368.62270	332.76306	1
259	H	83.73942	77.40908	76.71833	524.38866	2297.69985	1367.20941	1
260	C	84.69226	76.88550	78.57078	46.50277	-774.29190	-147.97904	1

261	H	84.23989	76.37764	79.45400	1676.51875	1883.29066	1032.55549	1
262	C	85.88665	76.06015	77.85928	-559.41456	-34.19198	-556.30433	1
263	H	86.32539	76.67930	77.04119	-64.66664	395.18769	2695.05373	1
264	H	86.72057	75.86861	78.57541	-2703.44278	-60.40056	333.79418	1
265	C	85.33820	74.77298	77.30603	-519.76435	377.31045	459.42366	1
266	H	84.41895	75.00799	76.72264	-1746.74323	1667.50644	-1261.73691	1
267	C	86.34959	74.12242	76.37036	570.95554	16.46261	-545.27700	1
268	H	85.95281	73.17301	75.92714	2391.58273	28.05277	-1305.07271	1
269	H	86.62116	74.79876	75.51922	175.75588	917.63458	2559.43867	1
270	H	87.30005	73.86640	76.90546	-1063.97851	-2155.34650	1283.00462	1
271	C	84.96608	73.80413	78.42035	193.76014	2.62946	-765.53141	1
272	H	84.56312	72.84112	78.01313	507.39394	-846.55087	2539.60089	1
273	H	85.85124	73.55043	79.05890	1337.57841	1818.19054	1526.01994	1
274	H	84.17996	74.23297	79.09433	1100.88635	-1172.91350	-2199.08909	1
275	C	85.23943	78.36301	78.89670	-549.21115	475.64486	-309.38218	1
276	O	84.78817	79.36918	78.40157	556.06106	-390.37755	-78.24250	1
277	O	86.32829	78.43394	79.79217	-572.27940	-310.19032	-209.75862	1
278	H	86.39802	77.46408	80.02351	-1380.08193	2212.14486	790.85944	1

Listing 3: C00003.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1294.6210	0.0000	300.0000
3	H	71.77912	76.43050	82.74316	-2043.14101	-1757.64893	399.89339		1
4	N	72.75468	76.32011	83.01133	426.75047	490.45733	-334.42467		1
5	H	73.02148	75.48974	82.49078	442.25559	-1110.30854	-2448.52907		1
6	C	73.56483	77.46236	82.83258	415.32972	-666.39213	83.73172		1
7	H	73.13756	78.22538	83.51705	879.32219	2491.00447	667.35213		1
8	C	75.09137	77.07199	83.16290	31.35357	477.41777	628.23362		1
9	H	75.41966	76.25962	82.47031	1168.38489	2240.25337	-1019.71136		1
10	H	75.76836	77.93790	82.96283	-360.43770	2534.90498	931.67112		1
11	C	75.19765	76.62076	84.59832	463.18208	512.70242	-382.34388		1
12	H	74.33912	75.94678	84.81867	1725.29117	1863.52247	-987.07854		1
13	C	76.48919	75.84276	84.81442	710.42801	-144.27427	-313.15367		1
14	H	76.59169	75.49677	85.87535	364.20195	-1033.13725	2494.72524		1
15	H	76.53957	74.93324	84.16136	2567.61904	335.80679	847.48802		1
16	H	77.38938	76.46811	84.58109	-2587.99029	680.92867	-512.16411		1
17	C	75.14559	77.80804	85.54967	268.17616	741.64379	-40.42634		1
18	H	75.23623	77.48602	86.61933	1283.54314	-1945.37420	-1411.27812		1
19	H	75.97759	78.53198	85.34971	-1258.57796	1317.15249	-2026.02085		1
20	H	74.18374	78.37486	85.45383	-2502.84526	909.80597	575.92391		1
21	C	73.50629	77.94797	81.28548	619.36578	-458.64843	-172.09273		1
22	O	73.70025	79.10643	81.00759	-81.40433	433.87611	522.34594		1
23	N	73.36478	76.90946	80.45897	175.23996	-622.20190	341.55523		1
24	H	73.11560	75.95588	80.77442	-876.57256	-303.22879	-2561.90213		1
25	C	73.03596	77.17891	79.09421	-571.88214	-534.10783	-106.15033		1
26	H	72.77501	78.25854	79.00565	-2713.20841	-16.25800	-248.80809		1
27	C	74.35268	76.77910	78.25164	166.60354	288.16399	-716.09568		1
28	H	74.89632	75.99848	78.85044	-2097.85574	1636.78449	-586.18044		1
29	O	75.29080	77.84593	78.06236	-317.80580	-363.38227	484.43082		1
30	H	76.09042	77.47512	78.50323	1863.74748	-1451.84923	1357.29467		1
31	C	73.81915	76.11113	76.93491	503.80731	517.99032	318.51606		1
32	H	74.65583	75.70599	76.31874	640.61020	-2157.10410	-1536.29104		1
33	H	73.11940	75.26497	77.14547	1687.88455	465.60692	2087.56452		1
34	H	73.26539	76.84192	76.29851	-1293.07895	-1899.88581	-1463.57452		1
35	C	71.82639	76.12004	78.92209	-153.07550	-733.68902	248.70981		1
36	O	71.81462	75.15474	79.65998	186.15459	-480.78787	-449.34387		1
37	N	71.01398	76.44598	77.91620	-487.53139	543.18517	42.03850		1
38	C	69.92385	75.59205	77.53171	-699.35871	69.34393	360.10701		1
39	H	69.31991	75.42302	78.45065	2.81126	-221.99807	-2715.58072		1
40	C	69.19019	76.41313	76.39836	-507.46439	-592.59194	122.07761		1

41	H	68.70934	75.75696	75.63656	-1975.08116	525.87560	-1801.71556	1
42	H	68.37770	77.04738	76.81912	1588.27743	-1913.22100	1113.83566	1
43	C	70.34532	77.28773	75.81522	-613.62442	-457.55993	-194.14490	1
44	H	70.98963	76.69043	75.13194	1707.54637	-721.27992	1996.92523	1
45	H	69.99083	78.16995	75.23640	758.23357	2100.81767	1560.55011	1
46	C	71.11997	77.67818	77.14722	-352.41524	704.96076	49.21465	1
47	H	72.19622	77.94411	77.01653	1714.76886	-2070.42778	443.35792	1
48	H	70.61483	78.46376	77.75807	1224.15040	1801.50881	1636.97633	1
49	C	70.58426	74.19629	76.96745	566.85117	537.05831	117.62814	1
50	O	71.42291	74.14408	76.10025	-550.26779	-406.08867	4.21666	1
51	N	69.94137	73.22292	77.59625	566.34832	-425.77725	180.18749	1
52	H	69.23502	73.47057	78.28826	644.44502	2646.80550	-52.73430	1
53	C	70.35109	71.87513	77.42525	612.34801	-281.48662	411.56221	1
54	H	71.17917	71.95883	76.68534	1667.23498	-1490.75142	1556.16753	1
55	C	70.89155	71.49863	78.89372	-714.45746	-175.43074	286.98927	1
56	H	70.30785	72.10747	79.63997	-787.09484	1763.03619	-1922.46060	1
57	O	72.25491	71.92687	79.11010	-429.46514	516.51932	-128.40526	1
58	H	72.10430	72.83649	79.45604	1981.82785	436.16847	-1818.18182	1
59	C	70.56304	69.98341	79.11749	630.79189	-468.94448	76.03230	1
60	H	70.99439	69.60747	80.07545	-1775.71861	2062.30353	131.89849	1
61	H	69.46041	69.80454	79.15589	-1855.14608	88.94118	1993.53760	1
62	H	70.96009	69.34137	78.29188	-1504.82350	-780.94249	-2132.90992	1
63	C	69.12498	70.97363	76.85106	288.57638	618.62814	-397.00270	1
64	O	69.20622	69.74631	76.88590	321.70495	-185.26452	574.37218	1
65	N	68.16264	71.71367	76.35279	-447.05792	-446.53431	367.76425	1
66	H	68.34165	72.71605	76.35154	350.31316	1975.63644	-1843.31522	1
67	C	67.01339	71.19116	75.69536	-511.23061	374.03917	-471.51480	1
68	H	66.72640	70.31074	76.31352	2234.79579	-898.70890	-1273.45190	1
69	C	65.97478	72.41034	75.67613	529.53781	-159.34528	563.72604	1
70	H	65.05717	72.03617	75.15308	654.59388	2347.94251	1217.51488	1
71	H	65.66767	72.64561	76.73048	-1526.55661	2103.42026	817.87394	1
72	O	66.47313	73.64464	75.08819	-554.84278	14.12789	399.58769	1
73	H	66.59340	73.33449	74.16665	1297.06236	2061.84854	1220.68812	1
74	C	67.42156	70.74871	74.18860	-662.15484	-412.13544	123.62687	1
75	O	66.96850	71.30507	73.22519	-540.01537	-317.05804	274.91456	1
76	N	68.31185	69.74449	74.26101	-202.76299	-690.00100	-131.49145	1
77	H	68.61972	69.49197	75.23567	-702.62132	-2617.37191	281.70413	1
78	C	68.28684	68.61954	73.30473	-491.73914	576.34187	222.73509	1
79	H	67.80407	67.79839	73.88208	1977.17978	-1823.58850	-434.68928	1
80	C	67.57000	68.94052	72.01937	-649.50797	-328.66843	306.11224	1
81	H	67.78089	70.00545	71.75247	2075.07803	1452.16490	-1004.45904	1
82	C	68.05217	68.06395	70.87505	-615.18735	-489.99689	-70.96352	1
83	H	67.51968	68.30137	69.91369	-1226.32661	-1724.38906	-1716.47170	1
84	H	69.15406	68.19532	70.68986	2381.64273	-969.84735	900.46860	1
85	H	67.88201	66.97364	71.09155	2122.74991	1702.23946	-141.36228	1
86	C	66.06456	68.78200	72.15492	-501.86074	-479.61276	-376.42482	1
87	H	65.53285	69.03665	71.19743	993.79261	-2246.95401	-1177.81305	1
88	H	65.77985	67.72814	72.42466	42.71279	-626.15391	-2651.37258	1
89	H	65.65013	69.45708	72.95492	-2026.39012	-1590.33709	-887.82922	1
90	C	69.89286	68.28072	73.05772	-672.89153	382.57394	-156.34072	1
91	O	70.31828	67.17166	73.28438	410.04627	221.86223	500.35950	1
92	N	70.53569	69.31977	72.54473	-378.11782	-443.79414	-441.10984	1
93	H	69.99725	70.18161	72.48390	2404.15973	-568.14894	1149.30085	1
94	C	71.94668	69.24327	72.36096	-544.54484	466.16019	331.29119	1
95	H	72.21085	68.19656	72.64059	-1409.80988	-170.17955	2325.32679	1
96	C	72.21456	69.59747	70.83097	-184.48284	116.78282	-758.89137	1
97	H	71.73657	68.84862	70.16034	1893.78641	1861.14652	611.04528	1
98	H	71.75455	70.57584	70.56937	-2170.79665	-974.19311	1327.50117	1
99	C	73.75806	69.64129	70.62615	389.51668	672.81878	-138.49152	1
100	H	74.21973	70.29173	71.40033	510.64577	1933.03327	1851.02484	1
101	H	74.20094	68.63782	70.81192	-2302.30869	-1105.72939	-948.89774	1
102	C	74.17685	70.16131	69.19708	-559.93427	-126.34590	542.30857	1

103	O	75.33440	70.40306	68.97417	-670.36003	-111.83166	76.36448	1
104	N	73.15137	70.27000	68.32650	-216.06729	-537.07037	446.51379	1
105	H	72.15468	70.06252	68.46100	-1251.96487	1074.12894	-2168.52500	1
106	H	73.25751	70.55922	67.34812	-2451.83023	-720.73851	944.84612	1
107	C	72.60422	70.39333	73.30180	546.24052	-563.88337	-85.11809	1
108	O	72.70719	71.53876	72.87822	71.70702	-307.40463	606.69673	1
109	N	72.92535	69.91699	74.49934	479.90863	-504.50129	222.86849	1
110	C	73.27882	70.81746	75.56127	75.51268	-600.91904	506.73700	1
111	H	72.73622	71.76884	75.35499	-2033.61562	1795.30103	254.89480	1
112	C	72.78865	69.97780	76.81384	523.79067	517.99274	284.45581	1
113	H	73.21897	70.34020	77.77860	1599.61665	-1127.00911	1895.98173	1
114	H	71.68056	70.02055	76.91708	-1881.83093	1275.82488	-1501.55016	1
115	C	73.23505	68.53763	76.41467	-600.05639	-404.05026	316.64485	1
116	H	74.34113	68.41896	76.50622	-2597.05260	496.36221	657.73249	1
117	H	72.76946	67.73418	77.02943	-1666.24518	1294.38985	-1723.90591	1
118	C	72.76570	68.52143	74.89805	493.57570	-129.95376	-602.56394	1
119	H	73.38535	67.88894	74.22024	-1469.08415	-637.84797	2204.22581	1
120	H	71.68430	68.28037	74.74450	-1038.97840	1068.88701	-2280.71789	1
121	C	74.90305	71.00006	75.56643	188.88100	241.05089	-727.87821	1
122	O	75.65064	70.14661	75.97628	531.88613	-49.19943	427.07960	1
123	N	75.22168	72.22720	75.11212	708.14833	26.93417	-179.73509	1
124	H	74.42148	72.73395	74.72968	-2232.69501	-1179.09831	1023.94816	1
125	C	76.58440	72.42496	74.59569	-738.32412	259.92548	104.42456	1
126	H	76.99592	71.38661	74.57060	2028.89123	1260.02983	1311.33324	1
127	C	76.48241	73.06755	73.22718	-258.65678	-345.52513	661.28459	1
128	H	75.95249	74.04053	73.33931	-1826.06090	-1801.46097	-918.64554	1
129	C	77.86101	73.35129	72.65774	-541.23400	531.92970	-218.41428	1
130	H	77.80468	73.89858	71.67627	1311.73218	-2219.18200	882.19023	1
131	H	78.45125	73.99520	73.37602	-1048.71298	1223.58118	-2196.97971	1
132	H	78.44910	72.40760	72.48712	419.06414	1903.92898	1903.44670	1
133	C	75.70011	72.21420	72.24698	-423.86431	152.66566	-648.55262	1
134	H	75.66103	72.68201	71.22573	105.68386	-2342.50080	1387.51238	1
135	H	76.17043	71.19983	72.12189	-1695.63603	-1484.73621	-1531.02793	1
136	H	74.62713	72.04825	72.58749	-1853.57121	-487.39031	1936.59343	1
137	C	77.42348	73.36377	75.67457	539.71428	-510.58232	267.58633	1
138	O	78.64637	73.43868	75.57804	-15.93758	-278.34085	-624.49402	1
139	N	76.62585	74.00756	76.51107	-676.81886	12.05292	276.17960	1
140	H	75.67742	73.72813	76.24299	-1694.44250	-373.84189	-2100.66098	1
141	C	76.91294	74.24577	77.88700	412.33078	-664.70360	108.35451	1
142	H	75.90389	74.44876	78.30552	1765.77476	1294.44366	1621.76594	1
143	C	77.57381	72.94549	78.50029	-179.66635	-721.95667	-264.73915	1
144	H	76.93559	72.04664	78.34290	-607.34922	2587.87032	-598.10018	1
145	H	78.54389	72.71909	78.00256	-359.69332	-1479.13954	-2259.74260	1
146	C	77.76868	73.27283	80.01869	-240.01076	616.02425	431.85322	1
147	H	78.33624	74.22710	80.12626	-1359.17131	782.54425	2227.99181	1
148	H	76.78572	73.45245	80.50869	-820.36667	85.81767	-2596.78715	1
149	C	78.54297	72.10221	80.74481	-513.07015	236.18570	-551.87280	1
150	H	77.92720	71.17441	80.78844	1816.11944	-1183.11722	-1650.94321	1
151	H	79.47154	71.82765	80.19326	-1800.04429	-1361.53473	1526.34643	1
152	C	78.87416	72.63224	82.16051	726.08972	-253.19732	-179.64713	1
153	H	79.59569	73.47351	82.17751	1224.27271	-456.51798	-2390.90304	1
154	H	77.98841	72.88465	82.77696	1206.40339	-1150.93514	-2154.90344	1
155	N	79.58982	71.48858	82.95322	329.70796	-633.68968	-155.67358	1
156	H	79.89498	71.73942	83.93796	1348.31305	1938.76845	1359.00643	1
157	H	79.03527	70.60036	83.12726	2096.92035	1446.54551	-966.48890	1
158	H	80.49340	71.10820	82.54635	-1197.07217	-2303.53719	827.28733	1
159	C	77.96962	75.46071	78.18913	-378.01186	-556.17301	-413.96481	1
160	O	77.74457	76.19358	79.12283	-409.44433	-307.55053	-453.30833	1
161	N	79.07300	75.35377	77.46420	-429.02477	524.70884	274.08502	1
162	H	79.11570	74.65426	76.67754	1706.34263	-1425.96036	1574.38926	1
163	C	79.99828	76.44883	77.51336	-45.25864	-626.22952	478.93267	1
164	H	79.84387	76.87936	78.53120	1988.63164	570.90773	1772.87287	1

165	C	81.41329	75.76615	77.29242	551.77128	-20.49526	-564.54996	1
166	H	81.58527	75.03045	78.10926	1434.61535	-1753.10253	1513.99471	1
167	H	81.39138	75.15990	76.36139	-714.67738	1819.09770	1898.36494	1
168	C	82.61664	76.76296	77.22908	446.99263	-555.77305	338.97221	1
169	H	82.59115	77.34617	76.27832	1953.68466	1892.25957	-161.67766	1
170	H	82.57920	77.49788	78.06526	-403.03785	2688.07032	-188.43591	1
171	C	83.95730	75.92585	77.28006	567.86262	335.74681	434.04421	1
172	H	84.07170	75.40237	78.25670	-1080.02275	1568.26081	-1948.78900	1
173	H	83.94982	75.12784	76.50499	-919.54108	2111.34692	1456.13463	1
174	C	85.12489	76.91412	77.02486	195.81897	173.33862	-745.11536	1
175	H	84.94563	77.62850	76.19554	1405.67949	-2301.21089	-390.08113	1
176	H	85.48243	77.45749	77.92340	-940.37328	-1118.32446	2299.72133	1
177	N	86.32928	76.07576	76.52136	319.26422	656.36007	-42.02424	1
178	H	87.21462	76.62762	76.32510	1961.03633	619.91968	1787.09422	1
179	H	86.70763	75.34180	77.18780	854.14343	-2156.80752	1429.08711	1
180	H	86.14128	75.52894	75.57743	1237.02905	-1378.50857	-1998.28500	1
181	C	79.53537	77.48110	76.35296	532.53319	-268.57236	517.55729	1
182	O	78.41266	77.42778	75.84487	266.16714	-290.73804	-558.88002	1
183	N	80.46823	78.38079	76.15435	-226.25352	640.49678	-270.32839	1
184	H	81.30565	78.34466	76.73150	2007.69063	-1035.27229	1523.50231	1
185	C	80.33337	79.33246	75.09544	-540.76542	-573.33303	49.50000	1
186	H	79.28048	79.66751	75.22793	-2374.20950	-1036.76023	843.75774	1
187	C	81.44047	80.45201	75.31765	-77.09082	666.87422	-415.84136	1
188	H	82.45192	80.00648	75.10982	-985.81834	617.19825	2463.91927	1
189	O	81.51627	81.00857	76.64602	293.29899	-391.65602	-477.80926	1
190	H	82.43765	80.79562	76.89168	2528.72714	-681.76262	-751.27122	1
191	C	81.07744	81.47223	74.17517	252.47363	-605.14473	440.05134	1
192	H	81.81108	82.31022	74.13188	-2052.65063	1456.49051	-1043.51830	1
193	H	81.06910	80.98800	73.16898	-2152.98800	-1661.97574	-161.70652	1
194	H	80.07085	81.92279	74.33599	-473.12726	-1584.27339	2165.61725	1
195	C	80.53538	78.56014	73.66226	360.36307	488.46713	505.10056	1
196	O	81.48861	78.76495	72.95359	-200.08817	-528.03552	-385.82850	1
197	N	79.47317	77.79608	73.45081	-597.54095	-226.44775	355.20479	1
198	H	78.73136	77.67637	74.19076	2179.23655	-1300.70981	-991.33835	1
199	C	79.49313	76.89726	72.35717	-687.68921	297.39807	-249.45179	1
200	H	80.11735	77.35365	71.55689	-349.16256	-2467.37713	-1101.72831	1
201	C	80.02610	75.49211	72.88208	672.47345	361.54328	-201.62880	1
202	H	79.42144	75.19024	73.77589	1541.41502	582.18425	2169.97026	1
203	H	79.82611	74.73065	72.09396	-2534.67717	60.25153	997.72295	1
204	C	81.52321	75.38681	73.25409	574.26774	-389.43119	-377.02542	1
205	C	82.56416	76.13539	72.63848	688.82679	-287.33580	-257.96133	1
206	H	82.33290	76.92179	71.89748	331.14182	1470.38163	2269.80013	1
207	C	81.83290	74.37632	74.20696	-383.52382	-675.04808	144.24917	1
208	H	81.02799	73.78327	74.67609	4.09847	1517.59662	2262.86397	1
209	C	83.89976	75.85254	72.99871	-134.76730	428.45285	-649.50303	1
210	H	84.71695	76.42222	72.51817	-903.23433	1600.49020	2011.53387	1
211	C	83.18638	74.13196	74.52545	-335.53281	-615.00040	-364.39058	1
212	H	83.42317	73.33943	75.25968	1596.45398	-1369.33862	1732.02659	1
213	C	84.24029	74.86233	73.94139	585.48547	-340.24194	-406.23938	1
214	O	85.69454	74.60185	74.28971	-419.15649	-173.04408	-511.94141	1
215	H	85.54043	73.77649	74.77144	-1071.84350	1559.71507	-1960.13012	1
216	C	77.90359	76.62228	72.02665	291.41878	-183.13091	710.72246	1
217	O	77.16190	76.18271	72.88178	379.87695	523.47396	-222.23622	1
218	N	77.62021	76.96257	70.77958	564.30591	373.09380	277.24371	1
219	H	78.38170	77.33131	70.21054	-120.59931	-2436.07824	-1214.35098	1
220	C	76.29496	76.94893	70.26773	404.07514	-299.37480	608.84009	1
221	H	76.44414	77.04686	69.16901	-1071.07882	-841.69025	2359.66467	1
222	C	75.60070	75.58260	70.68902	-683.12807	68.71770	-390.13096	1
223	H	76.25603	74.72189	70.42822	2068.88918	1596.58590	770.89603	1
224	H	75.47671	75.53873	71.80054	1379.86429	2342.49779	-179.85638	1
225	C	74.22087	75.46126	69.97453	-176.39967	537.49466	550.97268	1
226	H	73.55887	76.31350	70.25181	-396.28051	1942.22168	1869.33314	1

227	H	74.34964	75.53567	68.87213	-94.44700	586.00678	-2659.20016	1
228	C	73.52600	74.07520	70.37055	-291.69381	-718.18079	-150.72929	1
229	H	74.05603	73.16663	69.98514	-2303.38776	1089.76242	964.62032	1
230	H	73.28208	73.92375	71.45267	884.16729	2568.80533	-207.74283	1
231	N	72.33172	74.20934	69.64461	-594.49522	-252.81478	342.29276	1
232	H	72.36110	74.82416	68.84494	-1735.17426	2084.05705	-263.71605	1
233	C	71.23646	73.60473	69.88445	595.23177	-271.52487	442.22352	1
234	N	71.17140	72.73100	70.96618	585.53813	-424.79750	-105.81303	1
235	H	71.91856	72.49230	71.65960	959.88797	1327.56823	-2177.11905	1
236	H	70.31179	72.23805	71.23390	1578.48647	16.27378	-2220.76233	1
237	N	70.24878	73.95408	68.94655	-452.17763	-390.33541	-421.51853	1
238	H	70.27129	74.61184	68.16975	470.26107	1974.25629	-1817.92087	1
239	H	69.29416	73.59709	68.98420	1856.67307	-1573.97321	-1224.35416	1
240	C	75.37440	78.16946	70.84382	-531.47271	-581.45780	-55.06206	1
241	O	74.36124	78.44158	70.24867	-243.00837	192.73507	609.52485	1
242	N	75.86026	78.77183	71.94248	343.49288	-644.25607	38.09164	1
243	H	76.70075	78.31539	72.29519	-1691.16043	-1535.97525	-1484.73099	1
244	C	74.93519	79.44153	72.88481	542.66492	350.14337	454.42563	1
245	H	74.09615	78.72480	73.04289	1209.57979	-2396.95920	463.86744	1
246	C	75.72987	79.74981	74.13594	-737.14309	145.93010	242.71942	1
247	H	76.73833	80.10015	73.81857	-1050.18303	159.36419	-2509.06125	1
248	C	75.08650	80.86059	74.94693	-706.77696	-252.88343	-245.16230	1
249	H	75.69854	81.12523	75.85320	-1624.64039	-1665.49085	1417.86935	1
250	H	74.96647	81.79899	74.33642	2566.10521	598.51109	693.22305	1
251	H	74.06191	80.56980	75.30891	-1972.69758	107.10018	-1876.34312	1
252	C	75.92417	78.52312	75.00768	412.85148	672.58832	-27.69222	1
253	H	76.57518	78.74451	75.90216	1447.02277	1762.76533	-1490.78944	1
254	H	74.94576	78.14065	75.41000	1320.77379	-145.20455	2378.68491	1
255	H	76.41281	77.67335	74.44539	-1512.10848	1470.52031	1724.75147	1
256	C	74.43888	80.80427	72.11204	-607.11113	499.56689	73.73769	1
257	O	73.32089	81.21589	72.27664	357.97126	460.81534	356.68785	1
258	N	75.47077	81.39144	71.48159	536.55407	-368.62270	332.76306	1
259	H	76.34473	80.83736	71.48968	524.38866	2297.69985	1367.20941	1
260	C	75.16134	81.88074	70.15564	46.50277	-774.29190	-147.97904	1
261	H	74.23785	81.34333	69.84685	1676.51875	1883.29066	1032.55549	1
262	C	74.96080	83.47753	70.18908	-559.41456	-34.19198	-556.30433	1
263	H	75.89035	83.95177	70.58554	-64.66664	395.18769	2695.05373	1
264	H	74.83038	83.87715	69.15471	-2703.44278	-60.40056	333.79418	1
265	C	73.78053	83.84731	71.04959	-519.76435	377.31045	459.42366	1
266	H	73.90551	83.35758	72.04456	-1746.74323	1667.50644	-1261.73691	1
267	C	73.72194	85.35471	71.26084	570.95554	16.46261	-545.27700	1
268	H	72.85751	85.64646	71.91160	2391.58273	28.05277	-1305.07271	1
269	H	74.65212	85.73982	71.75276	175.75588	917.63458	2559.43867	1
270	H	73.60732	85.90370	70.29106	-1063.97851	-2155.34650	1283.00462	1
271	C	72.47428	83.36039	70.43803	193.76014	2.62946	-765.53141	1
272	H	71.58602	83.73228	71.01104	507.39394	-846.55087	2539.60089	1
273	H	72.35587	83.70387	69.37786	1337.57841	1818.19054	1526.01994	1
274	H	72.41866	82.23857	70.44163	1100.88635	-1172.91350	-2199.08909	1
275	C	76.45972	81.50748	69.31065	-549.21115	475.64486	-309.38218	1
276	O	77.40070	80.92064	69.79484	556.06106	-390.37755	-78.24250	1
277	O	76.48698	81.90403	67.95446	-572.27940	-310.19032	-209.75862	1
278	H	75.57769	82.30803	67.89199	-1380.08193	2212.14486	790.85944	1

Listing 4: C00004.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1294.3757	0.0000	300.0000
3	H	77.81839	58.44812	77.61439	-2043.14101	-1757.64893	399.89339		1
4	N	77.51883	59.13719	76.92911	426.75047	490.45733	-334.42467		1
5	H	76.97371	58.57081	76.28335	442.25559	-1110.30854	-2448.52907		1
6	C	78.54976	59.90111	76.34119	415.32972	-666.39213	83.73172		1

7	H	79.17710	60.18057	77.21432	879.32219	2491.00447	667.35213	1
8	C	79.36550	59.03481	75.25830	31.35357	477.41777	628.23362	1
9	H	78.68825	58.76305	74.41335	1168.38489	2240.25337	-1019.71136	1
10	H	80.16368	59.67409	74.80997	-360.43770	2534.90498	931.67112	1
11	C	79.96424	57.79406	75.86951	463.18208	512.70242	-382.34388	1
12	H	79.13858	57.14407	76.23611	1725.29117	1863.52247	-987.07854	1
13	C	80.75676	57.02638	74.81798	710.42801	-144.27427	-313.15367	1
14	H	81.18865	56.07966	75.23369	364.20195	-1033.13725	2494.72524	1
15	H	80.11922	56.74502	73.94057	2567.61904	335.80679	847.48802	1
16	H	81.61198	57.63407	74.42394	-2587.99029	680.92867	-512.16411	1
17	C	80.87728	58.12211	77.04285	268.17616	741.64379	-40.42634	1
18	H	81.37357	57.20296	77.44898	1283.54314	-1945.37420	-1411.27812	1
19	H	81.69031	58.83382	76.74585	-1258.57796	1317.15249	-2026.02085	1
20	H	80.31540	58.59381	77.88956	-2502.84526	909.80597	575.92391	1
21	C	77.87242	61.17762	75.60520	619.36578	-458.64843	-172.09273	1
22	O	78.29060	61.58407	74.53370	-81.40433	433.87611	522.34594	1
23	N	76.88932	61.66940	76.34805	175.23996	-622.20190	341.55523	1
24	H	76.71099	61.19434	77.23248	-876.57256	-303.22879	-2561.90213	1
25	C	76.32441	62.93561	76.00838	-571.88214	-534.10783	-106.15033	1
26	H	76.23982	62.90828	74.90143	-2713.20841	-16.25800	-248.80809	1
27	C	74.93450	63.04420	76.78460	166.60354	288.16399	-716.09568	1
28	H	75.13228	62.96087	77.88838	-2097.85574	1636.78449	-586.18044	1
29	O	73.96214	62.02784	76.47574	-317.80580	-363.38227	484.43082	1
30	H	73.84909	61.59728	77.34580	1863.74748	-1451.84923	1357.29467	1
31	C	74.51615	64.52097	76.43976	503.80731	517.99032	318.51606	1
32	H	73.57639	64.81050	76.96457	640.61020	-2157.10410	-1536.29104	1
33	H	75.30313	65.25304	76.73689	1687.88455	465.60692	2087.56452	1
34	H	74.33559	64.65079	75.34759	-1293.07895	-1899.88581	-1463.57452	1
35	C	77.36041	64.08298	76.54361	-153.07550	-733.68902	248.70981	1
36	O	77.53546	64.20191	77.72656	186.15459	-480.78787	-449.34387	1
37	N	77.85726	64.82224	75.52690	-487.53139	543.18517	42.03850	1
38	C	78.92849	65.72637	75.72731	-699.35871	69.34393	360.10701	1
39	H	79.45616	65.41172	76.65429	2.81126	-221.99807	-2715.58072	1
40	C	79.73829	65.60984	74.38070	-507.46439	-592.59194	122.07761	1
41	H	80.40239	66.48510	74.19535	-1975.08116	525.87560	-1801.71556	1
42	H	80.38527	64.70358	74.36688	1588.27743	-1913.22100	1113.83566	1
43	C	78.56801	65.48261	73.34968	-613.62442	-457.55993	-194.14490	1
44	H	78.07293	66.46441	73.17692	1707.54637	-721.27992	1996.92523	1
45	H	78.88612	65.10302	72.35273	758.23357	2100.81767	1560.55011	1
46	C	77.61741	64.48123	74.12514	-352.41524	704.96076	49.21465	1
47	H	76.52876	64.59478	73.90785	1714.76886	-2070.42778	443.35792	1
48	H	77.91674	63.38368	74.05261	1224.15040	1801.50881	1636.97633	1
49	C	78.40042	67.32679	75.80556	566.85117	537.05831	117.62814	1
50	O	79.20709	68.25353	75.96055	-550.26779	-406.08867	4.21666	1
51	N	77.14163	67.43054	75.64919	566.34832	-425.77725	180.18749	1
52	H	76.66975	66.55495	75.52845	644.44502	2646.80550	-52.73430	1
53	C	75.51595	69.59666	76.06148	612.34801	-281.48662	411.56221	2
54	H	76.22583	68.77264	75.71585	1667.23498	-1490.75142	1556.16753	2
55	C	74.50374	68.97590	77.06757	-714.45746	-175.43074	286.98927	2
56	H	75.05304	68.60857	77.97237	-787.09484	1763.03619	-1922.46060	2
57	O	73.76548	67.82967	76.50625	-429.46514	516.51932	-128.40526	2
58	H	74.02671	67.13678	77.12877	1981.82785	436.16847	-1818.18182	2
59	C	73.61919	70.21436	77.45989	630.79189	-468.94448	76.03230	2
60	H	72.84715	69.93799	78.21536	-1775.71861	2062.30353	131.89849	2
61	H	74.23300	71.03908	77.89861	-1855.14608	88.94118	1993.53760	2
62	H	73.08478	70.63184	76.57502	-1504.82350	-780.94249	-2132.90992	2
63	C	76.35637	70.81232	76.64082	288.57638	618.62814	-397.00270	2
64	O	76.47110	71.06953	77.82175	321.70495	-185.26452	574.37218	2
65	N	76.89658	71.45599	75.59320	-447.05792	-446.53431	367.76425	2
66	H	76.79116	71.09529	74.64559	350.31316	1975.63644	-1843.31522	2
67	C	77.66713	72.63345	75.84380	-511.23061	374.03917	-471.51480	2
68	H	77.01578	73.17388	76.56681	2234.79579	-898.70890	-1273.45190	2

69	C	79.00544	72.12939	76.56780	529.53781	-159.34528	563.72604	2
70	H	79.49185	73.04194	77.00857	654.59388	2347.94251	1217.51488	2
71	H	78.68257	71.48557	77.43143	-1526.55661	2103.42026	817.87394	2
72	O	79.96690	71.44134	75.73393	-554.84278	14.12789	399.58769	2
73	H	79.66992	70.51174	75.86286	1297.06236	2061.84854	1220.68812	2
74	C	77.83024	73.38241	74.41884	-662.15484	-412.13544	123.62687	2
75	O	76.88657	73.49949	73.66287	-540.01537	-317.05804	274.91456	2
76	N	79.06534	73.85739	74.27301	-202.76299	-690.00100	-131.49145	2
77	H	79.72762	73.58563	75.00178	-702.62132	-2617.37191	281.70413	2
78	C	79.49695	74.64146	73.12359	-491.73914	576.34187	222.73509	2
79	H	80.60556	74.61285	73.24481	1977.17978	-1823.58850	-434.68928	2
80	C	79.03052	73.96689	71.84759	-649.50797	-328.66843	306.11224	2
81	H	77.91219	73.95466	71.84628	2075.07803	1452.16490	-1004.45904	2
82	C	79.52011	74.69173	70.60807	-615.18735	-489.99689	-70.96352	2
83	H	79.23572	74.13207	69.66657	-1226.32661	-1724.38906	-1716.47170	2
84	H	79.09585	75.72983	70.52354	2381.64273	-969.84735	900.46860	2
85	H	80.63970	74.79455	70.60749	2122.74991	1702.23946	-141.36228	2
86	C	79.48706	72.51820	71.79291	-501.86074	-479.61276	-376.42482	2
87	H	79.07680	71.98443	70.89260	993.79261	-2246.95401	-1177.81305	2
88	H	80.60753	72.43986	71.74766	42.71279	-626.15391	-2651.37258	2
89	H	79.15285	71.95014	72.70466	-2026.39012	-1590.33709	-887.82922	2
90	C	78.93393	76.18744	73.41685	-672.89153	382.57394	-156.34072	2
91	O	79.42767	76.80471	74.33329	410.04627	221.86223	500.35950	2
92	N	78.07191	76.60414	72.51109	-378.11782	-443.79414	-441.10984	2
93	H	77.73603	75.87813	71.88409	2404.15973	-568.14894	1149.30085	2
94	C	77.26823	77.78639	72.72993	-544.54484	466.16019	331.29119	2
95	H	76.48583	77.43757	73.44026	-1409.80988	-170.17955	2325.32679	2
96	C	78.17458	78.90920	73.37899	-184.48284	116.78282	-758.89137	2
97	H	78.45679	78.63496	74.42940	1893.78641	1861.14652	611.04528	2
98	H	79.14209	78.99491	72.83244	-2170.79665	-974.19311	1327.50117	2
99	C	77.39729	80.26407	73.37705	389.51668	672.81878	-138.49152	2
100	H	77.10035	80.53661	72.33987	510.64577	1933.03327	1851.02484	2
101	H	76.43000	80.15873	73.91516	-2302.30869	-1105.72939	-948.89774	2
102	C	78.23566	81.43376	74.01960	-559.93427	-126.34590	542.30857	2
103	O	77.71717	82.50626	74.19729	-670.36003	-111.83166	76.36448	2
104	N	79.51488	81.10888	74.30864	-216.06729	-537.07037	446.51379	2
105	H	80.01773	80.22587	74.16232	-1251.96487	1074.12894	-2168.52500	2
106	H	80.20565	81.77322	74.67367	-2451.83023	-720.73851	944.84612	2
107	C	76.62124	78.07911	71.28328	546.24052	-563.88337	-85.11809	2
108	O	75.51910	77.55843	71.09638	71.70702	-307.40463	606.69673	2
109	N	77.38548	78.70094	70.39557	479.90863	-504.50129	222.86849	2
110	C	76.86641	79.13409	69.12328	75.51268	-600.91904	506.73700	2
111	H	75.88583	79.61891	69.33236	-2033.61562	1795.30103	254.89480	2
112	C	78.00256	80.11112	68.60543	523.79067	517.99274	284.45581	2
113	H	77.98097	80.24781	67.50047	1599.61665	-1127.00911	1895.98173	2
114	H	77.90865	81.12433	69.05645	-1881.83093	1275.82488	-1501.55016	2
115	C	79.28491	79.38055	69.11494	-600.05639	-404.05026	316.64485	2
116	H	79.52949	78.50233	68.47699	-2597.05260	496.36221	657.73249	2
117	H	80.19092	80.02734	69.12682	-1666.24518	1294.38985	-1723.90591	2
118	C	78.81533	78.93685	70.56560	493.57570	-129.95376	-602.56394	2
119	H	79.27414	77.99900	70.95765	-1469.08415	-637.84797	2204.22581	2
120	H	78.90225	79.74442	71.33142	-1038.97840	1068.88701	-2280.71789	2
121	C	76.71628	77.89371	68.07888	188.88100	241.05089	-727.87821	2
122	O	76.58862	78.11676	66.90039	531.88613	-49.19943	427.07960	2
123	N	76.74601	76.70547	68.68527	708.14833	26.93417	-179.73509	2
124	H	76.87970	76.72241	69.69873	-2232.69501	-1179.09831	1023.94816	2
125	C	76.57871	75.45986	67.92629	-738.32412	259.92548	104.42456	2
126	H	75.98387	75.78467	67.03734	2028.89123	1260.02983	1311.33324	2
127	C	77.96703	74.98488	67.51832	-258.65678	-345.52513	661.28459	2
128	H	78.56216	74.86356	68.45724	-1826.06090	-1801.46097	-918.64554	2
129	C	77.94470	73.65584	66.78963	-541.23400	531.92970	-218.41428	2
130	H	78.98154	73.31040	66.52135	1311.73218	-2219.18200	882.19023	2

131	H	77.46892	72.84141	67.41448	-1048.71298	1223.58118	-2196.97971	2
132	H	77.35757	73.72092	65.83190	419.06414	1903.92898	1903.44670	2
133	C	78.67188	76.01389	66.65275	-423.86431	152.66566	-648.55262	2
134	H	79.76216	75.77366	66.51595	105.68386	-2342.50080	1387.51238	2
135	H	78.21042	76.07447	65.62867	-1695.63603	-1484.73621	-1531.02793	2
136	H	78.59959	77.04587	67.09882	-1853.57121	-487.39031	1936.59343	2
137	C	75.78423	74.39982	68.89814	539.71428	-510.58232	267.58633	2
138	O	75.81731	73.21836	68.63813	-15.93758	-278.34085	-624.49402	2
139	N	75.13176	74.97280	69.90216	-676.81886	12.05292	276.17960	2
140	H	75.14173	75.99448	70.02281	-1694.44250	-373.84189	-2100.66098	2
141	C	74.12613	74.11816	70.49267	412.33078	-664.70360	108.35451	2
142	H	73.68556	73.60081	69.61041	1765.77476	1294.44366	1621.76594	2
143	C	74.88813	73.08351	71.41018	-179.66635	-721.95667	-264.73915	2
144	H	75.67963	72.56064	70.82308	-607.34922	2587.87032	-598.10018	2
145	H	75.42705	73.58992	72.25955	-359.69332	-1479.13954	-2259.74260	2
146	C	73.81625	72.06834	71.94864	-240.01076	616.02425	431.85322	2
147	H	73.09856	72.58499	72.62849	-1359.17131	782.54425	2227.99181	2
148	H	73.20684	71.65953	71.11028	-820.36667	85.81767	-2596.78715	2
149	C	74.57010	70.91891	72.69138	-513.07015	236.18570	-551.87280	2
150	H	75.29087	70.40958	72.01504	1816.11944	-1183.11722	-1650.94321	2
151	H	75.18037	71.32917	73.52471	-1800.04429	-1361.53473	1526.34643	2
152	C	73.46916	69.88608	73.22807	726.08972	-253.19732	-179.64713	2
153	H	72.92267	70.25389	74.13193	1224.27271	-456.51798	-2390.90304	2
154	H	72.73568	69.58276	72.44015	1206.40339	-1150.93514	-2154.90344	2
155	N	74.15748	68.69003	73.61006	329.70796	-633.68968	-155.67358	2
156	H	73.91042	68.30087	74.52238	1348.31305	1938.76845	1359.00643	2
157	H	74.01617	67.89514	72.99197	2096.92035	1446.54551	-966.48890	2
158	H	74.99038	69.93007	75.14194	-1197.07217	-2303.53719	827.28733	2
159	C	73.03608	74.95469	71.37642	-378.01186	-556.17301	-413.96481	2
160	O	71.91070	74.51994	71.44304	-409.44433	-307.55053	-453.30833	2
161	N	73.58741	75.98863	71.98159	-429.02477	524.70884	274.08502	2
162	H	74.58175	76.23995	71.78861	1706.34263	-1425.96036	1574.38926	2
163	C	72.83818	76.90187	72.77157	-45.25864	-626.22952	478.93267	2
164	H	73.38580	77.86136	72.63483	1988.63164	570.90773	1772.87287	2
165	C	71.33241	76.94008	72.29356	551.77128	-20.49526	-564.54996	2
166	H	71.26780	77.11538	71.19518	1434.61535	-1753.10253	1513.99471	2
167	H	70.82362	75.95700	72.47750	-714.67738	1819.09770	1898.36494	2
168	C	70.64597	78.09095	73.10454	446.99263	-555.77305	338.97221	2
169	H	70.66938	77.86114	74.19396	1953.68466	1892.25957	-161.67766	2
170	H	71.20301	79.04640	72.98442	-403.03785	2688.07032	-188.43591	2
171	C	69.15755	78.25033	72.59852	567.86262	335.74681	434.04421	2
172	H	69.12838	78.67868	71.57001	-1080.02275	1568.26081	-1948.78900	2
173	H	68.64844	77.26126	72.53172	-919.54108	2111.34692	1456.13463	2
174	C	68.43687	79.17031	73.61295	195.81897	173.33862	-745.11536	2
175	H	68.19912	78.69044	74.58341	1405.67949	-2301.21089	-390.08113	2
176	H	68.93922	80.13978	73.78783	-940.37328	-1118.32446	2299.72133	2
177	N	67.05017	79.56218	73.00494	319.26422	656.36007	-42.02424	2
178	H	66.44024	80.18045	73.61432	1961.03633	619.91968	1787.09422	2
179	H	67.05242	80.10301	72.09102	854.14343	-2156.80752	1429.08711	2
180	H	66.38653	78.76385	72.78795	1237.02905	-1378.50857	-1998.28500	2
181	C	72.86251	76.40228	74.34475	532.53319	-268.57236	517.55729	2
182	O	72.53166	75.30645	74.72575	266.16714	-290.73804	-558.88002	2
183	N	73.19468	77.47158	75.05543	-226.25352	640.49678	-270.32839	2
184	H	73.40822	78.34966	74.58457	2007.69063	-1035.27229	1523.50231	2
185	C	73.24662	77.36895	76.46716	-540.76542	-573.33303	49.50000	2
186	H	72.85560	76.35743	76.73047	-2374.20950	-1036.76023	843.75774	2
187	C	74.79115	77.59417	76.86794	-77.09082	666.87422	-415.84136	2
188	H	75.12755	78.56999	76.42248	-985.81834	617.19825	2463.91927	2
189	O	75.70622	76.59699	76.38977	293.29899	-391.65602	-477.80926	2
190	H	76.27584	77.12829	75.79734	2528.72714	-681.76262	-751.27122	2
191	C	74.71549	77.74050	78.43001	252.47363	-605.14473	440.05134	2
192	H	75.71589	77.96568	78.86667	-2052.65063	1456.49051	-1043.51830	2

193	H	74.02627	78.56065	78.74150	-2152.98800	-1661.97574	-161.70652	2
194	H	74.35165	76.80176	78.90853	-473.12726	-1584.27339	2165.61725	2
195	C	72.39680	78.63601	77.04659	360.36307	488.46713	505.10056	2
196	O	72.45922	79.75167	76.53736	-200.08817	-528.03552	-385.82850	2
197	N	71.75839	78.26010	78.13389	-597.54095	-226.44775	355.20479	2
198	H	71.86322	77.29885	78.45178	2179.23655	-1300.70981	-991.33835	2
199	C	71.08439	79.25838	78.89473	-687.68921	297.39807	-249.45179	2
200	H	70.60028	79.89125	78.11631	-349.16256	-2467.37713	-1101.72831	2
201	C	70.13143	78.62209	80.00257	672.47345	361.54328	-201.62880	2
202	H	70.75825	78.19938	80.82495	1541.41502	582.18425	2169.97026	2
203	H	69.51477	79.43684	80.45271	-2534.67717	60.25153	997.72295	2
204	C	69.22927	77.53711	79.39411	574.26774	-389.43119	-377.02542	2
205	C	68.03093	77.92898	78.72660	688.82679	-287.33580	-257.96133	2
206	H	67.75474	78.99951	78.64105	331.14182	1470.38163	2269.80013	2
207	C	69.59264	76.16085	79.49832	-383.52382	-675.04808	144.24917	2
208	H	70.52502	75.86037	80.01014	4.09847	1517.59662	2262.86397	2
209	C	67.21672	76.93062	78.19144	-134.76730	428.45285	-649.50303	2
210	H	66.28384	77.22797	77.68144	-903.23433	1600.49020	2011.53387	2
211	C	68.74377	75.20014	78.94291	-335.53281	-615.00040	-364.39058	2
212	H	69.02974	74.13720	79.02954	1596.45398	-1369.33862	1732.02659	2
213	C	67.53165	75.54314	78.27569	585.48547	-340.24194	-406.23938	2
214	O	66.66166	74.57356	77.71164	-419.15649	-173.04408	-511.94141	2
215	H	67.15452	73.75177	77.94523	-1071.84350	1559.71507	-1960.13012	2
216	C	72.19233	80.07112	79.78057	291.41878	-183.13091	710.72246	2
217	O	72.24545	79.92888	80.97978	379.87695	523.47396	-222.23622	2
218	N	72.94800	80.81606	78.97768	564.30591	373.09380	277.24371	2
219	H	72.80656	80.76960	77.94205	-120.59931	-2436.07824	-1214.35098	2
220	C	73.94118	81.62199	79.59792	404.07514	-299.37480	608.84009	2
221	H	74.00829	81.26256	80.65340	-1071.07882	-841.69025	2359.66467	2
222	C	75.27444	81.46476	78.74849	-683.12807	68.71770	-390.13096	2
223	H	75.53389	80.39212	78.60625	2068.88918	1596.58590	770.89603	2
224	H	75.13487	81.87649	77.72371	1379.86429	2342.49779	-179.85638	2
225	C	76.40667	82.22208	79.50583	-176.39967	537.49466	550.97268	2
226	H	76.10189	83.27067	79.73345	-396.28051	1942.22168	1869.33314	2
227	H	76.61535	81.75093	80.49236	-94.44700	586.00678	-2659.20016	2
228	C	77.69163	82.18476	78.55693	-291.69381	-718.18079	-150.72929	2
229	H	78.08168	81.16637	78.30297	-2303.38776	1089.76242	964.62032	2
230	H	77.59968	82.76429	77.60261	884.16729	2568.80533	-207.74283	2
231	N	78.65099	82.82390	79.35547	-594.49522	-252.81478	342.29276	2
232	H	78.32951	83.22152	80.22462	-1735.17426	2084.05705	-263.71605	2
233	C	79.88068	82.93561	79.05202	595.23177	-271.52487	442.22352	2
234	N	80.29971	82.38189	77.83721	585.53813	-424.79750	-105.81303	2
235	H	79.75183	81.91445	77.11527	959.88797	1327.56823	-2177.11905	2
236	H	81.25328	82.41913	77.47642	1578.48647	16.27378	-2220.76233	2
237	N	80.58198	83.62135	80.05333	-452.17763	-390.33541	-421.51853	2
238	H	80.26609	84.02221	80.93537	470.26107	1974.25629	-1817.92087	2
239	H	81.58265	83.81621	80.00344	1856.67307	-1573.97321	-1224.35416	2
240	C	73.51274	83.20168	79.48615	-531.47271	-581.45780	-55.06206	2
241	O	73.99972	84.01420	80.23560	-243.00837	192.73507	609.52485	2
242	N	72.72827	83.42064	78.43377	343.49288	-644.25607	38.09164	2
243	H	72.48785	82.59204	77.89465	-1691.16043	-1535.97525	-1484.73099	2
244	C	72.05492	84.70896	78.23562	542.66492	350.14337	454.42563	2
245	H	71.90093	85.08209	79.27654	1209.57979	-2396.95920	463.86744	2
246	C	72.98445	85.61824	77.44661	-737.14309	145.93010	242.71942	2
247	H	73.15220	85.14828	76.45174	-1050.18303	159.36419	-2509.06125	2
248	C	72.37756	86.99022	77.22515	-706.77696	-252.88343	-245.16230	2
249	H	73.03287	87.63851	76.58026	-1624.64039	-1665.49085	1417.86935	2
250	H	71.36624	86.91447	76.71764	2566.10521	598.51109	693.22305	2
251	H	72.22170	87.53634	78.19617	-1972.69758	107.10018	-1876.34312	2
252	C	74.33785	85.76122	78.11978	412.85148	672.58832	-27.69222	2
253	H	75.03420	86.42247	77.53432	1447.02277	1762.76533	-1490.78944	2
254	H	74.23854	86.19995	79.15137	1320.77379	-145.20455	2378.68491	2

255	H	74.84180	84.76172	78.24534	-1512.10848	1470.52031	1724.75147	2
256	C	70.65087	84.39596	77.42692	-607.11113	499.56689	73.73769	2
257	O	70.13424	85.26606	76.75879	357.97126	460.81534	356.68785	2
258	N	70.19649	83.17845	77.66219	536.55407	-368.62270	332.76306	2
259	H	70.72694	82.57466	78.28721	524.38866	2297.69985	1367.20941	2
260	C	69.03043	82.74078	76.97027	46.50277	-774.29190	-147.97904	2
261	H	68.48966	83.67894	76.70259	1676.51875	1883.29066	1032.55549	2
262	C	69.46518	81.89294	75.69090	-559.41456	-34.19198	-556.30433	2
263	H	70.05736	81.00519	76.00652	-64.66664	395.18769	2695.05373	2
264	H	68.56433	81.49542	75.17463	-2703.44278	-60.40056	333.79418	2
265	C	70.31348	82.77114	74.71334	-519.76435	377.31045	459.42366	2
266	H	71.18532	83.20345	75.25223	-1746.74323	1667.50644	-1261.73691	2
267	C	70.79599	81.87244	73.51640	570.95554	16.46261	-545.27700	2
268	H	71.48070	82.43051	72.83657	2391.58273	28.05277	-1305.07271	2
269	H	71.34775	80.97418	73.87886	175.75588	917.63458	2559.43867	2
270	H	69.94123	81.51602	72.89637	-1063.97851	-2155.34650	1283.00462	2
271	C	69.41882	83.91200	74.10527	193.76014	2.62946	-765.53141	2
272	H	69.94958	84.45809	73.29090	507.39394	-846.55087	2539.60089	2
273	H	68.47278	83.50933	73.67399	1337.57841	1818.19054	1526.01994	2
274	H	69.14312	84.66816	74.88213	1100.88635	-1172.91350	-2199.08909	2
275	C	68.22474	81.70479	77.92184	-549.21115	475.64486	-309.38218	2
276	O	68.74920	81.05336	78.78778	556.06106	-390.37755	-78.24250	2
277	O	66.87903	81.46901	77.56241	-572.27940	-310.19032	-209.75862	2
278	H	66.78980	82.16604	76.85032	-1380.08193	2212.14486	790.85944	2

Listing 5: C00005.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1294.3184	0.0000	300.0000
3	H	70.86210	62.77071	79.43633	-2043.14101	-1757.64893	399.89339		1
4	N	71.07610	62.99383	78.46748	426.75047	490.45733	-334.42467		1
5	H	70.22577	63.44856	78.14689	442.25559	-1110.30854	-2448.52907		1
6	C	72.28532	63.67621	78.23128	415.32972	-666.39213	83.73172		1
7	H	73.04240	63.13716	78.83873	879.32219	2491.00447	667.35213		1
8	C	72.59916	63.65851	76.64949	31.35357	477.41777	628.23362		1
9	H	71.69606	64.01455	76.09289	1168.38489	2240.25337	-1019.71136		1
10	H	73.40661	64.39551	76.42848	-360.43770	2534.90498	931.67112		1
11	C	72.99864	62.28180	76.18253	463.18208	512.70242	-382.34388		1
12	H	72.21796	61.55828	76.50831	1725.29117	1863.52247	-987.07854		1
13	C	73.08745	62.25901	74.66156	710.42801	-144.27427	-313.15367		1
14	H	73.29467	61.22877	74.27265	364.20195	-1033.13725	2494.72524		1
15	H	72.13594	62.61211	74.18524	2567.61904	335.80679	847.48802		1
16	H	73.90987	62.92355	74.29047	-2587.99029	680.92867	-512.16411		1
17	C	74.33816	61.86699	76.77479	268.17616	741.64379	-40.42634		1
18	H	74.67898	60.87729	76.37435	1283.54314	-1945.37420	-1411.27812		1
19	H	75.13994	62.61430	76.53882	-1258.57796	1317.15249	-2026.02085		1
20	H	74.29001	61.77416	77.89037	-2502.84526	909.80597	575.92391		1
21	C	72.19985	65.24717	78.60636	619.36578	-458.64843	-172.09273		1
22	O	73.17326	65.95857	78.34761	-81.40433	433.87611	522.34594		1
23	N	71.06168	65.56875	79.16943	175.23996	-622.20190	341.55523		1
24	H	70.41754	64.79796	79.33097	-876.57256	-303.22879	-2561.90213		1
25	C	70.60077	66.88582	79.46867	-571.88214	-534.10783	-106.15033		1
26	H	69.50353	66.70141	79.47127	-2713.20841	-16.25800	-248.80809		1
27	C	71.02945	67.20385	80.97300	166.60354	288.16399	-716.09568		1
28	H	72.14754	67.28646	81.05363	-2097.85574	1636.78449	-586.18044		1
29	O	70.67218	66.20091	81.94875	-317.80580	-363.38227	484.43082		1
30	H	71.55217	65.94316	82.28243	1863.74748	-1451.84923	1357.29467		1
31	C	70.35649	68.61040	81.17571	503.80731	517.99032	318.51606		1
32	H	70.65892	69.07113	82.14454	640.61020	-2157.10410	-1536.29104		1
33	H	70.62377	69.32638	80.36409	1687.88455	465.60692	2087.56452		1
34	H	69.24506	68.52650	81.18567	-1293.07895	-1899.88581	-1463.57452		1

35	C	70.98469	67.91199	78.25409	-153.07550	-733.68902	248.70981	1
36	O	70.21648	67.86483	77.32476	186.15459	-480.78787	-449.34387	1
37	N	72.07054	68.68472	78.38492	-487.53139	543.18517	42.03850	1
38	C	72.38031	69.64698	77.36258	-699.35871	69.34393	360.10701	1
39	H	71.45126	70.23712	77.19081	2.81126	-221.99807	-2715.58072	1
40	C	73.59337	70.46110	77.98629	-507.46439	-592.59194	122.07761	1
41	H	74.26505	70.90055	77.20876	-1975.08116	525.87560	-1801.71556	1
42	H	73.23619	71.30707	78.61467	1588.27743	-1913.22100	1113.83566	1
43	C	74.30541	69.37525	78.85067	-613.62442	-457.55993	-194.14490	1
44	H	74.92932	68.70463	78.21796	1707.54637	-721.27992	1996.92523	1
45	H	74.98140	69.79497	79.62905	758.23357	2100.81767	1560.55011	1
46	C	73.05065	68.60644	79.45504	-352.41524	704.96076	49.21465	1
47	H	73.22199	67.52138	79.68173	1714.76886	-2070.42778	443.35792	1
48	H	72.60086	69.11268	80.34131	1224.15040	1801.50881	1636.97633	1
49	C	72.86060	68.89699	75.99510	566.85117	537.05831	117.62814	1
50	O	72.79350	69.51431	74.95856	-550.26779	-406.08867	4.21666	1
51	N	73.40063	67.71250	76.23714	566.34832	-425.77725	180.18749	1
52	H	73.34834	67.29152	77.19346	644.44502	2646.80550	-52.73430	1
53	C	73.83366	66.89460	75.15332	612.34801	-281.48662	411.56221	1
54	H	74.18468	65.96765	75.65598	1667.23498	-1490.75142	1556.16753	1
55	C	72.51380	66.60001	74.30478	-714.45746	-175.43074	286.98927	1
56	H	72.10073	67.58799	73.95905	-787.09484	1763.03619	-1922.46060	1
57	O	71.43828	65.98607	75.06251	-429.46514	516.51932	-128.40526	1
58	H	71.05838	66.76765	75.50992	1981.82785	436.16847	-1818.18182	1
59	C	72.99311	65.75478	73.07572	630.79189	-468.94448	76.03230	1
60	H	72.13655	65.46983	72.42060	-1775.71861	2062.30353	131.89849	1
61	H	73.72882	66.31098	72.43942	-1855.14608	88.94118	1993.53760	1
62	H	73.48611	64.80989	73.40258	-1504.82350	-780.94249	-2132.90992	1
63	C	75.06223	67.61741	74.36100	288.57638	618.62814	-397.00270	1
64	O	75.44811	67.15937	73.30759	321.70495	-185.26452	574.37218	1
65	N	75.59261	68.61837	75.04631	-447.05792	-446.53431	367.76425	1
66	H	75.14022	68.93143	75.90470	350.31316	1975.63644	-1843.31522	1
67	C	76.60656	69.43379	74.45100	-511.23061	374.03917	-471.51480	1
68	H	77.39720	68.74048	74.08881	2234.79579	-898.70890	-1273.45190	1
69	C	75.90174	70.15715	73.20650	529.53781	-159.34528	563.72604	1
70	H	76.69970	70.66306	72.59728	654.59388	2347.94251	1217.51488	1
71	H	75.48973	69.32171	72.57580	-1526.55661	2103.42026	817.87394	1
72	O	74.88992	71.14482	73.50390	-554.84278	14.12789	399.58769	1
73	H	74.19663	70.56442	73.89281	1297.06236	2061.84854	1220.68812	1
74	C	77.06829	70.44893	75.62606	-662.15484	-412.13544	123.62687	1
75	O	76.36553	70.70117	76.57964	-540.01537	-317.05804	274.91456	1
76	N	78.26913	70.92031	75.31810	-202.76299	-690.00100	-131.49145	1
77	H	78.80715	70.68059	74.46415	-702.62132	-2617.37191	281.70413	1
78	C	79.01620	71.65614	76.29276	-491.73914	576.34187	222.73509	1
79	H	78.34144	72.41997	76.73949	1977.17978	-1823.58850	-434.68928	1
80	C	79.55413	70.63071	77.38321	-649.50797	-328.66843	306.11224	1
81	H	80.16064	69.83572	76.89891	2075.07803	1452.16490	-1004.45904	1
82	C	80.40194	71.40881	78.44513	-615.18735	-489.99689	-70.96352	1
83	H	80.75416	70.73913	79.26476	-1226.32661	-1724.38906	-1716.47170	1
84	H	81.30855	71.87725	77.99031	2381.64273	-969.84735	900.46860	1
85	H	79.81198	72.22912	78.91901	2122.74991	1702.23946	-141.36228	1
86	C	78.35791	69.99292	78.17257	-501.86074	-479.61276	-376.42482	1
87	H	78.70493	69.47267	79.09651	993.79261	-2246.95401	-1177.81305	1
88	H	77.61345	70.76595	78.48337	42.71279	-626.15391	-2651.37258	1
89	H	77.81582	69.23647	77.55497	-2026.39012	-1590.33709	-887.82922	1
90	C	80.20202	72.21071	75.32351	-672.89153	382.57394	-156.34072	1
91	O	80.37830	71.64601	74.25143	410.04627	221.86223	500.35950	1
92	N	80.87544	73.17429	75.90919	-378.11782	-443.79414	-441.10984	1
93	H	80.59463	73.45147	76.85730	2404.15973	-568.14894	1149.30085	1
94	C	81.86289	73.97760	75.25461	-544.54484	466.16019	331.29119	1
95	H	82.64671	74.11587	76.03105	-1409.80988	-170.17955	2325.32679	1
96	C	82.36554	73.24211	73.94250	-184.48284	116.78282	-758.89137	1

97	H	82.59985	72.17331	74.15845	1893.78641	1861.14652	611.04528	1
98	H	81.54526	73.22340	73.18479	-2170.79665	-974.19311	1327.50117	1
99	C	83.60903	73.99539	73.37558	389.51668	672.81878	-138.49152	1
100	H	83.39891	75.08511	73.31170	510.64577	1933.03327	1851.02484	1
101	H	84.46236	73.92056	74.08484	-2302.30869	-1105.72939	-948.89774	1
102	C	84.04920	73.46434	71.95834	-559.93427	-126.34590	542.30857	1
103	O	84.85750	74.08263	71.31341	-670.36003	-111.83166	76.36448	1
104	N	83.45848	72.30472	71.59919	-216.06729	-537.07037	446.51379	1
105	H	82.79668	71.72037	72.12345	-1251.96487	1074.12894	-2168.52500	1
106	H	83.67459	71.79342	70.73657	-2451.83023	-720.73851	944.84612	1
107	C	81.16524	75.37383	74.81371	546.24052	-563.88337	-85.11809	1
108	O	80.10241	75.37511	74.20540	71.70702	-307.40463	606.69673	1
109	N	81.93925	76.40707	75.13054	479.90863	-504.50129	222.86849	1
110	C	81.49130	77.76021	74.92130	75.51268	-600.91904	506.73700	1
111	H	80.42715	77.76618	75.25396	-2033.61562	1795.30103	254.89480	1
112	C	82.50316	78.60690	75.80314	523.79067	517.99274	284.45581	1
113	H	82.60425	79.65776	75.44911	1599.61665	-1127.00911	1895.98173	1
114	H	82.18376	78.65542	76.86831	-1881.83093	1275.82488	-1501.55016	1
115	C	83.81331	77.77619	75.63832	-600.05639	-404.05026	316.64485	1
116	H	84.26641	77.94424	74.63487	-2597.05260	496.36221	657.73249	1
117	H	84.59768	78.01766	76.39049	-1666.24518	1294.38985	-1723.90591	1
118	C	83.23922	76.30035	75.77914	493.57570	-129.95376	-602.56394	1
119	H	83.83994	75.51119	75.27316	-1469.08415	-637.84797	2204.22581	1
120	H	83.03902	75.98919	76.83151	-1038.97840	1068.88701	-2280.71789	1
121	C	81.63714	78.13509	73.34384	188.88100	241.05089	-727.87821	1
122	O	82.44485	78.93604	72.96072	531.88613	-49.19943	427.07960	1
123	N	80.72871	77.45834	72.62901	708.14833	26.93417	-179.73509	1
124	H	80.13820	76.72193	73.08921	-2232.69501	-1179.09831	1023.94816	1
125	C	80.68392	77.66865	71.18057	-738.32412	259.92548	104.42456	1
126	H	81.32411	78.56708	71.00143	2028.89123	1260.02983	1311.33324	1
127	C	81.20542	76.39550	70.52691	-258.65678	-345.52513	661.28459	1
128	H	80.67597	75.53756	70.99834	-1826.06090	-1801.46097	-918.64554	1
129	C	80.92114	76.37081	69.03785	-541.23400	531.92970	-218.41428	1
130	H	81.27214	75.41271	68.56252	1311.73218	-2219.18200	882.19023	1
131	H	79.81914	76.46704	68.82598	-1048.71298	1223.58118	-2196.97971	1
132	H	81.43649	77.21697	68.50357	419.06414	1903.92898	1903.44670	1
133	C	82.69063	76.21802	70.77814	-423.86431	152.66566	-648.55262	1
134	H	83.05911	75.20211	70.45333	105.68386	-2342.50080	1387.51238	1
135	H	83.30040	76.98535	70.22464	-1695.63603	-1484.73621	-1531.02793	1
136	H	82.93604	76.33275	71.87018	-1853.57121	-487.39031	1936.59343	1
137	C	79.08419	77.86198	70.79310	539.71428	-510.58232	267.58633	1
138	O	78.24441	77.07258	71.22662	-15.93758	-278.34085	-624.49402	1
139	N	78.95246	78.82319	69.92018	-676.81886	12.05292	276.17960	1
140	H	79.82906	79.29856	69.71724	-1694.44250	-373.84189	-2100.66098	1
141	C	77.69326	79.35592	69.52678	412.33078	-664.70360	108.35451	1
142	H	77.99106	80.08402	68.73941	1765.77476	1294.44366	1621.76594	1
143	C	76.80083	78.17400	68.97464	-179.66635	-721.95667	-264.73915	1
144	H	77.35289	77.59140	68.20348	-607.34922	2587.87032	-598.10018	1
145	H	76.57146	77.44037	69.78297	-359.69332	-1479.13954	-2259.74260	1
146	C	75.49551	78.79848	68.37603	-240.01076	616.02425	431.85322	1
147	H	74.98735	79.45088	69.12084	-1359.17131	782.54425	2227.99181	1
148	H	75.72887	79.45581	67.50906	-820.36667	85.81767	-2596.78715	1
149	C	74.55131	77.60632	67.94449	-513.07015	236.18570	-551.87280	1
150	H	75.00651	77.01905	67.11416	1816.11944	-1183.11722	-1650.94321	1
151	H	74.41115	76.88594	68.78320	-1800.04429	-1361.53473	1526.34643	1
152	C	73.19591	78.21678	67.51658	726.08972	-253.19732	-179.64713	1
153	H	72.61256	78.66771	68.34420	1224.27271	-456.51798	-2390.90304	1
154	H	73.25582	78.92537	66.66658	1206.40339	-1150.93514	-2154.90344	1
155	N	72.30384	77.04497	66.98724	329.70796	-633.68968	-155.67358	1
156	H	71.32289	77.30874	66.68097	1348.31305	1938.76845	1359.00643	1
157	H	72.65934	76.53703	66.12670	2096.92035	1446.54551	-966.48890	1
158	H	72.11053	76.24015	67.65204	-1197.07217	-2303.53719	827.28733	1

159	C	77.06716	80.13880	70.82838	-378.01186	-556.17301	-413.96481	1
160	O	77.62695	81.13683	71.22193	-409.44433	-307.55053	-453.30833	1
161	N	75.94350	79.59770	71.27830	-429.02477	524.70884	274.08502	1
162	H	75.59462	78.73278	70.86772	1706.34263	-1425.96036	1574.38926	1
163	C	75.29565	80.22496	72.37687	-45.25864	-626.22952	478.93267	1
164	H	75.80442	81.21370	72.48197	1988.63164	570.90773	1772.87287	1
165	C	73.74556	80.32271	72.04785	551.77128	-20.49526	-564.54996	1
166	H	73.57904	80.98497	71.16939	1434.61535	-1753.10253	1513.99471	1
167	H	73.32716	79.33298	71.75868	-714.67738	1819.09770	1898.36494	1
168	C	73.03338	80.88011	73.32352	446.99263	-555.77305	338.97221	1
169	H	72.77474	80.04868	74.02363	1953.68466	1892.25957	-161.67766	1
170	H	73.72451	81.54688	73.88925	-403.03785	2688.07032	-188.43591	1
171	C	71.73157	81.67114	72.89329	567.86262	335.74681	434.04421	1
172	H	71.97055	82.48040	72.16593	-1080.02275	1568.26081	-1948.78900	1
173	H	71.00241	81.00450	72.37814	-919.54108	2111.34692	1456.13463	1
174	C	71.13618	82.25329	74.19697	195.81897	173.33862	-745.11536	1
175	H	70.78209	81.48859	74.91649	1405.67949	-2301.21089	-390.08113	1
176	H	71.77812	82.99630	74.71213	-940.37328	-1118.32446	2299.72133	1
177	N	69.83347	83.03388	73.83172	319.26422	656.36007	-42.02424	1
178	H	69.35280	83.51462	74.64551	1961.03633	619.91968	1787.09422	1
179	H	69.87671	83.80784	73.10638	854.14343	-2156.80752	1429.08711	1
180	H	69.04493	82.42052	73.47692	1237.02905	-1378.50857	-1998.28500	1
181	C	75.43417	79.30537	73.73193	532.53319	-268.57236	517.55729	1
182	O	74.91530	79.71758	74.74297	266.16714	-290.73804	-558.88002	1
183	N	76.18686	78.22718	73.54553	-226.25352	640.49678	-270.32839	1
184	H	76.52603	78.10834	72.58874	2007.69063	-1035.27229	1523.50231	1
185	C	75.96040	77.05029	74.34748	-540.76542	-573.33303	49.50000	1
186	H	74.89739	76.76189	74.19923	-2374.20950	-1036.76023	843.75774	1
187	C	76.97644	75.99716	73.71186	-77.09082	666.87422	-415.84136	1
188	H	77.93480	76.54998	73.48155	-985.81834	617.19825	2463.91927	1
189	O	76.54903	75.48098	72.45697	293.29899	-391.65602	-477.80926	1
190	H	77.19016	75.99676	71.82971	2528.72714	-681.76262	-751.27122	1
191	C	77.27469	74.94937	74.84500	252.47363	-605.14473	440.05134	1
192	H	78.12562	74.28267	74.55740	-2052.65063	1456.49051	-1043.51830	1
193	H	77.55845	75.44262	75.80544	-2152.98800	-1661.97574	-161.70652	1
194	H	76.39219	74.29845	75.04901	-473.12726	-1584.27339	2165.61725	1
195	C	76.27795	77.41046	75.89473	360.36307	488.46713	505.10056	1
196	O	77.21159	78.11912	76.22190	-200.08817	-528.03552	-385.82850	1
197	N	75.49184	76.65615	76.64948	-597.54095	-226.44775	355.20479	1
198	H	74.83019	76.04124	76.17377	2179.23655	-1300.70981	-991.33835	1
199	C	75.28407	76.94128	78.02915	-687.68921	297.39807	-249.45179	1
200	H	75.03293	75.94538	78.45682	-349.16256	-2467.37713	-1101.72831	1
201	C	76.56079	77.61996	78.71584	672.47345	361.54328	-201.62880	1
202	H	76.80605	78.59323	78.21708	1541.41502	582.18425	2169.97026	1
203	H	76.30116	77.86486	79.77280	-2534.67717	60.25153	997.72295	1
204	C	77.77196	76.67185	78.68179	574.26774	-389.43119	-377.02542	1
205	C	77.75215	75.47687	79.45908	688.82679	-287.33580	-257.96133	1
206	H	76.87065	75.21813	80.07279	331.14182	1470.38163	2269.80013	1
207	C	78.92017	77.00678	77.90085	-383.52382	-675.04808	144.24917	1
208	H	78.95159	77.94482	77.30512	4.09847	1517.59662	2262.86397	1
209	C	78.87837	74.64705	79.44072	-134.76730	428.45285	-649.50303	1
210	H	78.86655	73.73266	80.05884	-903.23433	1600.49020	2011.53387	1
211	C	80.01883	76.13595	77.90797	-335.53281	-615.00040	-364.39058	1
212	H	80.89725	76.39996	77.29317	1596.45398	-1369.33862	1732.02659	1
213	C	80.04020	74.93824	78.67339	585.48547	-340.24194	-406.23938	1
214	O	81.17070	74.04961	78.68374	-419.15649	-173.04408	-511.94141	1
215	H	81.78853	74.58442	78.13683	-1071.84350	1559.71507	-1960.13012	1
216	C	74.04347	77.96772	78.20826	291.41878	-183.13091	710.72246	1
217	O	73.81633	78.42183	79.30475	379.87695	523.47396	-222.23622	1
218	N	73.33880	78.14440	77.09529	564.30591	373.09380	277.24371	1
219	H	73.57198	77.76454	76.15896	-120.59931	-2436.07824	-1214.35098	1
220	C	72.27202	79.10836	77.10113	404.07514	-299.37480	608.84009	1

221	H	71.66259	78.93265	78.01590	-1071.07882	-841.69025	2359.66467	1
222	C	72.98121	80.52762	77.13766	-683.12807	68.71770	-390.13096	1
223	H	73.80934	80.50839	77.88215	2068.88918	1596.58590	770.89603	1
224	H	73.47059	80.74384	76.15906	1379.86429	2342.49779	-179.85638	1
225	C	71.94438	81.62964	77.51568	-176.39967	537.49466	550.97268	1
226	H	71.12744	81.70029	76.76572	-396.28051	1942.22168	1869.33314	1
227	H	71.44195	81.39177	78.47940	-94.44700	586.00678	-2659.20016	1
228	C	72.76114	82.99938	77.62284	-291.69381	-718.18079	-150.72929	1
229	H	73.54785	83.03725	78.41863	-2303.38776	1089.76242	964.62032	1
230	H	73.22643	83.34637	76.66512	884.16729	2568.80533	-207.74283	1
231	N	71.76031	83.91913	77.96827	-594.49522	-252.81478	342.29276	1
232	H	70.80694	83.59989	77.89322	-1735.17426	2084.05705	-263.71605	1
233	C	71.97257	85.11109	78.35472	595.23177	-271.52487	442.22352	1
234	N	73.29968	85.54581	78.44330	585.53813	-424.79750	-105.81303	1
235	H	74.16276	85.04423	78.23801	959.88797	1327.56823	-2177.11905	1
236	H	73.58793	86.47859	78.74067	1578.48647	16.27378	-2220.76233	1
237	N	70.77014	85.78074	78.62309	-452.17763	-390.33541	-421.51853	1
238	H	69.80249	85.46551	78.57491	470.26107	1974.25629	-1817.92087	1
239	H	70.73280	86.74489	78.95647	1856.67307	-1573.97321	-1224.35416	1
240	C	71.57877	78.72731	75.68682	-531.47271	-581.45780	-55.06206	1
241	O	72.20245	78.03014	74.90083	-243.00837	192.73507	609.52485	1
242	N	70.37747	79.25339	75.57193	343.49288	-644.25607	38.09164	1
243	H	69.91748	79.85080	76.28405	-1691.16043	-1535.97525	-1484.73099	1
244	C	69.64181	79.10930	74.35211	542.66492	350.14337	454.42563	1
245	H	70.35859	79.26208	73.51577	1209.57979	-2396.95920	463.86744	1
246	C	69.01675	77.64620	74.29996	-737.14309	145.93010	242.71942	1
247	H	68.47916	77.41838	75.24503	-1050.18303	159.36419	-2509.06125	1
248	C	68.04735	77.52108	73.07709	-706.77696	-252.88343	-245.16230	1
249	H	67.72544	76.46524	72.91535	-1624.64039	-1665.49085	1417.86935	1
250	H	67.10897	78.12964	73.24182	2566.10521	598.51109	693.22305	1
251	H	68.52444	77.87046	72.13101	-1972.69758	107.10018	-1876.34312	1
252	C	70.16157	76.60144	74.05587	412.85148	672.58832	-27.69222	1
253	H	69.76569	75.63885	73.65365	1447.02277	1762.76533	-1490.78944	1
254	H	70.91736	76.98389	73.32719	1320.77379	-145.20455	2378.68491	1
255	H	70.70448	76.36233	75.00243	-1512.10848	1470.52031	1724.75147	1
256	C	68.54649	80.29091	74.56634	-607.11113	499.56689	73.73769	1
257	O	68.50603	80.86422	75.64646	357.97126	460.81534	356.68785	1
258	N	67.87042	80.53932	73.45211	536.55407	-368.62270	332.76306	1
259	H	68.04031	79.92418	72.65745	524.38866	2297.69985	1367.20941	1
260	C	66.66096	81.28354	73.53249	46.50277	-774.29190	-147.97904	1
261	H	66.88105	82.10053	74.25420	1676.51875	1883.29066	1032.55549	1
262	C	66.23089	81.75747	72.05261	-559.41456	-34.19198	-556.30433	1
263	H	65.99407	80.84979	71.44703	-64.66664	395.18769	2695.05373	1
264	H	65.28386	82.34776	72.09354	-2703.44278	-60.40056	333.79418	1
265	C	67.32652	82.54890	71.38589	-519.76435	377.31045	459.42366	1
266	H	68.29881	82.04690	71.58931	-1746.74323	1667.50644	-1261.73691	1
267	C	67.11311	82.57893	69.87743	570.95554	16.46261	-545.27700	1
268	H	67.92839	83.14223	69.35452	2391.58273	28.05277	-1305.07271	1
269	H	67.08862	81.54702	69.44107	175.75588	917.63458	2559.43867	1
270	H	66.14432	83.07406	69.60922	-1063.97851	-2155.34650	1283.00462	1
271	C	67.37960	83.97300	71.92165	193.76014	2.62946	-765.53141	1
272	H	68.23180	84.54943	71.47732	507.39394	-846.55087	2539.60089	1
273	H	66.44050	84.53628	71.68427	1337.57841	1818.19054	1526.01994	1
274	H	67.50500	83.99487	73.03464	1100.88635	-1172.91350	-2199.08909	1
275	C	65.49004	80.30857	74.05239	-549.21115	475.64486	-309.38218	1
276	O	65.49901	79.11028	73.89802	556.06106	-390.37755	-78.24250	1
277	O	64.34355	80.95569	74.56183	-572.27940	-310.19032	-209.75862	1
278	H	64.67618	81.89790	74.53791	-1380.08193	2212.14486	790.85944	1

Listing 6: C00006.xmolout

2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1294.2957	0.0000	300.0000
3	H	68.71586	73.12670	87.63958	-2043.14101	-1757.64893	399.89339	1	
4	N	69.69982	72.89536	87.76675	426.75047	490.45733	-334.42467	1	
5	H	69.77453	71.97324	87.32632	442.25559	-1110.30854	-2448.52907	1	
6	C	70.60064	73.82037	87.19173	415.32972	-666.39213	83.73172	1	
7	H	70.06952	74.79272	87.09080	879.32219	2491.00447	667.35213	1	
8	C	71.89726	73.91184	88.15399	31.35357	477.41777	628.23362	1	
9	H	72.33084	72.89196	88.28333	1168.38489	2240.25337	-1019.71136	1	
10	H	72.69809	74.53150	87.68561	-360.43770	2534.90498	931.67112	1	
11	C	71.47677	74.48055	89.48159	463.18208	512.70242	-382.34388	1	
12	H	70.56731	73.93188	89.81759	1725.29117	1863.52247	-987.07854	1	
13	C	72.57305	74.27785	90.52052	710.42801	-144.27427	-313.15367	1	
14	H	72.26330	74.65786	91.52802	364.20195	-1033.13725	2494.72524	1	
15	H	72.83441	73.19478	90.64038	2567.61904	335.80679	847.48802	1	
16	H	73.51364	74.81683	90.23775	-2587.99029	680.92867	-512.16411	1	
17	C	71.14426	75.96270	89.37375	268.17616	741.64379	-40.42634	1	
18	H	70.84191	76.39108	90.36411	1283.54314	-1945.37420	-1411.27812	1	
19	H	72.01938	76.55961	89.00601	-1258.57796	1317.15249	-2026.02085	1	
20	H	70.30037	76.14966	88.66134	-2502.84526	909.80597	575.92391	1	
21	C	71.03218	73.14590	85.78698	619.36578	-458.64843	-172.09273	1	
22	O	70.76081	71.96616	85.51313	-81.40433	433.87611	522.34594	1	
23	N	71.62319	74.05010	85.04905	175.23996	-622.20190	341.55523	1	
24	H	71.74939	74.95829	85.49496	-876.57256	-303.22879	-2561.90213	1	
25	C	72.45813	73.70947	83.92647	-571.88214	-534.10783	-106.15033	1	
26	H	73.42167	73.40215	84.38907	-2713.20841	-16.25800	-248.80809	1	
27	C	71.80477	72.48761	83.12522	166.60354	288.16399	-716.09568	1	
28	H	70.69119	72.53526	83.30584	-2097.85574	1636.78449	-586.18044	1	
29	O	72.18951	71.19537	83.59389	-317.80580	-363.38227	484.43082	1	
30	H	71.51958	71.09623	84.37667	1863.74748	-1451.84923	1357.29467	1	
31	C	72.13108	72.80559	81.62241	503.80731	517.99032	318.51606	1	
32	H	71.67047	72.05684	80.93679	640.61020	-2157.10410	-1536.29104	1	
33	H	71.75966	73.81135	81.31500	1687.88455	465.60692	2087.56452	1	
34	H	73.23054	72.79217	81.43657	-1293.07895	-1899.88581	-1463.57452	1	
35	C	72.65052	75.07021	83.07933	-153.07550	-733.68902	248.70981	1	
36	O	73.79297	75.26855	82.70007	186.15459	-480.78787	-449.34387	1	
37	N	71.55040	75.77496	82.81250	-487.53139	543.18517	42.03850	1	
38	C	71.59856	77.03954	82.13358	-699.35871	69.34393	360.10701	1	
39	H	72.32924	76.91098	81.30223	2.81126	-221.99807	-2715.58072	1	
40	C	70.09541	77.27115	81.69720	-507.46439	-592.59194	122.07761	1	
41	H	69.85295	78.35086	81.56442	-1975.08116	525.87560	-1801.71556	1	
42	H	69.86783	76.76995	80.72948	1588.27743	-1913.22100	1113.83566	1	
43	C	69.32374	76.60408	82.88032	-613.62442	-457.55993	-194.14490	1	
44	H	69.32964	77.25990	83.77968	1707.54637	-721.27992	1996.92523	1	
45	H	68.25743	76.38111	82.65166	758.23357	2100.81767	1560.55011	1	
46	C	70.20374	75.30106	83.10670	-352.41524	704.96076	49.21465	1	
47	H	70.20349	74.88836	84.14460	1714.76886	-2070.42778	443.35792	1	
48	H	69.99955	74.47534	82.38511	1224.15040	1801.50881	1636.97633	1	
49	C	72.05888	78.21365	83.17870	566.85117	537.05831	117.62814	1	
50	O	71.51446	79.29068	83.17675	-550.26779	-406.08867	4.21666	1	
51	N	73.09589	77.79947	83.89728	566.34832	-425.77725	180.18749	1	
52	H	73.48488	76.85668	83.73309	644.44502	2646.80550	-52.73430	1	
53	C	73.62577	78.67076	84.88045	612.34801	-281.48662	411.56221	1	
54	H	73.01604	79.60360	84.82139	1667.23498	-1490.75142	1556.16753	1	
55	C	73.57367	77.91017	86.29081	-714.45746	-175.43074	286.98927	1	
56	H	74.27422	77.03154	86.24003	-787.09484	1763.03619	-1922.46060	1	
57	O	72.30028	77.37821	86.69044	-429.46514	516.51932	-128.40526	1	
58	H	72.49218	76.41830	86.69993	1981.82785	436.16847	-1818.18182	1	
59	C	74.17993	79.01905	87.22723	630.79189	-468.94448	76.03230	1	
60	H	74.31587	78.64528	88.26822	-1775.71861	2062.30353	131.89849	1	
61	H	75.17543	79.36782	86.86513	-1855.14608	88.94118	1993.53760	1	
62	H	73.51429	79.91170	87.28245	-1504.82350	-780.94249	-2132.90992	1	

63	C	75.21167	78.81865	84.46830	288.57638	618.62814	-397.00270	1
64	O	75.99092	77.88263	84.66973	321.70495	-185.26452	574.37218	1
65	N	75.41637	79.97875	83.90055	-447.05792	-446.53431	367.76425	1
66	H	74.58367	80.56654	83.85513	350.31316	1975.63644	-1843.31522	1
67	C	76.56429	80.36460	83.16319	-511.23061	374.03917	-471.51480	1
68	H	76.46498	81.47252	83.14001	2234.79579	-898.70890	-1273.45190	1
69	C	77.88146	79.86846	83.92281	529.53781	-159.34528	563.72604	1
70	H	78.73985	80.53102	83.61934	654.59388	2347.94251	1217.51488	1
71	H	77.69014	80.05238	85.01405	-1526.55661	2103.42026	817.87394	1
72	O	78.29853	78.52027	83.69052	-554.84278	14.12789	399.58769	1
73	H	77.50217	78.03164	84.13853	1297.06236	2061.84854	1220.68812	1
74	C	76.56242	79.76427	81.65030	-662.15484	-412.13544	123.62687	1
75	O	77.13987	80.35981	80.77361	-540.01537	-317.05804	274.91456	1
76	N	75.86630	78.59228	81.52475	-202.76299	-690.00100	-131.49145	1
77	H	75.57224	78.33417	82.47288	-702.62132	-2617.37191	281.70413	1
78	C	76.48512	77.52312	80.69611	-491.73914	576.34187	222.73509	1
79	H	77.56719	77.54306	80.96236	1977.17978	-1823.58850	-434.68928	1
80	C	75.78220	76.23934	81.05329	-649.50797	-328.66843	306.11224	1
81	H	74.73404	76.48683	81.37650	2075.07803	1452.16490	-1004.45904	1
82	C	75.67863	75.30147	79.86456	-615.18735	-489.99689	-70.96352	1
83	H	75.11535	74.36183	80.12232	-1226.32661	-1724.38906	-1716.47170	1
84	H	75.13428	75.79475	79.00558	2381.64273	-969.84735	900.46860	1
85	H	76.69245	74.99573	79.48380	2122.74991	1702.23946	-141.36228	1
86	C	76.46446	75.54184	82.21691	-501.86074	-479.61276	-376.42482	1
87	H	75.93978	74.58094	82.48629	993.79261	-2246.95401	-1177.81305	1
88	H	77.53495	75.28575	81.98120	42.71279	-626.15391	-2651.37258	1
89	H	76.46578	76.19156	83.14048	-2026.39012	-1590.33709	-887.82922	1
90	C	76.19777	77.89969	79.12383	-672.89153	382.57394	-156.34072	1
91	O	75.08336	78.05846	78.68718	410.04627	221.86223	500.35950	1
92	N	77.34136	77.80439	78.43389	-378.11782	-443.79414	-441.10984	1
93	H	78.19641	77.71263	78.98275	2404.15973	-568.14894	1149.30085	1
94	C	77.35545	78.56582	77.21362	-544.54484	466.16019	331.29119	1
95	H	76.34310	78.38692	76.77986	-1409.80988	-170.17955	2325.32679	1
96	C	77.58973	80.06872	77.65372	-184.48284	116.78282	-758.89137	1
97	H	76.91016	80.33684	78.49919	1893.78641	1861.14652	611.04528	1
98	H	78.62493	80.20971	78.04147	-2170.79665	-974.19311	1327.50117	1
99	C	77.33024	80.96341	76.40230	389.51668	672.81878	-138.49152	1
100	H	78.03543	80.69352	75.58403	510.64577	1933.03327	1851.02484	1
101	H	76.32602	80.74630	75.97533	-2302.30869	-1105.72939	-948.89774	1
102	C	77.44469	82.50245	76.71944	-559.93427	-126.34590	542.30857	1
103	O	77.30385	83.30136	75.82998	-670.36003	-111.83166	76.36448	1
104	N	77.68488	82.78496	78.01805	-216.06729	-537.07037	446.51379	1
105	H	77.79062	82.15480	78.82262	-1251.96487	1074.12894	-2168.52500	1
106	H	77.76732	83.73730	78.39011	-2451.83023	-720.73851	944.84612	1
107	C	78.61675	77.99217	76.34891	546.24052	-563.88337	-85.11809	1
108	O	79.72848	78.38085	76.58865	71.70702	-307.40463	606.69673	1
109	N	78.20882	77.04727	75.49055	479.90863	-504.50129	222.86849	1
110	C	79.09489	76.54048	74.48533	75.51268	-600.91904	506.73700	1
111	H	80.10972	76.47926	74.94209	-2033.61562	1795.30103	254.89480	1
112	C	78.42340	75.14860	74.11639	523.79067	517.99274	284.45581	1
113	H	78.68008	74.81464	73.07625	1599.61665	-1127.00911	1895.98173	1
114	H	78.75800	74.34017	74.80451	-1881.83093	1275.82488	-1501.55016	1
115	C	76.90461	75.45250	74.29814	-600.05639	-404.05026	316.64485	1
116	H	76.49932	75.99689	73.41736	-2597.05260	496.36221	657.73249	1
117	H	76.28518	74.53561	74.41795	-1666.24518	1294.38985	-1723.90591	1
118	C	76.91950	76.37856	75.58981	493.57570	-129.95376	-602.56394	1
119	H	76.11871	77.15520	75.63009	-1469.08415	-637.84797	2204.22581	1
120	H	76.93832	75.83096	76.56216	-1038.97840	1068.88701	-2280.71789	1
121	C	79.04961	77.54183	73.20031	188.88100	241.05089	-727.87821	1
122	O	78.13803	78.29830	72.95086	531.88613	-49.19943	427.07960	1
123	N	80.19079	77.36884	72.45844	708.14833	26.93417	-179.73509	1
124	H	80.60934	76.54684	72.90760	-2232.69501	-1179.09831	1023.94816	1

125	C	80.05306	77.41000	70.98864	-738.32412	259.92548	104.42456	1
126	H	79.58915	78.40132	70.78014	2028.89123	1260.02983	1311.33324	1
127	C	81.43396	77.23756	70.40035	-258.65678	-345.52513	661.28459	1
128	H	81.78867	76.21454	70.66060	-1826.06090	-1801.46097	-918.64554	1
129	C	81.42292	77.36787	68.88883	-541.23400	531.92970	-218.41428	1
130	H	82.44594	77.20477	68.45161	1311.73218	-2219.18200	882.19023	1
131	H	80.72102	76.61047	68.39736	-1048.71298	1223.58118	-2196.97971	1
132	H	81.08558	78.39050	68.56566	419.06414	1903.92898	1903.44670	1
133	C	82.42737	78.22903	70.98386	-423.86431	152.66566	-648.55262	1
134	H	83.47068	78.04785	70.60663	105.68386	-2342.50080	1387.51238	1
135	H	82.15588	79.28732	70.72006	-1695.63603	-1484.73621	-1531.02793	1
136	H	82.45759	78.16737	72.10606	-1853.57121	-487.39031	1936.59343	1
137	C	79.07390	76.14246	70.57935	539.71428	-510.58232	267.58633	1
138	O	79.14817	75.04977	71.10257	-15.93758	-278.34085	-624.49402	1
139	N	78.25717	76.53348	69.61231	-676.81886	12.05292	276.17960	1
140	H	78.42340	77.47101	69.25275	-1694.44250	-373.84189	-2100.66098	1
141	C	77.62779	75.50492	68.83324	412.33078	-664.70360	108.35451	1
142	H	77.12215	74.83478	69.56199	1765.77476	1294.44366	1621.76594	1
143	C	76.66526	76.24044	67.82389	-179.66635	-721.95667	-264.73915	1
144	H	75.92395	76.87005	68.36466	-607.34922	2587.87032	-598.10018	1
145	H	77.24053	76.94061	67.17713	-359.69332	-1479.13954	-2259.74260	1
146	C	75.94879	75.14716	66.96128	-240.01076	616.02425	431.85322	1
147	H	76.68780	74.50387	66.43044	-1359.17131	782.54425	2227.99181	1
148	H	75.34662	74.46010	67.60031	-820.36667	85.81767	-2596.78715	1
149	C	75.02700	75.92292	65.93814	-513.07015	236.18570	-551.87280	1
150	H	74.29301	76.56450	66.47806	1816.11944	-1183.11722	-1650.94321	1
151	H	75.62817	76.61398	65.30363	-1800.04429	-1361.53473	1526.34643	1
152	C	74.29819	74.86908	65.07044	726.08972	-253.19732	-179.64713	1
153	H	74.94787	74.33356	64.34807	1224.27271	-456.51798	-2390.90304	1
154	H	73.69454	74.12755	65.66100	1206.40339	-1150.93514	-2154.90344	1
155	N	73.25538	75.63389	64.19507	329.70796	-633.68968	-155.67358	1
156	H	72.65556	75.03376	63.55852	1348.31305	1938.76845	1359.00643	1
157	H	72.51637	76.18761	64.71756	2096.92035	1446.54551	-966.48890	1
158	H	73.63127	76.35516	63.51245	-1197.07217	-2303.53719	827.28733	1
159	C	78.79941	74.73692	67.98285	-378.01186	-556.17301	-413.96481	1
160	O	79.67195	75.31901	67.36789	-409.44433	-307.55053	-453.30833	1
161	N	78.54835	73.44221	68.04445	-429.02477	524.70884	274.08502	1
162	H	77.76783	73.10650	68.60627	1706.34263	-1425.96036	1574.38926	1
163	C	79.37709	72.54999	67.30901	-45.25864	-626.22952	478.93267	1
164	H	79.93545	73.20726	66.60192	1988.63164	570.90773	1772.87287	1
165	C	80.32083	71.83440	68.36132	551.77128	-20.49526	-564.54996	1
166	H	80.96341	72.58306	68.87646	1434.61535	-1753.10253	1513.99471	1
167	H	79.73155	71.35173	69.17229	-714.67738	1819.09770	1898.36494	1
168	C	81.18846	70.78703	67.58882	446.99263	-555.77305	338.97221	1
169	H	80.54474	70.02249	67.09553	1953.68466	1892.25957	-161.67766	1
170	H	81.76066	71.27939	66.77095	-403.03785	2688.07032	-188.43591	1
171	C	82.16946	70.11241	68.63031	567.86262	335.74681	434.04421	1
172	H	82.72727	70.88564	69.20675	-1080.02275	1568.26081	-1948.78900	1
173	H	81.60245	69.52182	69.38667	-919.54108	2111.34692	1456.13463	1
174	C	83.14911	69.21247	67.84194	195.81897	173.33862	-745.11536	1
175	H	82.68032	68.33656	67.35065	1405.67949	-2301.21089	-390.08113	1
176	H	83.79000	69.75362	67.11739	-940.37328	-1118.32446	2299.72133	1
177	N	84.15922	68.60147	68.87139	319.26422	656.36007	-42.02424	1
178	H	84.91161	67.97698	68.46002	1961.03633	619.91968	1787.09422	1
179	H	84.74276	69.28204	69.43985	854.14343	-2156.80752	1429.08711	1
180	H	83.75744	67.97352	69.62685	1237.02905	-1378.50857	-1998.28500	1
181	C	78.32445	71.51417	66.58105	532.53319	-268.57236	517.55729	1
182	O	77.89317	71.78097	65.48352	266.16714	-290.73804	-558.88002	1
183	N	78.01737	70.49629	67.37287	-226.25352	640.49678	-270.32839	1
184	H	78.43369	70.43554	68.30091	2007.69063	-1035.27229	1523.50231	1
185	C	77.02630	69.57470	66.94700	-540.76542	-573.33303	49.50000	1
186	H	76.82438	69.88052	65.89215	-2374.20950	-1036.76023	843.75774	1

187	C	77.62531	68.09792	67.09945	-77.09082	666.87422	-415.84136	1
188	H	77.59858	67.80863	68.18546	-985.81834	617.19825	2463.91927	1
189	O	78.98364	67.91099	66.66600	293.29899	-391.65602	-477.80926	1
190	H	79.40824	67.61581	67.49706	2528.72714	-681.76262	-751.27122	1
191	C	76.54646	67.27028	66.30888	252.47363	-605.14473	440.05134	1
192	H	76.74921	66.17572	66.36586	-2052.65063	1456.49051	-1043.51830	1
193	H	75.51663	67.44187	66.71121	-2152.98800	-1661.97574	-161.70652	1
194	H	76.53460	67.54609	65.22836	-473.12726	-1584.27339	2165.61725	1
195	C	75.74827	69.77619	67.96060	360.36307	488.46713	505.10056	1
196	O	75.08822	68.83325	68.33479	-200.08817	-528.03552	-385.82850	1
197	N	75.57095	71.06580	68.22115	-597.54095	-226.44775	355.20479	1
198	H	76.21110	71.72167	67.77399	2179.23655	-1300.70981	-991.33835	1
199	C	74.54227	71.46815	69.10256	-687.68921	297.39807	-249.45179	1
200	H	74.10295	70.52133	69.49237	-349.16256	-2467.37713	-1101.72831	1
201	C	75.17994	72.41861	70.23035	672.47345	361.54328	-201.62880	1
202	H	75.50926	73.38824	69.79569	1541.41502	582.18425	2169.97026	1
203	H	74.40444	72.67213	70.99173	-2534.67717	60.25153	997.72295	1
204	C	76.36879	71.68707	70.87043	574.26774	-389.43119	-377.02542	1
205	C	76.19809	70.33203	71.28926	688.82679	-287.33580	-257.96133	1
206	H	75.21144	69.84031	71.21535	331.14182	1470.38163	2269.80013	1
207	C	77.64343	72.31768	71.01321	-383.52382	-675.04808	144.24917	1
208	H	77.79593	73.38514	70.75107	4.09847	1517.59662	2262.86397	1
209	C	77.30274	69.62111	71.75689	-134.76730	428.45285	-649.50303	1
210	H	77.16349	68.56856	72.06016	-903.23433	1600.49020	2011.53387	1
211	C	78.72068	71.56445	71.48463	-335.53281	-615.00040	-364.39058	1
212	H	79.70106	72.06524	71.56763	1596.45398	-1369.33862	1732.02659	1
213	C	78.60445	70.19295	71.85571	585.48547	-340.24194	-406.23938	1
214	O	79.70278	69.41886	72.31173	-419.15649	-173.04408	-511.94141	1
215	H	80.40724	70.10975	72.30402	-1071.84350	1559.71507	-1960.13012	1
216	C	73.50095	72.37920	68.23862	291.41878	-183.13091	710.72246	1
217	O	73.77968	72.88982	67.16807	379.87695	523.47396	-222.23622	1
218	N	72.38246	72.50718	68.94155	564.30591	373.09380	277.24371	1
219	H	72.33871	72.02478	69.83805	-120.59931	-2436.07824	-1214.35098	1
220	C	71.25044	73.06014	68.28645	404.07514	-299.37480	608.84009	1
221	H	71.59697	73.33685	67.26242	-1071.07882	-841.69025	2359.66467	1
222	C	70.13826	71.92799	68.33635	-683.12807	68.71770	-390.13096	1
223	H	70.48401	71.00754	67.81492	2068.88918	1596.58590	770.89603	1
224	H	69.95249	71.61890	69.38925	1379.86429	2342.49779	-179.85638	1
225	C	68.83107	72.48280	67.69487	-176.39967	537.49466	550.97268	1
226	H	68.59721	73.49911	68.08546	-396.28051	1942.22168	1869.33314	1
227	H	68.93438	72.59914	66.59317	-94.44700	586.00678	-2659.20016	1
228	C	67.67722	71.44316	68.07460	-291.69381	-718.18079	-150.72929	1
229	H	67.79780	70.40311	67.67893	-2303.38776	1089.76242	964.62032	1
230	H	67.45524	71.37692	69.17064	884.16729	2568.80533	-207.74283	1
231	N	66.56728	72.02895	67.44977	-594.49522	-252.81478	342.29276	1
232	H	66.66763	72.99017	67.16113	-1735.17426	2084.05705	-263.71605	1
233	C	65.45568	71.44627	67.24373	595.23177	-271.52487	442.22352	1
234	N	65.32259	70.11941	67.66526	585.53813	-424.79750	-105.81303	1
235	H	65.99417	69.52106	68.14458	959.88797	1327.56823	-2177.11905	1
236	H	64.47912	69.55457	67.56072	1578.48647	16.27378	-2220.76233	1
237	N	64.55361	72.30946	66.60676	-452.17763	-390.33541	-421.51853	1
238	H	64.65790	73.27538	66.29960	470.26107	1974.25629	-1817.92087	1
239	H	63.60531	72.03521	66.34755	1856.67307	-1573.97321	-1224.35416	1
240	C	70.65334	74.32966	69.14013	-531.47271	-581.45780	-55.06206	1
241	O	70.29033	75.34285	68.59457	-243.00837	192.73507	609.52485	1
242	N	70.39534	73.97044	70.44360	343.49288	-644.25607	38.09164	1
243	H	71.00377	73.15141	70.55548	-1691.16043	-1535.97525	-1484.73099	1
244	C	70.40512	75.03991	71.45849	542.66492	350.14337	454.42563	1
245	H	70.18657	75.97553	70.89186	1209.57979	-2396.95920	463.86744	1
246	C	69.33040	74.66236	72.45309	-737.14309	145.93010	242.71942	1
247	H	69.64830	73.72188	72.95693	-1050.18303	159.36419	-2509.06125	1
248	C	69.12892	75.72703	73.51629	-706.77696	-252.88343	-245.16230	1

249	H	68.32395	75.43742	74.24645	-1624.64039	-1665.49085	1417.86935	1
250	H	70.06865	75.90284	74.11143	2566.10521	598.51109	693.22305	1
251	H	68.82944	76.71293	73.06529	-1972.69758	107.10018	-1876.34312	1
252	C	68.00735	74.38344	71.75860	412.85148	672.58832	-27.69222	1
253	H	67.21934	74.03304	72.47942	1447.02277	1762.76533	-1490.78944	1
254	H	67.60936	75.30216	71.24751	1320.77379	-145.20455	2378.68491	1
255	H	68.11908	73.59176	70.96764	-1512.10848	1470.52031	1724.75147	1
256	C	71.92503	74.99661	72.10841	-607.11113	499.56689	73.73769	1
257	O	72.61721	74.00806	72.05694	357.97126	460.81534	356.68785	1
258	N	72.20331	76.17182	72.66217	536.55407	-368.62270	332.76306	1
259	H	71.46934	76.87776	72.66429	524.38866	2297.69985	1367.20941	1
260	C	73.35139	76.25739	73.48879	46.50277	-774.29190	-147.97904	1
261	H	74.01804	75.44119	73.12892	1676.51875	1883.29066	1032.55549	1
262	C	73.96648	77.74533	73.39216	-559.41456	-34.19198	-556.30433	1
263	H	73.23063	78.46528	73.82459	-64.66664	395.18769	2695.05373	1
264	H	74.88434	77.83567	74.02069	-2703.44278	-60.40056	333.79418	1
265	C	74.25913	78.10101	71.95752	-519.76435	377.31045	459.42366	1
266	H	73.38906	77.78636	71.33756	-1746.74323	1667.50644	-1261.73691	1
267	C	74.43462	79.60862	71.81848	570.95554	16.46261	-545.27700	1
268	H	74.63123	79.90758	70.75683	2391.58273	28.05277	-1305.07271	1
269	H	73.52318	80.16589	72.15715	175.75588	917.63458	2559.43867	1
270	H	75.29659	79.97932	72.43178	-1063.97851	-2155.34650	1283.00462	1
271	C	75.50435	77.39561	71.44224	193.76014	2.62946	-765.53141	1
272	H	75.69689	77.63329	70.36452	507.39394	-846.55087	2539.60089	1
273	H	76.42983	77.70778	72.01596	1337.57841	1818.19054	1526.01994	1
274	H	75.41516	76.28124	71.52176	1100.88635	-1172.91350	-2199.08909	1
275	C	72.87435	76.05752	75.02179	-549.21115	475.64486	-309.38218	1
276	O	71.80371	76.41503	75.43990	556.06106	-390.37755	-78.24250	1
277	O	73.86483	75.57257	75.90693	-572.27940	-310.19032	-209.75862	1
278	H	74.59200	75.40628	75.24407	-1380.08193	2212.14486	790.85944	1

Listing 7: C00007.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1294.2954	0.0000	300.0000
3	H	75.03646	64.16014	76.53732	-2043.14101	-1757.64893	399.89339		1
4	N	75.65288	64.16294	75.72699	426.75047	490.45733	-334.42467		1
5	H	74.98111	64.17967	74.96192	442.25559	-1110.30854	-2448.52907		1
6	C	76.60036	65.20996	75.71036	415.32972	-666.39213	83.73172		1
7	H	76.75542	65.47264	76.77773	879.32219	2491.00447	667.35213		1
8	C	77.93731	64.66330	74.99741	31.35357	477.41777	628.23362		1
9	H	77.70598	64.33986	73.95420	1168.38489	2240.25337	-1019.71136		1
10	H	78.69318	65.48011	74.90317	-360.43770	2534.90498	931.67112		1
11	C	78.48518	63.50581	75.79367	463.18208	512.70242	-382.34388		1
12	H	77.63470	62.84301	76.07197	1725.29117	1863.52247	-987.07854		1
13	C	79.46837	62.69952	74.95479	710.42801	-144.27427	-313.15367		1
14	H	79.88193	61.82799	75.52524	364.20195	-1033.13725	2494.72524		1
15	H	78.98620	62.29184	74.02889	2567.61904	335.80679	847.48802		1
16	H	80.33912	63.32437	74.62737	-2587.99029	680.92867	-512.16411		1
17	C	79.17220	63.98411	77.06514	268.17616	741.64379	-40.42634		1
18	H	79.58707	63.12807	77.65784	1283.54314	-1945.37420	-1411.27812		1
19	H	80.02619	64.67318	76.83690	-1258.57796	1317.15249	-2026.02085		1
20	H	78.46729	64.54055	77.73501	-2502.84526	909.80597	575.92391		1
21	C	75.97326	66.43891	74.83731	619.36578	-458.64843	-172.09273		1
22	O	75.78362	67.53800	75.32794	-81.40433	433.87611	522.34594		1
23	N	75.74928	66.05285	73.59013	175.23996	-622.20190	341.55523		1
24	H	75.91348	65.08106	73.33601	-876.57256	-303.22879	-2561.90213		1
25	C	75.20402	67.01206	72.68867	-571.88214	-534.10783	-106.15033		1
26	H	75.57714	67.98673	73.07565	-2713.20841	-16.25800	-248.80809		1
27	C	75.66815	66.62984	71.20686	166.60354	288.16399	-716.09568		1
28	H	75.19304	65.64902	70.92897	-2097.85574	1636.78449	-586.18044		1

29	O	77.08188	66.45913	71.01179	-317.80580	-363.38227	484.43082	1
30	H	77.12323	65.52606	70.71939	1863.74748	-1451.84923	1357.29467	1
31	C	74.99422	67.78938	70.38339	503.80731	517.99032	318.51606	1
32	H	75.10120	67.62591	69.28604	640.61020	-2157.10410	-1536.29104	1
33	H	73.90326	67.87712	70.60222	1687.88455	465.60692	2087.56452	1
34	H	75.45943	68.77754	70.61153	-1293.07895	-1899.88581	-1463.57452	1
35	C	73.57525	66.83432	72.77348	-153.07550	-733.68902	248.70981	1
36	O	73.07724	65.79683	72.42858	186.15459	-480.78787	-449.34387	1
37	N	72.98880	67.96048	73.21114	-487.53139	543.18517	42.03850	1
38	C	71.57205	68.04215	73.36008	-699.35871	69.34393	360.10701	1
39	H	71.19483	67.01141	73.55029	2.81126	-221.99807	-2715.58072	1
40	C	71.45060	69.06796	74.56610	-507.46439	-592.59194	122.07761	1
41	H	70.43972	69.55975	74.61291	-1975.08116	525.87560	-1801.71556	1
42	H	71.61433	68.56676	75.54654	1588.27743	-1913.22100	1113.83566	1
43	C	72.59974	70.07320	74.24435	-613.62442	-457.55993	-194.14490	1
44	H	72.28308	70.78820	73.45101	1707.54637	-721.27992	1996.92523	1
45	H	72.91645	70.68956	75.11954	758.23357	2100.81767	1560.55011	1
46	C	73.73873	69.10449	73.71435	-352.41524	704.96076	49.21465	1
47	H	74.33808	69.51119	72.86533	1714.76886	-2070.42778	443.35792	1
48	H	74.43784	68.68539	74.50488	1224.15040	1801.50881	1636.97633	1
49	C	70.91211	68.73191	72.02026	566.85117	537.05831	117.62814	1
50	O	71.46663	69.61759	71.41933	-550.26779	-406.08867	4.21666	1
51	N	69.67753	68.26090	71.88379	566.34832	-425.77725	180.18749	1
52	H	69.40269	67.48953	72.48889	644.44502	2646.80550	-52.73430	1
53	C	68.93463	68.56235	70.69044	612.34801	-281.48662	411.56221	1
54	H	69.64783	68.41784	69.84835	1667.23498	-1490.75142	1556.16753	1
55	C	67.69886	67.55270	70.67828	-714.45746	-175.43074	286.98927	1
56	H	67.09168	67.72067	71.60991	-787.09484	1763.03619	-1922.46060	1
57	O	68.05249	66.15571	70.68305	-429.46514	516.51932	-128.40526	1
58	H	67.63247	65.85397	71.51215	1981.82785	436.16847	-1818.18182	1
59	C	66.86790	68.03912	69.43501	630.79189	-468.94448	76.03230	1
60	H	65.93482	67.44195	69.31064	-1775.71861	2062.30353	131.89849	1
61	H	66.56414	69.10928	69.52756	-1855.14608	88.94118	1993.53760	1
62	H	67.45240	67.94054	68.49088	-1504.82350	-780.94249	-2132.90992	1
63	C	68.42999	70.09773	70.77965	288.57638	618.62814	-397.00270	1
64	O	68.17360	70.71370	69.77481	321.70495	-185.26452	574.37218	1
65	N	68.18337	70.45551	72.05181	-447.05792	-446.53431	367.76425	1
66	H	68.48328	69.83890	72.83646	350.31316	1975.63644	-1843.31522	1
67	C	68.41876	71.86326	72.31922	-511.23061	374.03917	-471.51480	1
68	H	69.28874	72.15426	71.68833	2234.79579	-898.70890	-1273.45190	1
69	C	67.08322	72.62409	71.87649	529.53781	-159.34528	563.72604	1
70	H	67.31260	73.72327	71.82951	654.59388	2347.94251	1217.51488	1
71	H	66.88605	72.28259	70.82280	-1526.55661	2103.42026	817.87394	1
72	O	65.92788	72.44868	72.73368	-554.84278	14.12789	399.58769	1
73	H	65.63610	71.56902	72.42666	1297.06236	2061.84854	1220.68812	1
74	C	68.72319	71.80132	73.89065	-662.15484	-412.13544	123.62687	1
75	O	68.80002	70.69852	74.43738	-540.01537	-317.05804	274.91456	1
76	N	69.03497	73.00263	74.38199	-202.76299	-690.00100	-131.49145	1
77	H	68.88699	73.74408	73.69085	-702.62132	-2617.37191	281.70413	1
78	C	68.61530	73.33799	75.73532	-491.73914	576.34187	222.73509	1
79	H	67.53997	73.61820	75.66552	1977.17978	-1823.58850	-434.68928	1
80	C	68.86018	72.08845	76.68931	-649.50797	-328.66843	306.11224	1
81	H	69.65424	71.42515	76.27372	2075.07803	1452.16490	-1004.45904	1
82	C	69.24979	72.59102	78.12261	-615.18735	-489.99689	-70.96352	1
83	H	69.43059	71.74342	78.82417	-1226.32661	-1724.38906	-1716.47170	1
84	H	70.17966	73.20928	78.09842	2381.64273	-969.84735	900.46860	1
85	H	68.44708	73.22614	78.56540	2122.74991	1702.23946	-141.36228	1
86	C	67.50041	71.33087	76.87818	-501.86074	-479.61276	-376.42482	1
87	H	67.61964	70.42978	77.52420	993.79261	-2246.95401	-1177.81305	1
88	H	66.72897	71.98123	77.35329	42.71279	-626.15391	-2651.37258	1
89	H	67.08463	70.98587	75.90054	-2026.39012	-1590.33709	-887.82922	1
90	C	69.54111	74.55152	76.17686	-672.89153	382.57394	-156.34072	1

91	O	70.77969	74.68781	75.87143	410.04627	221.86223	500.35950	1
92	N	68.91598	75.34184	77.00889	-378.11782	-443.79414	-441.10984	1
93	H	67.92408	75.18499	77.17583	2404.15973	-568.14894	1149.30085	1
94	C	69.60008	76.59231	77.19258	-544.54484	466.16019	331.29119	1
95	H	69.19551	77.22153	76.37518	-1409.80988	-170.17955	2325.32679	1
96	C	69.25528	77.15914	78.60336	-184.48284	116.78282	-758.89137	1
97	H	68.15775	77.31199	78.72689	1893.78641	1861.14652	611.04528	1
98	H	69.56020	76.43699	79.39566	-2170.79665	-974.19311	1327.50117	1
99	C	70.04078	78.51028	78.73710	389.51668	672.81878	-138.49152	1
100	H	71.12256	78.33895	78.53655	510.64577	1933.03327	1851.02484	1
101	H	69.72951	79.21980	77.94004	-2302.30869	-1105.72939	-948.89774	1
102	C	69.86848	79.19327	80.14241	-559.93427	-126.34590	542.30857	1
103	O	70.40215	80.25320	80.35672	-670.36003	-111.83166	76.36448	1
104	N	69.10526	78.49424	81.01091	-216.06729	-537.07037	446.51379	1
105	H	68.63230	77.59144	80.88847	-1251.96487	1074.12894	-2168.52500	1
106	H	68.90282	78.79970	81.96867	-2451.83023	-720.73851	944.84612	1
107	C	71.24728	76.22040	77.03740	546.24052	-563.88337	-85.11809	1
108	O	71.84628	75.62057	77.93498	71.70702	-307.40463	606.69673	1
109	N	71.80544	77.24209	76.28277	479.90863	-504.50129	222.86849	1
110	C	73.20388	77.31384	76.12346	75.51268	-600.91904	506.73700	1
111	H	73.52978	76.26392	76.33344	-2033.61562	1795.30103	254.89480	1
112	C	73.37264	77.81140	74.61259	523.79067	517.99274	284.45581	1
113	H	74.34590	78.32652	74.43979	1599.61665	-1127.00911	1895.98173	1
114	H	73.34758	76.95201	73.90669	-1881.83093	1275.82488	-1501.55016	1
115	C	72.13166	78.72821	74.41241	-600.05639	-404.05026	316.64485	1
116	H	72.30964	79.76163	74.78416	-2597.05260	496.36221	657.73249	1
117	H	71.82751	78.83228	73.34746	-1666.24518	1294.38985	-1723.90591	1
118	C	71.03727	77.97473	75.30390	493.57570	-129.95376	-602.56394	1
119	H	70.34173	78.65822	75.84841	-1469.08415	-637.84797	2204.22581	1
120	H	70.44115	77.20451	74.75565	-1038.97840	1068.88701	-2280.71789	1
121	C	73.83049	78.33274	77.26259	188.88100	241.05089	-727.87821	1
122	O	74.05730	77.87874	78.37904	531.88613	-49.19943	427.07960	1
123	N	73.97143	79.56308	76.83475	708.14833	26.93417	-179.73509	1
124	H	73.70680	79.73235	75.86773	-2232.69501	-1179.09831	1023.94816	1
125	C	74.82176	80.48115	77.52201	-738.32412	259.92548	104.42456	1
126	H	74.67467	81.43090	76.96279	2028.89123	1260.02983	1311.33324	1
127	C	74.33057	80.56350	79.02958	-258.65678	-345.52513	661.28459	1
128	H	74.31421	79.54595	79.49973	-1826.06090	-1801.46097	-918.64554	1
129	C	75.23732	81.54623	79.84645	-541.23400	531.92970	-218.41428	1
130	H	74.88911	81.63807	80.90226	1311.73218	-2219.18200	882.19023	1
131	H	76.29797	81.20225	79.87653	-1048.71298	1223.58118	-2196.97971	1
132	H	75.23315	82.57010	79.40551	419.06414	1903.92898	1903.44670	1
133	C	72.88162	81.16221	79.02998	-423.86431	152.66566	-648.55262	1
134	H	72.45478	81.21446	80.06172	105.68386	-2342.50080	1387.51238	1
135	H	72.85952	82.19323	78.60596	-1695.63603	-1484.73621	-1531.02793	1
136	H	72.18672	80.53602	78.42166	-1853.57121	-487.39031	1936.59343	1
137	C	76.33300	79.89848	77.28360	539.71428	-510.58232	267.58633	1
138	O	76.86393	80.08548	76.19227	-15.93758	-278.34085	-624.49402	1
139	N	76.79591	79.27879	78.34338	-676.81886	12.05292	276.17960	1
140	H	76.17396	79.21520	79.14715	-1694.44250	-373.84189	-2100.66098	1
141	C	78.03696	78.58928	78.33560	412.33078	-664.70360	108.35451	1
142	H	78.43342	78.72724	77.30353	1765.77476	1294.44366	1621.76594	1
143	C	78.92498	79.28172	79.46053	-179.66635	-721.95667	-264.73915	1
144	H	78.91992	80.38758	79.33947	-607.34922	2587.87032	-598.10018	1
145	H	78.48380	79.09174	80.46403	-359.69332	-1479.13954	-2259.74260	1
146	C	80.38208	78.72505	79.39083	-240.01076	616.02425	431.85322	1
147	H	80.37227	77.60356	79.41503	-1359.17131	782.54425	2227.99181	1
148	H	80.87107	79.01029	78.43306	-820.36667	85.81767	-2596.78715	1
149	C	81.18979	79.30171	80.62399	-513.07015	236.18570	-551.87280	1
150	H	81.27545	80.41090	80.55763	1816.11944	-1183.11722	-1650.94321	1
151	H	80.66038	79.09180	81.58167	-1800.04429	-1361.53473	1526.34643	1
152	C	82.58805	78.64221	80.61639	726.08972	-253.19732	-179.64713	1

153	H	82.58504	77.54922	80.80076	1224.27271	-456.51798	-2390.90304	1
154	H	83.19945	78.87481	79.72198	1206.40339	-1150.93514	-2154.90344	1
155	N	83.40122	79.24618	81.80954	329.70796	-633.68968	-155.67358	1
156	H	84.39244	78.88617	81.92458	1348.31305	1938.76845	1359.00643	1
157	H	83.56086	80.29436	81.78281	2096.92035	1446.54551	-966.48890	1
158	H	83.01174	79.10477	82.78683	-1197.07217	-2303.53719	827.28733	1
159	C	77.81143	77.03066	78.75789	-378.01186	-556.17301	-413.96481	1
160	O	78.75248	76.36107	79.12070	-409.44433	-307.55053	-453.30833	1
161	N	76.53574	76.66383	78.68405	-429.02477	524.70884	274.08502	1
162	H	75.81041	77.32650	78.35479	1706.34263	-1425.96036	1574.38926	1
163	C	76.29153	75.25973	78.54494	-45.25864	-626.22952	478.93267	1
164	H	77.17416	74.74645	78.99753	1988.63164	570.90773	1772.87287	1
165	C	74.90933	74.98832	79.27231	551.77128	-20.49526	-564.54996	1
166	H	74.92827	75.41545	80.30004	1434.61535	-1753.10253	1513.99471	1
167	H	74.05934	75.50047	78.75434	-714.67738	1819.09770	1898.36494	1
168	C	74.71284	73.43795	79.31234	446.99263	-555.77305	338.97221	1
169	H	74.43872	73.04511	78.30514	1953.68466	1892.25957	-161.67766	1
170	H	75.66290	72.92981	79.59317	-403.03785	2688.07032	-188.43591	1
171	C	73.59110	73.11936	80.38057	567.86262	335.74681	434.04421	1
172	H	73.84177	73.57477	81.36641	-1080.02275	1568.26081	-1948.78900	1
173	H	72.61614	73.56615	80.07672	-919.54108	2111.34692	1456.13463	1
174	C	73.49180	71.58061	80.50219	195.81897	173.33862	-745.11536	1
175	H	73.07391	71.07349	79.60979	1405.67949	-2301.21089	-390.08113	1
176	H	74.43026	71.08092	80.81627	-940.37328	-1118.32446	2299.72133	1
177	N	72.48382	71.26675	81.65733	319.26422	656.36007	-42.02424	1
178	H	72.30440	70.23840	81.84669	1961.03633	619.91968	1787.09422	1
179	H	72.73502	71.61605	82.62807	854.14343	-2156.80752	1429.08711	1
180	H	71.49633	71.63491	81.53887	1237.02905	-1378.50857	-1998.28500	1
181	C	76.08660	74.93989	76.95521	532.53319	-268.57236	517.55729	1
182	O	75.60740	75.76412	76.17533	266.16714	-290.73804	-558.88002	1
183	N	76.41833	73.68905	76.75764	-226.25352	640.49678	-270.32839	1
184	H	76.79813	73.21764	77.57767	2007.69063	-1035.27229	1523.50231	1
185	C	76.20571	72.95837	75.56283	-540.76542	-573.33303	49.50000	1
186	H	76.45132	71.91257	75.85293	-2374.20950	-1036.76023	843.75774	1
187	C	74.68086	73.13486	75.09743	-77.09082	666.87422	-415.84136	1
188	H	74.45566	74.22855	74.95227	-985.81834	617.19825	2463.91927	1
189	O	73.67420	72.63392	75.98994	293.29899	-391.65602	-477.80926	1
190	H	73.08417	73.41601	76.07915	2528.72714	-681.76262	-751.27122	1
191	C	74.80298	72.43549	73.69535	252.47363	-605.14473	440.05134	1
192	H	73.88487	72.57571	73.07916	-2052.65063	1456.49051	-1043.51830	1
193	H	75.67313	72.84017	73.11306	-2152.98800	-1661.97574	-161.70652	1
194	H	74.96933	71.33927	73.80236	-473.12726	-1584.27339	2165.61725	1
195	C	77.20640	73.49704	74.37291	360.36307	488.46713	505.10056	1
196	O	77.85679	72.68238	73.76661	-200.08817	-528.03552	-385.82850	1
197	N	77.06792	74.79804	74.14824	-597.54095	-226.44775	355.20479	1
198	H	76.41700	75.37880	74.74183	2179.23655	-1300.70981	-991.33835	1
199	C	78.07654	75.43553	73.37730	-687.68921	297.39807	-249.45179	1
200	H	78.79238	74.60730	73.16693	-349.16256	-2467.37713	-1101.72831	1
201	C	77.37581	75.99054	72.04627	672.47345	361.54328	-201.62880	1
202	H	76.56116	76.70824	72.29612	1541.41502	582.18425	2169.97026	1
203	H	78.11768	76.53483	71.41801	-2534.67717	60.25153	997.72295	1
204	C	76.82337	74.77793	71.28474	574.26774	-389.43119	-377.02542	1
205	C	77.74454	73.90019	70.63654	688.82679	-287.33580	-257.96133	1
206	H	78.82749	74.12045	70.63810	331.14182	1470.38163	2269.80013	1
207	C	75.42539	74.48681	71.27519	-383.52382	-675.04808	144.24917	1
208	H	74.70698	75.16130	71.77486	4.09847	1517.59662	2262.86397	1
209	C	77.25602	72.74392	70.02912	-134.76730	428.45285	-649.50303	1
210	H	77.97419	72.05913	69.54495	-903.23433	1600.49020	2011.53387	1
211	C	74.98440	73.31955	70.64560	-335.53281	-615.00040	-364.39058	1
212	H	73.90236	73.10084	70.65006	1596.45398	-1369.33862	1732.02659	1
213	C	75.87243	72.40069	70.01327	585.48547	-340.24194	-406.23938	1
214	O	75.43364	71.20245	69.39095	-419.15649	-173.04408	-511.94141	1

215	H	74.46205	71.28315	69.54090	-1071.84350	1559.71507	-1960.13012	1
216	C	78.69149	76.60955	74.32770	291.41878	-183.13091	710.72246	1
217	O	79.04234	76.38051	75.46209	379.87695	523.47396	-222.23622	1
218	N	78.86628	77.73572	73.63823	564.30591	373.09380	277.24371	1
219	H	78.54609	77.77358	72.67205	-120.59931	-2436.07824	-1214.35098	1
220	C	78.91068	78.97567	74.38203	404.07514	-299.37480	608.84009	1
221	H	78.12181	78.91110	75.17937	-1071.07882	-841.69025	2359.66467	1
222	C	80.36663	79.02826	74.99647	-683.12807	68.71770	-390.13096	1
223	H	80.58212	78.06932	75.52609	2068.88918	1596.58590	770.89603	1
224	H	81.12587	79.10353	74.18556	1379.86429	2342.49779	-179.85638	1
225	C	80.47237	80.23814	75.97640	-176.39967	537.49466	550.97268	1
226	H	80.24257	81.19684	75.46007	-396.28051	1942.22168	1869.33314	1
227	H	79.72768	80.15877	76.79851	-94.44700	586.00678	-2659.20016	1
228	C	81.96796	80.22429	76.54110	-291.69381	-718.18079	-150.72929	1
229	H	82.33226	79.24393	76.94099	-2303.38776	1089.76242	964.62032	1
230	H	82.74344	80.60953	75.83120	884.16729	2568.80533	-207.74283	1
231	N	81.88859	81.11544	77.62113	-594.49522	-252.81478	342.29276	1
232	H	81.04006	81.65359	77.70304	-1735.17426	2084.05705	-263.71605	1
233	C	82.80425	81.29047	78.48490	595.23177	-271.52487	442.22352	1
234	N	83.98046	80.54364	78.35481	585.53813	-424.79750	-105.81303	1
235	H	84.24625	79.87371	77.63427	959.88797	1327.56823	-2177.11905	1
236	H	84.78504	80.61268	78.97894	1578.48647	16.27378	-2220.76233	1
237	N	82.42268	82.24204	79.44172	-452.17763	-390.33541	-421.51853	1
238	H	81.57692	82.80353	79.52779	470.26107	1974.25629	-1817.92087	1
239	H	83.03205	82.53617	80.20591	1856.67307	-1573.97321	-1224.35416	1
240	C	78.63418	80.10234	73.26267	-531.47271	-581.45780	-55.06206	1
241	O	79.31655	80.18466	72.24452	-243.00837	192.73507	609.52485	1
242	N	77.59406	80.85431	73.61269	343.49288	-644.25607	38.09164	1
243	H	77.09617	80.67400	74.51420	-1691.16043	-1535.97525	-1484.73099	1
244	C	76.92491	81.40840	72.45711	542.66492	350.14337	454.42563	1
245	H	77.14260	80.62763	71.69250	1209.57979	-2396.95920	463.86744	1
246	C	75.38683	81.62234	72.75298	-737.14309	145.93010	242.71942	1
247	H	75.23728	82.20384	73.68844	-1050.18303	159.36419	-2509.06125	1
248	C	74.76060	82.35864	71.51675	-706.77696	-252.88343	-245.16230	1
249	H	73.65805	82.48484	71.62396	-1624.64039	-1665.49085	1417.86935	1
250	H	75.20100	83.37727	71.38608	2566.10521	598.51109	693.22305	1
251	H	74.94125	81.79685	70.57030	-1972.69758	107.10018	-1876.34312	1
252	C	74.68541	80.22232	72.84094	412.85148	672.58832	-27.69222	1
253	H	73.58538	80.32470	72.98924	1447.02277	1762.76533	-1490.78944	1
254	H	74.83803	79.62865	71.90913	1320.77379	-145.20455	2378.68491	1
255	H	75.08670	79.61761	73.69055	-1512.10848	1470.52031	1724.75147	1
256	C	77.65029	82.81972	72.05527	-607.11113	499.56689	73.73769	1
257	O	77.20099	83.89502	72.36495	357.97126	460.81534	356.68785	1
258	N	78.72424	82.53450	71.32597	536.55407	-368.62270	332.76306	1
259	H	79.07557	81.55054	71.20937	524.38866	2297.69985	1367.20941	1
260	C	79.52043	83.62594	70.89567	46.50277	-774.29190	-147.97904	1
261	H	78.84930	84.51535	70.91974	1676.51875	1883.29066	1032.55549	1
262	C	80.76680	83.76125	71.92024	-559.41456	-34.19198	-556.30433	1
263	H	81.30427	82.78487	71.97560	-64.66664	395.18769	2695.05373	1
264	H	81.50921	84.50322	71.54231	-2703.44278	-60.40056	333.79418	1
265	C	80.25273	84.15788	73.27632	-519.76435	377.31045	459.42366	1
266	H	79.45082	83.44226	73.57122	-1746.74323	1667.50644	-1261.73691	1
267	C	81.36551	84.08663	74.31449	570.95554	16.46261	-545.27700	1
268	H	80.99931	84.37604	75.33314	2391.58273	28.05277	-1305.07271	1
269	H	81.79007	83.05270	74.39632	175.75588	917.63458	2559.43867	1
270	H	82.21191	84.77470	74.05844	-1063.97851	-2155.34650	1283.00462	1
271	C	79.65827	85.55978	73.24859	193.76014	2.62946	-765.53141	1
272	H	79.40457	85.92300	74.27743	507.39394	-846.55087	2539.60089	1
273	H	80.36572	86.30267	72.79750	1337.57841	1818.19054	1526.01994	1
274	H	78.70943	85.58888	72.64855	1100.88635	-1172.91350	-2199.08909	1
275	C	80.11279	83.25523	69.44340	-549.21115	475.64486	-309.38218	1
276	O	79.97609	82.18168	68.91827	556.06106	-390.37755	-78.24250	1

277	O	80.86744	84.27409	68.81103	-572.27940	-310.19032	-209.75862	1
278	H	80.75806	84.99098	69.49435	-1380.08193	2212.14486	790.85944	1

Listing 8: C00008.xmolout

1		276						
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750
		0.2500	300.00	0.00	0.00	0.00	-1294.2694	0.0000
								300.0000
3	H	75.32361	62.83301	77.20589	-2043.14101	-1757.64893	399.89339	1
4	N	75.45345	63.21380	76.27261	426.75047	490.45733	-334.42467	1
5	H	74.53795	63.60506	76.06979	442.25559	-1110.30854	-2448.52907	1
6	C	76.56277	64.07660	76.09664	415.32972	-666.39213	83.73172	1
7	H	77.37782	63.57045	76.66102	879.32219	2491.00447	667.35213	1
8	C	76.89748	64.16346	74.51107	31.35357	477.41777	628.23362	1
9	H	76.04080	64.63315	73.97316	1168.38489	2240.25337	-1019.71136	1
10	H	77.77343	64.83111	74.33509	-360.43770	2534.90498	931.67112	1
11	C	77.15274	62.78050	73.98923	463.18208	512.70242	-382.34388	1
12	H	76.31747	62.12412	74.32545	1725.29117	1863.52247	-987.07854	1
13	C	77.19027	62.77222	72.46506	710.42801	-144.27427	-313.15367	1
14	H	77.36369	61.74130	72.06215	364.20195	-1033.13725	2494.72524	1
15	H	76.23003	63.14348	72.02377	2567.61904	335.80679	847.48802	1
16	H	78.01110	63.42384	72.06984	-2587.99029	680.92867	-512.16411	1
17	C	78.46287	62.21336	74.52269	268.17616	741.64379	-40.42634	1
18	H	78.67028	61.19338	74.10843	1283.54314	-1945.37420	-1411.27812	1
19	H	79.33360	62.86444	74.25313	-1258.57796	1317.15249	-2026.02085	1
20	H	78.45128	62.11995	75.63851	-2502.84526	909.80597	575.92391	1
21	C	76.27261	65.52282	76.67263	619.36578	-458.64843	-172.09273	1
22	O	77.04869	66.52108	76.45343	-81.40433	433.87611	522.34594	1
23	N	75.22302	65.60285	77.44337	175.23996	-622.20190	341.55523	1
24	H	74.62034	64.79159	77.56017	-876.57256	-303.22879	-2561.90213	1
25	C	74.78048	66.95451	77.63425	-571.88214	-534.10783	-106.15033	1
26	H	74.06601	67.10613	76.80242	-2713.20841	-16.25800	-248.80809	1
27	C	74.07100	66.99335	79.03659	166.60354	288.16399	-716.09568	1
28	H	74.78776	66.61590	79.81665	-2097.85574	1636.78449	-586.18044	1
29	O	72.88585	66.16554	79.16514	-317.80580	-363.38227	484.43082	1
30	H	73.14689	65.56365	79.88488	1863.74748	-1451.84923	1357.29467	1
31	C	73.87457	68.54647	79.21229	503.80731	517.99032	318.51606	1
32	H	73.47257	68.79681	80.22158	640.61020	-2157.10410	-1536.29104	1
33	H	74.84216	69.09524	79.09037	1687.88455	465.60692	2087.56452	1
34	H	73.15910	68.95316	78.46160	-1293.07895	-1899.88581	-1463.57452	1
35	C	76.17223	67.91887	77.53622	-153.07550	-733.68902	248.70981	1
36	O	76.83238	68.09231	78.57543	186.15459	-480.78787	-449.34387	1
37	N	75.92251	68.93717	76.64073	-487.53139	543.18517	42.03850	1
38	C	76.93249	69.88754	76.34999	-699.35871	69.34393	360.10701	1
39	H	77.91741	69.38870	76.51361	2.81126	-221.99807	-2715.58072	1
40	C	76.58364	70.30644	74.84065	-507.46439	-592.59194	122.07761	1
41	H	77.00160	71.29811	74.55956	-1975.08116	525.87560	-1801.71556	1
42	H	76.98668	69.57020	74.11093	1588.27743	-1913.22100	1113.83566	1
43	C	75.03130	70.28009	74.87462	-613.62442	-457.55993	-194.14490	1
44	H	74.62833	71.18797	75.38013	1707.54637	-721.27992	1996.92523	1
45	H	74.55947	70.23355	73.86808	758.23357	2100.81767	1560.55011	1
46	C	74.78302	68.96565	75.75561	-352.41524	704.96076	49.21465	1
47	H	73.85303	68.98658	76.37357	1714.76886	-2070.42778	443.35792	1
48	H	74.82215	68.00866	75.17969	1224.15040	1801.50881	1636.97633	1
49	C	76.68937	71.16304	77.34654	566.85117	537.05831	117.62814	1
50	O	75.61041	71.76833	77.34647	-550.26779	-406.08867	4.21666	1
51	N	77.77415	71.41546	78.02611	566.34832	-425.77725	180.18749	1
52	H	78.57695	70.79889	77.90103	644.44502	2646.80550	-52.73430	1
53	C	77.68780	72.37912	79.07349	612.34801	-281.48662	411.56221	1
54	H	76.69392	72.86569	78.93081	1667.23498	-1490.75142	1556.16753	1
55	C	77.76311	71.52943	80.42700	-714.45746	-175.43074	286.98927	1
56	H	78.72185	70.94393	80.41446	-787.09484	1763.03619	-1922.46060	1

57	O	76.71617	70.54881	80.60012	-429.46514	516.51932	-128.40526	1
58	H	77.06227	69.80331	80.06453	1981.82785	436.16847	-1818.18182	1
59	C	77.82568	72.65746	81.51549	630.79189	-468.94448	76.03230	1
60	H	78.02500	72.23986	82.52970	-1775.71861	2062.30353	131.89849	1
61	H	78.62267	73.40541	81.30042	-1855.14608	88.94118	1993.53760	1
62	H	76.86212	73.21602	81.57229	-1504.82350	-780.94249	-2132.90992	1
63	C	78.94013	73.42241	78.88672	288.57638	618.62814	-397.00270	1
64	O	78.66550	74.62349	78.81521	321.70495	-185.26452	574.37218	1
65	N	80.10565	72.82853	78.88057	-447.05792	-446.53431	367.76425	1
66	H	80.00888	71.81549	78.93986	350.31316	1975.63644	-1843.31522	1
67	C	81.35137	73.43003	78.56726	-511.23061	374.03917	-471.51480	1
68	H	81.96984	72.54563	78.29417	2234.79579	-898.70890	-1273.45190	1
69	C	81.16345	74.43375	77.34779	529.53781	-159.34528	563.72604	1
70	H	82.14853	74.56255	76.82075	654.59388	2347.94251	1217.51488	1
71	H	80.47447	73.92075	76.62618	-1526.55661	2103.42026	817.87394	1
72	O	80.68738	75.77171	77.62657	-554.84278	14.12789	399.58769	1
73	H	79.81481	75.51173	78.12499	1297.06236	2061.84854	1220.68812	1
74	C	82.00790	74.22439	79.83589	-662.15484	-412.13544	123.62687	1
75	O	83.14418	74.63316	79.75364	-540.01537	-317.05804	274.91456	1
76	N	81.16016	74.36638	80.87075	-202.76299	-690.00100	-131.49145	1
77	H	80.29035	73.89323	80.63060	-702.62132	-2617.37191	281.70413	1
78	C	81.62560	74.48965	82.26189	-491.73914	576.34187	222.73509	1
79	H	80.73186	74.15500	82.84114	1977.17978	-1823.58850	-434.68928	1
80	C	82.83492	73.60568	82.49749	-649.50797	-328.66843	306.11224	1
81	H	83.60817	73.87680	81.73780	2075.07803	1452.16490	-1004.45904	1
82	C	83.43802	73.81150	83.87410	-615.18735	-489.99689	-70.96352	1
83	H	84.33578	73.15466	84.04085	-1226.32661	-1724.38906	-1716.47170	1
84	H	83.77304	74.88544	84.01941	2381.64273	-969.84735	900.46860	1
85	H	82.69960	73.58061	84.69025	2122.74991	1702.23946	-141.36228	1
86	C	82.49136	72.13750	82.31241	-501.86074	-479.61276	-376.42482	1
87	H	83.39535	71.47968	82.43129	993.79261	-2246.95401	-1177.81305	1
88	H	81.72976	71.79469	83.06519	42.71279	-626.15391	-2651.37258	1
89	H	82.06198	71.93985	81.29222	-2026.39012	-1590.33709	-887.82922	1
90	C	81.91819	76.09443	82.47869	-672.89153	382.57394	-156.34072	1
91	O	82.86425	76.48577	83.11827	410.04627	221.86223	500.35950	1
92	N	80.93096	76.80487	81.96975	-378.11782	-443.79414	-441.10984	1
93	H	80.16015	76.42025	81.39779	2404.15973	-568.14894	1149.30085	1
94	C	80.98364	78.23780	82.08846	-544.54484	466.16019	331.29119	1
95	H	81.22217	78.48887	83.14704	-1409.80988	-170.17955	2325.32679	1
96	C	82.17028	78.64906	81.11029	-184.48284	116.78282	-758.89137	1
97	H	83.10649	78.15600	81.46331	1893.78641	1861.14652	611.04528	1
98	H	81.98951	78.25091	80.08607	-2170.79665	-974.19311	1327.50117	1
99	C	82.33477	80.19762	81.08896	389.51668	672.81878	-138.49152	1
100	H	81.42354	80.67799	80.66464	510.64577	1933.03327	1851.02484	1
101	H	82.39341	80.59175	82.12945	-2302.30869	-1105.72939	-948.89774	1
102	C	83.61123	80.66908	80.29317	-559.93427	-126.34590	542.30857	1
103	O	83.84363	81.84585	80.19247	-670.36003	-111.83166	76.36448	1
104	N	84.36142	79.66136	79.79824	-216.06729	-537.07037	446.51379	1
105	H	84.22659	78.64516	79.85840	-1251.96487	1074.12894	-2168.52500	1
106	H	85.23948	79.80014	79.28626	-2451.83023	-720.73851	944.84612	1
107	C	79.49057	78.60408	81.59520	546.24052	-563.88337	-85.11809	1
108	O	78.89808	77.76602	80.94467	71.70702	-307.40463	606.69673	1
109	N	79.08821	79.81428	81.98543	479.90863	-504.50129	222.86849	1
110	C	77.86883	80.38112	81.48056	75.51268	-600.91904	506.73700	1
111	H	77.10756	79.57049	81.53026	-2033.61562	1795.30103	254.89480	1
112	C	77.62541	81.61032	82.44582	523.79067	517.99274	284.45581	1
113	H	77.03091	82.42233	81.96923	1599.61665	-1127.00911	1895.98173	1
114	H	77.07116	81.30706	83.36251	-1881.83093	1275.82488	-1501.55016	1
115	C	79.08992	82.03470	82.78122	-600.05639	-404.05026	316.64485	1
116	H	79.55276	82.56683	81.91885	-2597.05260	496.36221	657.73249	1
117	H	79.17334	82.70708	83.66443	-1666.24518	1294.38985	-1723.90591	1
118	C	79.75675	80.61008	83.00632	493.57570	-129.95376	-602.56394	1

119	H	80.85965	80.56674	82.84872	-1469.08415	-637.84797	2204.22581	1
120	H	79.50613	80.13007	83.98210	-1038.97840	1068.88701	-2280.71789	1
121	C	78.17494	80.85025	79.93641	188.88100	241.05089	-727.87821	1
122	O	78.85115	81.81368	79.67740	531.88613	-49.19943	427.07960	1
123	N	77.54738	80.01888	79.10979	708.14833	26.93417	-179.73509	1
124	H	77.05088	79.23417	79.53386	-2232.69501	-1179.09831	1023.94816	1
125	C	77.69782	80.09787	77.66836	-738.32412	259.92548	104.42456	1
126	H	78.26569	81.03817	77.46407	2028.89123	1260.02983	1311.33324	1
127	C	78.40797	78.82019	77.22280	-258.65678	-345.52513	661.28459	1
128	H	77.78626	77.95908	77.55741	-1826.06090	-1801.46097	-918.64554	1
129	C	78.53378	78.75333	75.71344	-541.23400	531.92970	-218.41428	1
130	H	79.04305	77.80767	75.37855	1311.73218	-2219.18200	882.19023	1
131	H	77.52534	78.78541	75.21278	-1048.71298	1223.58118	-2196.97971	1
132	H	79.13213	79.61518	75.30716	419.06414	1903.92898	1903.44670	1
133	C	79.75938	78.67306	77.88891	-423.86431	152.66566	-648.55262	1
134	H	80.21059	77.63401	77.70612	105.68386	-2342.50080	1387.51238	1
135	H	80.49617	79.43681	77.51376	-1695.63603	-1484.73621	-1531.02793	1
136	H	79.67655	78.80224	79.00725	-1853.57121	-487.39031	1936.59343	1
137	C	76.14094	80.06630	77.08343	539.71428	-510.58232	267.58633	1
138	O	75.25646	79.44669	77.66558	-15.93758	-278.34085	-624.49402	1
139	N	76.08286	80.69944	75.94172	-676.81886	12.05292	276.17960	1
140	H	76.96069	81.09536	75.61838	-1694.44250	-373.84189	-2100.66098	1
141	C	74.81520	80.90812	75.30346	412.33078	-664.70360	108.35451	1
142	H	74.15311	81.12127	76.17374	1765.77476	1294.44366	1621.76594	1
143	C	74.97605	82.08718	74.26552	-179.66635	-721.95667	-264.73915	1
144	H	75.52133	82.94823	74.71387	-607.34922	2587.87032	-598.10018	1
145	H	75.59318	81.75444	73.40063	-359.69332	-1479.13954	-2259.74260	1
146	C	73.54371	82.51046	73.79474	-240.01076	616.02425	431.85322	1
147	H	72.93884	81.62042	73.48399	-1359.17131	782.54425	2227.99181	1
148	H	72.97571	82.99225	74.62218	-820.36667	85.81767	-2596.78715	1
149	C	73.72278	83.49817	72.57370	-513.07015	236.18570	-551.87280	1
150	H	74.23937	84.43530	72.88511	1816.11944	-1183.11722	-1650.94321	1
151	H	74.36670	83.04229	71.78666	-1800.04429	-1361.53473	1526.34643	1
152	C	72.30941	83.79205	72.01818	726.08972	-253.19732	-179.64713	1
153	H	71.77071	82.90046	71.63835	1224.27271	-456.51798	-2390.90304	1
154	H	71.65372	84.36571	72.70319	1206.40339	-1150.93514	-2154.90344	1
155	N	72.48619	84.71412	70.76606	329.70796	-633.68968	-155.67358	1
156	H	71.59078	84.99628	70.27240	1348.31305	1938.76845	1359.00643	1
157	H	72.94372	85.65895	70.92395	2096.92035	1446.54551	-966.48890	1
158	H	73.05719	84.32677	69.95930	-1197.07217	-2303.53719	827.28733	1
159	C	74.37341	79.53685	74.53991	-378.01186	-556.17301	-413.96481	1
160	O	74.36087	79.43158	73.32228	-409.44433	-307.55053	-453.30833	1
161	N	74.01925	78.65506	75.44725	-429.02477	524.70884	274.08502	1
162	H	74.11802	78.86528	76.46811	1706.34263	-1425.96036	1574.38926	1
163	C	73.80121	77.31358	74.98669	-45.25864	-626.22952	478.93267	1
164	H	74.57496	77.18364	74.19574	1988.63164	570.90773	1772.87287	1
165	C	73.94500	76.37239	76.24420	551.77128	-20.49526	-564.54996	1
166	H	74.98197	76.40144	76.64983	1434.61535	-1753.10253	1513.99471	1
167	H	73.29154	76.73436	77.07002	-714.67738	1819.09770	1898.36494	1
168	C	73.54049	74.91860	75.82162	446.99263	-555.77305	338.97221	1
169	H	72.51566	74.91669	75.38237	1953.68466	1892.25957	-161.67766	1
170	H	74.21588	74.51743	75.03311	-403.03785	2688.07032	-188.43591	1
171	C	73.58101	74.02108	77.11837	567.86262	335.74681	434.04421	1
172	H	74.62367	73.67441	77.33547	-1080.02275	1568.26081	-1948.78900	1
173	H	73.25770	74.59932	78.01459	-919.54108	2111.34692	1456.13463	1
174	C	72.63149	72.81655	76.88281	195.81897	173.33862	-745.11536	1
175	H	71.55322	73.03331	77.02606	1405.67949	-2301.21089	-390.08113	1
176	H	72.78818	72.28692	75.92097	-940.37328	-1118.32446	2299.72133	1
177	N	73.01395	71.77048	77.96111	319.26422	656.36007	-42.02424	1
178	H	72.48422	70.85169	77.93706	1961.03633	619.91968	1787.09422	1
179	H	74.07838	71.48268	77.90139	854.14343	-2156.80752	1429.08711	1
180	H	72.87139	72.05438	78.97399	1237.02905	-1378.50857	-1998.28500	1

181	C	72.28984	77.24796	74.35169	532.53319	-268.57236	517.55729	1
182	O	71.34807	76.78070	74.94461	266.16714	-290.73804	-558.88002	1
183	N	72.35204	77.72616	73.11476	-226.25352	640.49678	-270.32839	1
184	H	73.22542	78.18126	72.76449	2007.69063	-1035.27229	1523.50231	1
185	C	71.12161	77.81092	72.39569	-540.76542	-573.33303	49.50000	1
186	H	70.36449	77.41767	73.11899	-2374.20950	-1036.76023	843.75774	1
187	C	70.90763	79.33788	72.01142	-77.09082	666.87422	-415.84136	1
188	H	71.60846	79.60330	71.17203	-985.81834	617.19825	2463.91927	1
189	O	71.31489	80.32220	73.03168	293.29899	-391.65602	-477.80926	1
190	H	72.12650	79.88464	73.34640	2528.72714	-681.76262	-751.27122	1
191	C	69.42076	79.39480	71.53509	252.47363	-605.14473	440.05134	1
192	H	69.12927	80.42514	71.22189	-2052.65063	1456.49051	-1043.51830	1
193	H	69.23486	78.71555	70.65887	-2152.98800	-1661.97574	-161.70652	1
194	H	68.71928	79.08985	72.34827	-473.12726	-1584.27339	2165.61725	1
195	C	71.25583	76.91490	71.02931	360.36307	488.46713	505.10056	1
196	O	70.57663	77.17331	70.04979	-200.08817	-528.03552	-385.82850	1
197	N	72.11307	75.92529	71.18324	-597.54095	-226.44775	355.20479	1
198	H	72.56187	75.83697	72.09225	2179.23655	-1300.70981	-991.33835	1
199	C	72.32836	75.04231	70.08137	-687.68921	297.39807	-249.45179	1
200	H	72.50181	75.69376	69.19753	-349.16256	-2467.37713	-1101.72831	1
201	C	73.52448	74.05331	70.44176	672.47345	361.54328	-201.62880	1
202	H	73.26647	73.47606	71.35862	1541.41502	582.18425	2169.97026	1
203	H	73.64335	73.31546	69.61497	-2534.67717	60.25153	997.72295	1
204	C	74.84000	74.81867	70.65664	574.26774	-389.43119	-377.02542	1
205	C	75.60737	75.24998	69.53339	688.82679	-287.33580	-257.96133	1
206	H	75.24456	75.08370	68.50273	331.14182	1470.38163	2269.80013	1
207	C	75.30517	75.05521	71.98530	-383.52382	-675.04808	144.24917	1
208	H	74.70531	74.73525	72.85601	4.09847	1517.59662	2262.86397	1
209	C	76.83592	75.86996	69.76476	-134.76730	428.45285	-649.50303	1
210	H	77.43725	76.19258	68.89680	-903.23433	1600.49020	2011.53387	1
211	C	76.54261	75.67918	72.16528	-335.53281	-615.00040	-364.39058	1
212	H	76.89987	75.84382	73.19685	1596.45398	-1369.33862	1732.02659	1
213	C	77.35533	76.09972	71.07198	585.48547	-340.24194	-406.23938	1
214	O	78.62014	76.72091	71.24460	-419.15649	-173.04408	-511.94141	1
215	H	78.67552	76.71467	72.22919	-1071.84350	1559.71507	-1960.13012	1
216	C	70.98144	74.12767	69.92003	291.41878	-183.13091	710.72246	1
217	O	70.41290	73.59958	70.85028	379.87695	523.47396	-222.23622	1
218	N	70.75328	74.00777	68.61946	564.30591	373.09380	277.24371	1
219	H	71.36987	74.49586	67.97182	-120.59931	-2436.07824	-1214.35098	1
220	C	69.60824	73.30337	68.14764	404.07514	-299.37480	608.84009	1
221	H	69.79324	73.19824	67.05435	-1071.07882	-841.69025	2359.66467	1
222	C	69.56728	71.90951	68.91393	-683.12807	68.71770	-390.13096	1
223	H	70.58154	71.45002	68.91806	2068.88918	1596.58590	770.89603	1
224	H	69.30278	72.05949	69.99228	1379.86429	2342.49779	-179.85638	1
225	C	68.53642	70.96872	68.22120	-176.39967	537.49466	550.97268	1
226	H	67.50327	71.38042	68.30606	-396.28051	1942.22168	1869.33314	1
227	H	68.73797	70.87783	67.13059	-94.44700	586.00678	-2659.20016	1
228	C	68.67566	69.55455	68.95388	-291.69381	-718.18079	-150.72929	1
229	H	69.67262	69.05350	68.85969	-2303.38776	1089.76242	964.62032	1
230	H	68.39673	69.55490	70.03841	884.16729	2568.80533	-207.74283	1
231	N	67.73643	68.76443	68.27708	-594.49522	-252.81478	342.29276	1
232	H	67.12373	69.24111	67.63388	-1735.17426	2084.05705	-263.71605	1
233	C	67.60177	67.50980	68.43157	595.23177	-271.52487	442.22352	1
234	N	68.45416	66.86686	69.33607	585.53813	-424.79750	-105.81303	1
235	H	69.19013	67.25870	69.92205	959.88797	1327.56823	-2177.11905	1
236	H	68.43651	65.86859	69.54694	1578.48647	16.27378	-2220.76233	1
237	N	66.57198	67.01014	67.62192	-452.17763	-390.33541	-421.51853	1
238	H	65.94998	67.47989	66.96582	470.26107	1974.25629	-1817.92087	1
239	H	66.30503	66.02515	67.60367	1856.67307	-1573.97321	-1224.35416	1
240	C	68.26355	74.16662	68.45505	-531.47271	-581.45780	-55.06206	1
241	O	67.17980	73.64185	68.39210	-243.00837	192.73507	609.52485	1
242	N	68.53159	75.48071	68.60067	343.49288	-644.25607	38.09164	1

243	H	69.52255	75.70340	68.75339	-1691.16043	-1535.97525	-1484.73099	1
244	C	67.51174	76.38171	69.14405	542.66492	350.14337	454.42563	1
245	H	66.56401	75.97086	68.71914	1209.57979	-2396.95920	463.86744	1
246	C	67.56040	76.26296	70.65613	-737.14309	145.93010	242.71942	1
247	H	68.57379	76.59354	70.98441	-1050.18303	159.36419	-2509.06125	1
248	C	66.52304	77.14070	71.32900	-706.77696	-252.88343	-245.16230	1
249	H	66.62014	77.12263	72.44940	-1624.64039	-1665.49085	1417.86935	1
250	H	66.61902	78.21979	70.99351	2566.10521	598.51109	693.22305	1
251	H	65.47705	76.80985	71.07982	-1972.69758	107.10018	-1876.34312	1
252	C	67.38711	74.82074	71.09790	412.85148	672.58832	-27.69222	1
253	H	67.55447	74.69227	72.20222	1447.02277	1762.76533	-1490.78944	1
254	H	66.35381	74.44047	70.86607	1320.77379	-145.20455	2378.68491	1
255	H	68.11542	74.14473	70.55697	-1512.10848	1470.52031	1724.75147	1
256	C	67.86239	77.91197	68.62292	-607.11113	499.56689	73.73769	1
257	O	67.45626	78.87606	69.23552	357.97126	460.81534	356.68785	1
258	N	68.56082	77.89882	67.49857	536.55407	-368.62270	332.76306	1
259	H	68.78200	76.97948	67.11931	524.38866	2297.69985	1367.20941	1
260	C	68.79732	79.09970	66.79370	46.50277	-774.29190	-147.97904	1
261	H	68.21154	79.87926	67.33053	1676.51875	1883.29066	1032.55549	1
262	C	70.38899	79.39093	66.75572	-559.41456	-34.19198	-556.30433	1
263	H	70.90392	78.53496	66.25865	-64.66664	395.18769	2695.05373	1
264	H	70.60413	80.28685	66.12621	-2703.44278	-60.40056	333.79418	1
265	C	70.91213	79.57735	68.15253	-519.76435	377.31045	459.42366	1
266	H	70.56544	78.70778	68.78047	-1746.74323	1667.50644	-1261.73691	1
267	C	72.43565	79.58745	68.15379	570.95554	16.46261	-545.27700	1
268	H	72.84884	79.71083	69.18817	2391.58273	28.05277	-1305.07271	1
269	H	72.85558	78.63334	67.74250	175.75588	917.63458	2559.43867	1
270	H	72.84326	80.42553	67.53166	-1063.97851	-2155.34650	1283.00462	1
271	C	70.39442	80.87025	68.76760	193.76014	2.62946	-765.53141	1
272	H	70.84308	81.05988	69.77665	507.39394	-846.55087	2539.60089	1
273	H	70.63666	81.75775	68.12788	1337.57841	1818.19054	1526.01994	1
274	H	69.28153	80.84624	68.89897	1100.88635	-1172.91350	-2199.08909	1
275	C	68.36659	78.83277	65.25899	-549.21115	475.64486	-309.38218	1
276	O	68.36783	77.73963	64.75493	556.06106	-390.37755	-78.24250	1
277	O	68.13136	79.98815	64.47846	-572.27940	-310.19032	-209.75862	1
278	H	68.22753	80.67854	65.19159	-1380.08193	2212.14486	790.85944	1

Listing 9: C00009.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	1.8560	7424
		0.2500	300.00	0.00	0.00	0.00	-1294.2665	0.0000	300.0000
3	H	65.16994	75.22344	73.97829	-2043.14101	-1757.64893	399.89339		1
4	N	65.31837	75.30906	72.97283	426.75047	490.45733	-334.42467		1
5	H	64.38062	75.53283	72.61417	442.25559	-1110.30854	-2448.52907		1
6	C	66.27337	76.28642	72.61039	415.32972	-666.39213	83.73172		1
7	H	66.83387	76.54225	73.53671	879.32219	2491.00447	667.35213		1
8	C	67.23898	75.68363	71.46510	31.35357	477.41777	628.23362		1
9	H	66.62508	75.43729	70.56634	1168.38489	2240.25337	-1019.71136		1
10	H	67.97708	76.45213	71.13368	-360.43770	2534.90498	931.67112		1
11	C	67.93835	74.45309	71.97405	463.18208	512.70242	-382.34388		1
12	H	67.15729	73.74142	72.32721	1725.29117	1863.52247	-987.07854		1
13	C	68.74120	73.78352	70.86518	710.42801	-144.27427	-313.15367		1
14	H	69.17036	72.80558	71.20290	364.20195	-1033.13725	2494.72524		1
15	H	68.11076	73.57519	69.96270	2567.61904	335.80679	847.48802		1
16	H	69.60682	74.41769	70.53135	-2587.99029	680.92867	-512.16411		1
17	C	68.87257	74.76858	73.13499	268.17616	741.64379	-40.42634		1
18	H	69.44923	73.86233	73.45844	1283.54314	-1945.37420	-1411.27812		1
19	H	69.62384	75.55258	72.85888	-1258.57796	1317.15249	-2026.02085		1
20	H	68.31226	75.14246	74.03014	-2502.84526	909.80597	575.92391		1
21	C	65.35983	77.48888	72.03333	619.36578	-458.64843	-172.09273		1
22	O	64.12204	77.35689	71.98045	-81.40433	433.87611	522.34594		1

23	N	66.10993	78.50463	71.70992	175.23996	-622.20190	341.55523	1
24	H	67.11110	78.33601	71.80266	-876.57256	-303.22879	-2561.90213	1
25	C	65.66437	79.78136	71.24613	-571.88214	-534.10783	-106.15033	1
26	H	66.10565	79.83254	70.22664	-2713.20841	-16.25800	-248.80809	1
27	C	64.07257	79.89600	71.20819	166.60354	288.16399	-716.09568	1
28	H	63.68332	79.58082	72.21831	-2097.85574	1636.78449	-586.18044	1
29	O	63.42119	79.04499	70.26365	-317.80580	-363.38227	484.43082	1
30	H	63.31449	78.20349	70.84917	1863.74748	-1451.84923	1357.29467	1
31	C	63.82730	81.43575	71.01346	503.80731	517.99032	318.51606	1
32	H	62.73936	81.67906	71.00553	640.61020	-2157.10410	-1536.29104	1
33	H	64.29931	82.04026	71.82554	1687.88455	465.60692	2087.56452	1
34	H	64.25358	81.79441	70.04730	-1293.07895	-1899.88581	-1463.57452	1
35	C	66.35103	80.95450	72.14226	-153.07550	-733.68902	248.70981	1
36	O	66.56462	81.97250	71.53148	186.15459	-480.78787	-449.34387	1
37	N	66.50805	80.73533	73.45958	-487.53139	543.18517	42.03850	1
38	C	67.07386	81.74372	74.29697	-699.35871	69.34393	360.10701	1
39	H	66.85842	82.73005	73.82440	2.81126	-221.99807	-2715.58072	1
40	C	66.35323	81.45228	75.68396	-507.46439	-592.59194	122.07761	1
41	H	66.88379	81.90699	76.55043	-1975.08116	525.87560	-1801.71556	1
42	H	65.31207	81.84465	75.69915	1588.27743	-1913.22100	1113.83566	1
43	C	66.37454	79.89246	75.69445	-613.62442	-457.55993	-194.14490	1
44	H	67.38636	79.51179	75.96427	1707.54637	-721.27992	1996.92523	1
45	H	65.66116	79.43834	76.41847	758.23357	2100.81767	1560.55011	1
46	C	66.02505	79.56372	74.18000	-352.41524	704.96076	49.21465	1
47	H	66.55308	78.67252	73.77240	1714.76886	-2070.42778	443.35792	1
48	H	64.93787	79.48038	73.94876	1224.15040	1801.50881	1636.97633	1
49	C	68.68111	81.47653	74.51894	566.85117	537.05831	117.62814	1
50	O	69.29948	82.15628	75.30315	-550.26779	-406.08867	4.21666	1
51	N	69.10759	80.45851	73.78179	566.34832	-425.77725	180.18749	1
52	H	68.43955	80.02982	73.14324	644.44502	2646.80550	-52.73430	1
53	C	70.44700	80.02015	73.90807	612.34801	-281.48662	411.56221	1
54	H	70.88075	80.61745	74.74374	1667.23498	-1490.75142	1556.16753	1
55	C	70.36926	78.44672	74.19912	-714.45746	-175.43074	286.98927	1
56	H	69.88887	77.94098	73.31740	-787.09484	1763.03619	-1922.46060	1
57	O	69.57214	78.07354	75.34057	-429.46514	516.51932	-128.40526	1
58	H	68.89158	77.51423	74.91643	1981.82785	436.16847	-1818.18182	1
59	C	71.88053	78.02214	74.27149	630.79189	-468.94448	76.03230	1
60	H	71.98260	76.93359	74.48816	-1775.71861	2062.30353	131.89849	1
61	H	72.41597	78.21704	73.30693	-1855.14608	88.94118	1993.53760	1
62	H	72.42450	78.56897	75.07733	-1504.82350	-780.94249	-2132.90992	1
63	C	71.15223	80.29697	72.44885	288.57638	618.62814	-397.00270	1
64	O	70.53773	80.34385	71.41128	321.70495	-185.26452	574.37218	1
65	N	72.45453	80.40355	72.66074	-447.05792	-446.53431	367.76425	1
66	H	72.80688	80.29028	73.60938	350.31316	1975.63644	-1843.31522	1
67	C	73.38465	80.36444	71.54853	-511.23061	374.03917	-471.51480	1
68	H	73.16486	81.28202	70.95349	2234.79579	-898.70890	-1273.45190	1
69	C	74.80487	80.33025	72.17232	529.53781	-159.34528	563.72604	1
70	H	75.56326	80.23745	71.37165	654.59388	2347.94251	1217.51488	1
71	H	75.02552	81.25688	72.75052	-1526.55661	2103.42026	817.87394	1
72	O	75.07393	79.27593	73.38285	-554.84278	14.12789	399.58769	1
73	H	74.97865	78.51730	72.81081	1297.06236	2061.84854	1220.68812	1
74	C	73.13334	79.00661	70.66900	-662.15484	-412.13544	123.62687	1
75	O	72.82323	77.92555	71.15646	-540.01537	-317.05804	274.91456	1
76	N	73.47500	79.30078	69.42737	-202.76299	-690.00100	-131.49145	1
77	H	73.75323	80.27286	69.30299	-702.62132	-2617.37191	281.70413	1
78	C	72.79260	78.64333	68.34546	-491.73914	576.34187	222.73509	1
79	H	71.78018	78.45730	68.76686	1977.17978	-1823.58850	-434.68928	1
80	C	72.81882	79.62646	67.10789	-649.50797	-328.66843	306.11224	1
81	H	73.85986	79.96051	66.90640	2075.07803	1452.16490	-1004.45904	1
82	C	72.21001	78.92589	65.84338	-615.18735	-489.99689	-70.96352	1
83	H	72.16522	79.62002	64.97133	-1226.32661	-1724.38906	-1716.47170	1
84	H	72.82302	78.04373	65.53273	2381.64273	-969.84735	900.46860	1

85	H	71.17323	78.56195	66.03279	2122.74991	1702.23946	-141.36228	1
86	C	71.88945	80.85434	67.41127	-501.86074	-479.61276	-376.42482	1
87	H	71.88117	81.58219	66.56645	993.79261	-2246.95401	-1177.81305	1
88	H	70.83516	80.53515	67.58421	42.71279	-626.15391	-2651.37258	1
89	H	72.21684	81.40662	68.32257	-2026.39012	-1590.33709	-887.82922	1
90	C	73.56802	77.24347	68.02517	-672.89153	382.57394	-156.34072	1
91	O	74.17162	77.04789	66.99710	410.04627	221.86223	500.35950	1
92	N	73.35228	76.40953	69.03621	-378.11782	-443.79414	-441.10984	1
93	H	72.86300	76.71608	69.91337	2404.15973	-568.14894	1149.30085	1
94	C	73.91962	75.10915	68.94874	-544.54484	466.16019	331.29119	1
95	H	74.48236	75.07803	67.98653	-1409.80988	-170.17955	2325.32679	1
96	C	74.83464	75.03518	70.24722	-184.48284	116.78282	-758.89137	1
97	H	75.44810	75.96178	70.30085	1893.78641	1861.14652	611.04528	1
98	H	74.20679	75.04065	71.16633	-2170.79665	-974.19311	1327.50117	1
99	C	75.75311	73.77638	70.21724	389.51668	672.81878	-138.49152	1
100	H	75.13429	72.85202	70.22540	510.64577	1933.03327	1851.02484	1
101	H	76.30669	73.73338	69.25361	-2302.30869	-1105.72939	-948.89774	1
102	C	76.78680	73.73625	71.40958	-559.93427	-126.34590	542.30857	1
103	O	77.35001	72.70399	71.68551	-670.36003	-111.83166	76.36448	1
104	N	76.94128	74.91767	72.04390	-216.06729	-537.07037	446.51379	1
105	H	76.52041	75.83043	71.83632	-1251.96487	1074.12894	-2168.52500	1
106	H	77.62528	75.08451	72.78974	-2451.83023	-720.73851	944.84612	1
107	C	72.65183	74.07630	69.03885	546.24052	-563.88337	-85.11809	1
108	O	71.78421	74.25588	69.85652	71.70702	-307.40463	606.69673	1
109	N	72.79871	73.06375	68.17483	479.90863	-504.50129	222.86849	1
110	C	71.72448	72.15636	67.88366	75.51268	-600.91904	506.73700	1
111	H	70.81345	72.78882	67.77722	-2033.61562	1795.30103	254.89480	1
112	C	72.19419	71.44623	66.54395	523.79067	517.99274	284.45581	1
113	H	71.77354	70.42101	66.43369	1599.61665	-1127.00911	1895.98173	1
114	H	71.87112	72.01798	65.64542	-1881.83093	1275.82488	-1501.55016	1
115	C	73.74731	71.46019	66.69113	-600.05639	-404.05026	316.64485	1
116	H	74.09423	70.65577	67.37752	-2597.05260	496.36221	657.73249	1
117	H	74.28905	71.31607	65.72913	-1666.24518	1294.38985	-1723.90591	1
118	C	73.96860	72.90276	67.32398	493.57570	-129.95376	-602.56394	1
119	H	74.88548	73.01218	67.94721	-1469.08415	-637.84797	2204.22581	1
120	H	73.92263	73.73723	66.58368	-1038.97840	1068.88701	-2280.71789	1
121	C	71.52700	71.04658	69.05832	188.88100	241.05089	-727.87821	1
122	O	70.82186	70.08309	68.85359	531.88613	-49.19943	427.07960	1
123	N	72.25631	71.33039	70.14855	708.14833	26.93417	-179.73509	1
124	H	72.69443	72.25824	70.08724	-2232.69501	-1179.09831	1023.94816	1
125	C	71.67809	70.94799	71.41469	-738.32412	259.92548	104.42456	1
126	H	70.57944	71.06547	71.30507	2028.89123	1260.02983	1311.33324	1
127	C	72.10551	69.44405	71.65701	-258.65678	-345.52513	661.28459	1
128	H	72.97376	69.18785	71.01202	-1826.06090	-1801.46097	-918.64554	1
129	C	72.43451	69.18708	73.16875	-541.23400	531.92970	-218.41428	1
130	H	72.65619	68.11217	73.36660	1311.73218	-2219.18200	882.19023	1
131	H	73.32411	69.77614	73.50039	-1048.71298	1223.58118	-2196.97971	1
132	H	71.58561	69.48135	73.82952	419.06414	1903.92898	1903.44670	1
133	C	70.87503	68.53133	71.32250	-423.86431	152.66566	-648.55262	1
134	H	71.12603	67.44805	71.41210	105.68386	-2342.50080	1387.51238	1
135	H	70.01618	68.73077	72.00599	-1695.63603	-1484.73621	-1531.02793	1
136	H	70.51888	68.71476	70.26561	-1853.57121	-487.39031	1936.59343	1
137	C	72.33976	71.94928	72.51995	539.71428	-510.58232	267.58633	1
138	O	71.66226	72.52265	73.34547	-15.93758	-278.34085	-624.49402	1
139	N	73.65228	71.99010	72.32212	-676.81886	12.05292	276.17960	1
140	H	74.00409	71.43596	71.54118	-1694.44250	-373.84189	-2100.66098	1
141	C	74.55535	72.51748	73.28665	412.33078	-664.70360	108.35451	1
142	H	75.45630	72.75071	72.67654	1765.77476	1294.44366	1621.76594	1
143	C	73.88755	73.76699	73.98461	-179.66635	-721.95667	-264.73915	1
144	H	73.45138	74.45404	73.22389	-607.34922	2587.87032	-598.10018	1
145	H	73.03857	73.46535	74.65000	-359.69332	-1479.13954	-2259.74260	1
146	C	75.04382	74.45028	74.79462	-240.01076	616.02425	431.85322	1

147	H	75.24904	73.89562	75.74928	-1359.17131	782.54425	2227.99181	1
148	H	75.99243	74.43439	74.21148	-820.36667	85.81767	-2596.78715	1
149	C	74.60421	75.93615	75.08139	-513.07015	236.18570	-551.87280	1
150	H	74.33121	76.45804	74.13553	1816.11944	-1183.11722	-1650.94321	1
151	H	73.69233	75.96460	75.72071	-1800.04429	-1361.53473	1526.34643	1
152	C	75.79580	76.65287	75.77672	726.08972	-253.19732	-179.64713	1
153	H	75.95841	76.36304	76.83635	1224.27271	-456.51798	-2390.90304	1
154	H	76.75497	76.60039	75.22004	1206.40339	-1150.93514	-2154.90344	1
155	N	75.44170	78.15012	75.79851	329.70796	-633.68968	-155.67358	1
156	H	76.15737	78.76324	76.27862	1348.31305	1938.76845	1359.00643	1
157	H	75.28853	78.64264	74.77411	2096.92035	1446.54551	-966.48890	1
158	H	74.58093	78.40884	76.35508	-1197.07217	-2303.53719	827.28733	1
159	C	74.90096	71.36319	74.40947	-378.01186	-556.17301	-413.96481	1
160	O	74.12674	70.99376	75.26062	-409.44433	-307.55053	-453.30833	1
161	N	76.14777	70.96327	74.19087	-429.02477	524.70884	274.08502	1
162	H	76.69297	71.37344	73.42873	1706.34263	-1425.96036	1574.38926	1
163	C	76.64536	69.95457	75.07502	-45.25864	-626.22952	478.93267	1
164	H	75.73350	69.38747	75.37719	1988.63164	570.90773	1772.87287	1
165	C	77.71770	69.09487	74.29018	551.77128	-20.49526	-564.54996	1
166	H	77.30999	68.74196	73.31668	1434.61535	-1753.10253	1513.99471	1
167	H	78.61075	69.70764	74.03540	-714.67738	1819.09770	1898.36494	1
168	C	78.11076	67.89267	75.21213	446.99263	-555.77305	338.97221	1
169	H	78.60975	68.26009	76.14002	1953.68466	1892.25957	-161.67766	1
170	H	77.21413	67.32456	75.54815	-403.03785	2688.07032	-188.43591	1
171	C	79.07549	66.98180	74.35466	567.86262	335.74681	434.04421	1
172	H	78.50632	66.44946	73.55775	-1080.02275	1568.26081	-1948.78900	1
173	H	79.83440	67.61024	73.81109	-919.54108	2111.34692	1456.13463	1
174	C	79.80691	65.97636	75.27391	195.81897	173.33862	-745.11536	1
175	H	80.39105	66.43925	76.09451	1405.67949	-2301.21089	-390.08113	1
176	H	79.18005	65.15152	75.66828	-940.37328	-1118.32446	2299.72133	1
177	N	80.87811	65.30216	74.35191	319.26422	656.36007	-42.02424	1
178	H	81.57285	64.64358	74.80996	1961.03633	619.91968	1787.09422	1
179	H	80.51340	64.70713	73.55265	854.14343	-2156.80752	1429.08711	1
180	H	81.52108	65.97114	73.83705	1237.02905	-1378.50857	-1998.28500	1
181	C	77.36267	70.63228	76.38262	532.53319	-268.57236	517.55729	1
182	O	77.57833	69.89970	77.35068	266.16714	-290.73804	-558.88002	1
183	N	77.69905	71.88964	76.19395	-226.25352	640.49678	-270.32839	1
184	H	77.40833	72.19120	75.26495	2007.69063	-1035.27229	1523.50231	1
185	C	77.86662	72.83799	77.24267	-540.76542	-573.33303	49.50000	1
186	H	77.83621	73.81663	76.71534	-2374.20950	-1036.76023	843.75774	1
187	C	76.61613	72.65389	78.21267	-77.09082	666.87422	-415.84136	1
188	H	76.53840	71.56951	78.49867	-985.81834	617.19825	2463.91927	1
189	O	75.34058	72.99680	77.60568	293.29899	-391.65602	-477.80926	1
190	H	74.98167	72.10928	77.41423	2528.72714	-681.76262	-751.27122	1
191	C	77.00831	73.49691	79.47532	252.47363	-605.14473	440.05134	1
192	H	76.28109	73.34704	80.30771	-2052.65063	1456.49051	-1043.51830	1
193	H	78.01831	73.22840	79.86391	-2152.98800	-1661.97574	-161.70652	1
194	H	77.02848	74.58835	79.24664	-473.12726	-1584.27339	2165.61725	1
195	C	79.30955	72.63472	77.99550	360.36307	488.46713	505.10056	1
196	O	79.99891	73.61670	78.10658	-200.08817	-528.03552	-385.82850	1
197	N	79.48655	71.41154	78.47164	-597.54095	-226.44775	355.20479	1
198	H	78.76361	70.66725	78.26842	2179.23655	-1300.70981	-991.33835	1
199	C	80.76887	71.00050	78.92179	-687.68921	297.39807	-249.45179	1
200	H	80.66849	69.89692	79.02545	-349.16256	-2467.37713	-1101.72831	1
201	C	81.88511	71.41780	77.84865	672.47345	361.54328	-201.62880	1
202	H	81.83753	72.51679	77.66145	1541.41502	582.18425	2169.97026	1
203	H	82.89620	71.19679	78.26158	-2534.67717	60.25153	997.72295	1
204	C	81.65832	70.65405	76.53689	574.26774	-389.43119	-377.02542	1
205	C	82.15591	69.32433	76.39227	688.82679	-287.33580	-257.96133	1
206	H	82.66617	68.81772	77.23112	331.14182	1470.38163	2269.80013	1
207	C	80.96812	71.28906	75.46033	-383.52382	-675.04808	144.24917	1
208	H	80.54398	72.30187	75.58499	4.09847	1517.59662	2262.86397	1

209	C	82.00199	68.68698	75.15872	-134.76730	428.45285	-649.50303	1
210	H	82.39748	67.66281	75.04320	-903.23433	1600.49020	2011.53387	1
211	C	80.84921	70.61189	74.24202	-335.53281	-615.00040	-364.39058	1
212	H	80.33215	71.12067	73.40874	1596.45398	-1369.33862	1732.02659	1
213	C	81.36923	69.30189	74.04156	585.48547	-340.24194	-406.23938	1
214	O	81.25889	68.60456	72.79427	-419.15649	-173.04408	-511.94141	1
215	H	80.83039	69.31112	72.25934	-1071.84350	1559.71507	-1960.13012	1
216	C	81.13743	71.73241	80.32255	291.41878	-183.13091	710.72246	1
217	O	82.31517	71.85201	80.67119	379.87695	523.47396	-222.23622	1
218	N	80.04547	72.03154	80.98917	564.30591	373.09380	277.24371	1
219	H	79.18542	71.80286	80.49303	-120.59931	-2436.07824	-1214.35098	1
220	C	80.02994	72.80230	82.18338	404.07514	-299.37480	608.84009	1
221	H	78.95740	72.80526	82.48117	-1071.07882	-841.69025	2359.66467	1
222	C	80.97935	72.07128	83.22464	-683.12807	68.71770	-390.13096	1
223	H	80.64133	71.02393	83.39216	2068.88918	1596.58590	770.89603	1
224	H	82.01439	71.98284	82.81485	1379.86429	2342.49779	-179.85638	1
225	C	80.97924	72.87758	84.55873	-176.39967	537.49466	550.97268	1
226	H	81.26766	73.93927	84.38505	-396.28051	1942.22168	1869.33314	1
227	H	79.96373	72.90999	85.01212	-94.44700	586.00678	-2659.20016	1
228	C	82.02543	72.14420	85.52018	-291.69381	-718.18079	-150.72929	1
229	H	81.83736	71.05782	85.71364	-2303.38776	1089.76242	964.62032	1
230	H	83.09707	72.26154	85.21622	884.16729	2568.80533	-207.74283	1
231	N	81.84626	72.83258	86.72801	-594.49522	-252.81478	342.29276	1
232	H	81.33901	73.70270	86.67959	-1735.17426	2084.05705	-263.71605	1
233	C	82.28770	72.44717	87.85626	595.23177	-271.52487	442.22352	1
234	N	83.00580	71.24751	87.90473	585.53813	-424.79750	-105.81303	1
235	H	83.26285	70.61524	87.14784	959.88797	1327.56823	-2177.11905	1
236	H	83.41675	70.84670	88.74845	1578.48647	16.27378	-2220.76233	1
237	N	81.94416	73.35570	88.86695	-452.17763	-390.33541	-421.51853	1
238	H	81.42034	74.22888	88.83052	470.26107	1974.25629	-1817.92087	1
239	H	82.20363	73.22640	89.84566	1856.67307	-1573.97321	-1224.35416	1
240	C	80.57096	74.31751	81.87811	-531.47271	-581.45780	-55.06206	1
241	O	79.79896	75.22608	82.00362	-243.00837	192.73507	609.52485	1
242	N	81.88088	74.34142	81.61315	343.49288	-644.25607	38.09164	1
243	H	82.36631	73.42173	81.47168	-1691.16043	-1535.97525	-1484.73099	1
244	C	82.54039	75.57962	81.15482	542.66492	350.14337	454.42563	1
245	H	83.57924	75.38997	81.51189	1209.57979	-2396.95920	463.86744	1
246	C	82.47322	75.64916	79.64519	-737.14309	145.93010	242.71942	1
247	H	81.40138	75.70545	79.34735	-1050.18303	159.36419	-2509.06125	1
248	C	83.20770	76.86614	79.10807	-706.77696	-252.88343	-245.16230	1
249	H	83.09658	76.95865	77.99341	-1624.64039	-1665.49085	1417.86935	1
250	H	82.83096	77.82326	79.56142	2566.10521	598.51109	693.22305	1
251	H	84.30878	76.81138	79.32831	-1972.69758	107.10018	-1876.34312	1
252	C	83.04850	74.40481	78.99024	412.85148	672.58832	-27.69222	1
253	H	82.93910	74.43408	77.87138	1447.02277	1762.76533	-1490.78944	1
254	H	84.14285	74.28179	79.21832	1320.77379	-145.20455	2378.68491	1
255	H	82.52405	73.47588	79.36095	-1512.10848	1470.52031	1724.75147	1
256	C	81.85467	76.85367	81.95018	-607.11113	499.56689	73.73769	1
257	O	82.13012	77.02040	83.11201	357.97126	460.81534	356.68785	1
258	N	81.17573	77.66331	81.14092	536.55407	-368.62270	332.76306	1
259	H	80.96893	77.38996	80.17352	524.38866	2297.69985	1367.20941	1
260	C	80.18844	78.51078	81.73676	46.50277	-774.29190	-147.97904	1
261	H	79.92735	78.03681	82.70942	1676.51875	1883.29066	1032.55549	1
262	C	80.79021	79.99873	81.91604	-559.41456	-34.19198	-556.30433	1
263	H	81.08486	80.39163	80.91391	-64.66664	395.18769	2695.05373	1
264	H	80.00662	80.69491	82.29941	-2703.44278	-60.40056	333.79418	1
265	C	81.98050	79.97613	82.83587	-519.76435	377.31045	459.42366	1
266	H	82.66336	79.15782	82.50418	-1746.74323	1667.50644	-1261.73691	1
267	C	82.72982	81.30111	82.76765	570.95554	16.46261	-545.27700	1
268	H	83.63350	81.29994	83.42998	2391.58273	28.05277	-1305.07271	1
269	H	83.08061	81.52627	81.72766	175.75588	917.63458	2559.43867	1
270	H	82.08329	82.15684	83.09141	-1063.97851	-2155.34650	1283.00462	1

271	C	81.56812	79.69183	84.27379	193.76014	2.62946	-765.53141	1
272	H	82.43896	79.76765	84.97494	507.39394	-846.55087	2539.60089	1
273	H	80.78614	80.40941	84.63345	1337.57841	1818.19054	1526.01994	1
274	H	81.15291	78.65379	84.37755	1100.88635	-1172.91350	-2199.08909	1
275	C	79.02014	78.55962	80.64047	-549.21115	475.64486	-309.38218	1
276	O	79.15263	78.09426	79.53329	556.06106	-390.37755	-78.24250	1
277	O	77.84475	79.26033	80.98927	-572.27940	-310.19032	-209.75862	1
278	H	78.07431	79.48643	81.93443	-1380.08193	2212.14486	790.85944	1

Listing 10: C00010.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1294.2214	0.0000	300.0000
3	H	71.61414	87.28463	75.84055	-2043.14101	-1757.64893	399.89339		1
4	N	72.42419	87.12158	75.24494	426.75047	490.45733	-334.42467		1
5	H	71.96957	86.72832	74.42222	442.25559	-1110.30854	-2448.52907		1
6	C	73.17452	88.29579	74.98116	415.32972	-666.39213	83.73172		1
7	H	72.48753	89.15564	75.13823	879.32219	2491.00447	667.35213		1
8	C	74.42430	88.30739	75.99907	31.35357	477.41777	628.23362		1
9	H	74.94679	87.32529	75.92213	1168.38489	2240.25337	-1019.71136		1
10	H	75.16540	89.08760	75.69979	-360.43770	2534.90498	931.67112		1
11	C	73.94652	88.53769	77.41044	463.18208	512.70242	-382.34388		1
12	H	73.06655	87.88212	77.59695	1725.29117	1863.52247	-987.07854		1
13	C	75.04035	88.16323	78.40261	710.42801	-144.27427	-313.15367		1
14	H	74.72261	88.35204	79.46049	364.20195	-1033.13725	2494.72524		1
15	H	75.31401	87.07930	78.32614	2567.61904	335.80679	847.48802		1
16	H	75.97660	88.75366	78.22632	-2587.99029	680.92867	-512.16411		1
17	C	73.53363	89.98752	77.62208	268.17616	741.64379	-40.42634		1
18	H	73.18411	90.16948	78.67126	1283.54314	-1945.37420	-1411.27812		1
19	H	74.38612	90.68956	77.43078	-1258.57796	1317.15249	-2026.02085		1
20	H	72.69875	90.28776	76.93784	-2502.84526	909.80597	575.92391		1
21	C	73.71781	88.19152	73.45893	619.36578	-458.64843	-172.09273		1
22	O	73.78899	89.20302	72.75364	-81.40433	433.87611	522.34594		1
23	N	74.17657	86.97935	73.23133	175.23996	-622.20190	341.55523		1
24	H	74.00513	86.33728	74.00810	-876.57256	-303.22879	-2561.90213		1
25	C	74.22312	86.39767	71.91571	-571.88214	-534.10783	-106.15033		1
26	H	73.22879	85.91266	71.80919	-2713.20841	-16.25800	-248.80809		1
27	C	74.45121	87.51368	70.80439	166.60354	288.16399	-716.09568		1
28	H	75.18643	88.26896	71.21704	-2097.85574	1636.78449	-586.18044		1
29	O	73.30492	88.30213	70.47104	-317.80580	-363.38227	484.43082		1
30	H	73.40906	89.04688	71.17387	1863.74748	-1451.84923	1357.29467		1
31	C	75.09961	86.70738	69.62145	503.80731	517.99032	318.51606		1
32	H	75.39382	87.38047	68.78307	640.61020	-2157.10410	-1536.29104		1
33	H	76.01480	86.15571	69.94095	1687.88455	465.60692	2087.56452		1
34	H	74.38855	85.95499	69.20763	-1293.07895	-1899.88581	-1463.57452		1
35	C	75.35926	85.23428	71.99965	-153.07550	-733.68902	248.70981		1
36	O	74.93550	84.11810	71.84902	186.15459	-480.78787	-449.34387		1
37	N	76.62496	85.63935	72.19125	-487.53139	543.18517	42.03850		1
38	C	77.71914	84.72727	72.08409	-699.35871	69.34393	360.10701		1
39	H	77.43688	83.94098	71.34711	2.81126	-221.99807	-2715.58072		1
40	C	78.90732	85.69727	71.66514	-507.46439	-592.59194	122.07761		1
41	H	79.91146	85.25579	71.85332	-1975.08116	525.87560	-1801.71556		1
42	H	78.86617	85.95839	70.58434	1588.27743	-1913.22100	1113.83566		1
43	C	78.59282	86.93181	72.56534	-613.62442	-457.55993	-194.14490		1
44	H	78.86368	86.73873	73.62842	1707.54637	-721.27992	1996.92523		1
45	H	79.13080	87.85750	72.26057	758.23357	2100.81767	1560.55011		1
46	C	77.01790	87.03065	72.37954	-352.41524	704.96076	49.21465		1
47	H	76.45162	87.43669	73.25090	1714.76886	-2070.42778	443.35792		1
48	H	76.70680	87.57086	71.45529	1224.15040	1801.50881	1636.97633		1
49	C	78.15043	84.10924	73.54141	566.85117	537.05831	117.62814		1
50	O	79.07137	83.32834	73.60416	-550.26779	-406.08867	4.21666		1

51	N	77.41246	84.59692	74.53951	566.34832	-425.77725	180.18749	1
52	H	76.70252	85.27680	74.26861	644.44502	2646.80550	-52.73430	1
53	C	78.02751	84.59099	75.83869	612.34801	-281.48662	411.56221	1
54	H	79.11884	84.67985	75.64163	1667.23498	-1490.75142	1556.16753	1
55	C	77.40085	85.82075	76.63288	-714.45746	-175.43074	286.98927	1
56	H	76.28111	85.74277	76.59497	-787.09484	1763.03619	-1922.46060	1
57	O	77.74920	87.11373	76.09601	-429.46514	516.51932	-128.40526	1
58	H	76.86893	87.48778	75.91026	1981.82785	436.16847	-1818.18182	1
59	C	77.87820	85.53259	78.10380	630.79189	-468.94448	76.03230	1
60	H	77.46948	86.28239	78.82022	-1775.71861	2062.30353	131.89849	1
61	H	77.54844	84.52602	78.45360	-1855.14608	88.94118	1993.53760	1
62	H	78.98898	85.56703	78.18704	-1504.82350	-780.94249	-2132.90992	1
63	C	77.64399	83.15767	76.52177	288.57638	618.62814	-397.00270	1
64	O	76.48521	82.88953	76.84105	321.70495	-185.26452	574.37218	1
65	N	78.75054	82.49298	76.72185	-447.05792	-446.53431	367.76425	1
66	H	79.59083	82.94068	76.35689	350.31316	1975.63644	-1843.31522	1
67	C	78.86020	81.17969	77.24750	-511.23061	374.03917	-471.51480	1
68	H	79.86916	81.21976	77.71344	2234.79579	-898.70890	-1273.45190	1
69	C	77.69364	80.90123	78.30011	529.53781	-159.34528	563.72604	1
70	H	78.03477	80.06190	78.97012	654.59388	2347.94251	1217.51488	1
71	H	77.62689	81.82862	78.93049	-1526.55661	2103.42026	817.87394	1
72	O	76.40611	80.52447	77.80053	-554.84278	14.12789	399.58769	1
73	H	76.10624	81.44754	77.43373	1297.06236	2061.84854	1220.68812	1
74	C	78.92859	80.10463	76.01305	-662.15484	-412.13544	123.62687	1
75	O	80.00257	79.51413	75.88906	-540.01537	-317.05804	274.91456	1
76	N	77.83462	80.02924	75.30464	-202.76299	-690.00100	-131.49145	1
77	H	77.08828	80.64887	75.62844	-702.62132	-2617.37191	281.70413	1
78	C	77.61877	79.14746	74.20979	-491.73914	576.34187	222.73509	1
79	H	76.82004	79.64346	73.61362	1977.17978	-1823.58850	-434.68928	1
80	C	78.98229	78.97116	73.40617	-649.50797	-328.66843	306.11224	1
81	H	79.77479	78.54868	74.07106	2075.07803	1452.16490	-1004.45904	1
82	C	78.77313	78.04860	72.15782	-615.18735	-489.99689	-70.96352	1
83	H	79.71179	77.94407	71.56436	-1226.32661	-1724.38906	-1716.47170	1
84	H	78.45553	77.02154	72.45672	2381.64273	-969.84735	900.46860	1
85	H	77.99136	78.45333	71.47326	2122.74991	1702.23946	-141.36228	1
86	C	79.41307	80.37880	72.86929	-501.86074	-479.61276	-376.42482	1
87	H	80.37834	80.33185	72.31215	993.79261	-2246.95401	-1177.81305	1
88	H	78.64943	80.80971	72.17993	42.71279	-626.15391	-2651.37258	1
89	H	79.54610	81.10672	73.70800	-2026.39012	-1590.33709	-887.82922	1
90	C	77.12375	77.70212	74.77586	-672.89153	382.57394	-156.34072	1
91	O	77.41918	77.25099	75.88521	410.04627	221.86223	500.35950	1
92	N	76.45132	77.10637	73.82297	-378.11782	-443.79414	-441.10984	1
93	H	76.28630	77.62079	72.96254	2404.15973	-568.14894	1149.30085	1
94	C	76.05308	75.73442	73.99622	-544.54484	466.16019	331.29119	1
95	H	76.99531	75.18620	74.21095	-1409.80988	-170.17955	2325.32679	1
96	C	75.09842	75.75565	75.25813	-184.48284	116.78282	-758.89137	1
97	H	75.70117	75.95951	76.17657	1893.78641	1861.14652	611.04528	1
98	H	74.38692	76.60785	75.17019	-2170.79665	-974.19311	1327.50117	1
99	C	74.31378	74.41304	75.40369	389.51668	672.81878	-138.49152	1
100	H	73.76098	74.18517	74.46678	510.64577	1933.03327	1851.02484	1
101	H	75.00881	73.55153	75.51162	-2302.30869	-1105.72939	-948.89774	1
102	C	73.32172	74.48788	76.62469	-559.93427	-126.34590	542.30857	1
103	O	72.46066	73.65212	76.76537	-670.36003	-111.83166	76.36448	1
104	N	73.56861	75.51633	77.46017	-216.06729	-537.07037	446.51379	1
105	H	74.26708	76.26656	77.39899	-1251.96487	1074.12894	-2168.52500	1
106	H	73.01684	75.71980	78.30079	-2451.83023	-720.73851	944.84612	1
107	C	75.28336	75.25441	72.65022	546.24052	-563.88337	-85.11809	1
108	O	74.21330	75.74489	72.35276	71.70702	-307.40463	606.69673	1
109	N	75.95111	74.27478	72.03704	479.90863	-504.50129	222.86849	1
110	C	75.53555	73.77422	70.75635	75.51268	-600.91904	506.73700	1
111	H	75.14452	74.64747	70.18390	-2033.61562	1795.30103	254.89480	1
112	C	76.87345	73.09752	70.22235	523.79067	517.99274	284.45581	1

113	H	76.68681	72.35107	69.41810	1599.61665	-1127.00911	1895.98173	1
114	H	77.58263	73.84846	69.80876	-1881.83093	1275.82488	-1501.55016	1
115	C	77.41557	72.46085	71.53907	-600.05639	-404.05026	316.64485	1
116	H	76.84709	71.53554	71.79194	-2597.05260	496.36221	657.73249	1
117	H	78.48897	72.17037	71.48821	-1666.24518	1294.38985	-1723.90591	1
118	C	77.12488	73.61529	72.59210	493.57570	-129.95376	-602.56394	1
119	H	76.87122	73.26408	73.62062	-1469.08415	-637.84797	2204.22581	1
120	H	77.92084	74.39495	72.65069	-1038.97840	1068.88701	-2280.71789	1
121	C	74.42274	72.61514	71.01809	188.88100	241.05089	-727.87821	1
122	O	74.74702	71.44915	70.89812	531.88613	-49.19943	427.07960	1
123	N	73.22676	73.14344	71.27524	708.14833	26.93417	-179.73509	1
124	H	73.30152	74.16278	71.41898	-2232.69501	-1179.09831	1023.94816	1
125	C	72.21963	72.37449	72.05524	-738.32412	259.92548	104.42456	1
126	H	72.81020	72.04495	72.94483	2028.89123	1260.02983	1311.33324	1
127	C	71.08984	73.31747	72.39099	-258.65678	-345.52513	661.28459	1
128	H	70.75483	73.79447	71.44184	-1826.06090	-1801.46097	-918.64554	1
129	C	69.90599	72.58899	73.00459	-541.23400	531.92970	-218.41428	1
130	H	69.10482	73.30346	73.33982	1311.73218	-2219.18200	882.19023	1
131	H	69.43104	71.87613	72.27013	-1048.71298	1223.58118	-2196.97971	1
132	H	70.21806	71.98329	73.90099	419.06414	1903.92898	1903.44670	1
133	C	71.51848	74.42446	73.33789	-423.86431	152.66566	-648.55262	1
134	H	70.70752	75.19125	73.47450	105.68386	-2342.50080	1387.51238	1
135	H	71.75995	74.01776	74.35913	-1695.63603	-1484.73621	-1531.02793	1
136	H	72.44078	74.97131	72.95980	-1853.57121	-487.39031	1936.59343	1
137	C	71.71796	71.09350	71.16777	539.71428	-510.58232	267.58633	1
138	O	70.60836	71.03755	70.66606	-15.93758	-278.34085	-624.49402	1
139	N	72.64949	70.16334	71.15867	-676.81886	12.05292	276.17960	1
140	H	73.57899	70.34434	71.59634	-1694.44250	-373.84189	-2100.66098	1
141	C	72.53907	69.17530	70.12264	412.33078	-664.70360	108.35451	1
142	H	71.88792	69.66540	69.36077	1765.77476	1294.44366	1621.76594	1
143	C	74.00733	68.82490	69.65623	-179.66635	-721.95667	-264.73915	1
144	H	74.53344	69.73927	69.29381	-607.34922	2587.87032	-598.10018	1
145	H	74.61402	68.45377	70.51287	-359.69332	-1479.13954	-2259.74260	1
146	C	73.89202	67.73208	68.54223	-240.01076	616.02425	431.85322	1
147	H	73.37973	66.83052	68.95569	-1359.17131	782.54425	2227.99181	1
148	H	73.26343	68.08790	67.69533	-820.36667	85.81767	-2596.78715	1
149	C	75.35198	67.37788	68.04838	-513.07015	236.18570	-551.87280	1
150	H	75.85503	68.27512	67.61983	1816.11944	-1183.11722	-1650.94321	1
151	H	75.98981	67.05189	68.90184	-1800.04429	-1361.53473	1526.34643	1
152	C	75.23625	66.25470	66.99180	726.08972	-253.19732	-179.64713	1
153	H	74.83310	65.29767	67.37886	1224.27271	-456.51798	-2390.90304	1
154	H	74.70025	66.54414	66.06594	1206.40339	-1150.93514	-2154.90344	1
155	N	76.68684	65.90543	66.51553	329.70796	-633.68968	-155.67358	1
156	H	76.75740	65.13445	65.79041	1348.31305	1938.76845	1359.00643	1
157	H	77.24334	66.68023	66.05005	2096.92035	1446.54551	-966.48890	1
158	H	77.36662	65.55911	67.25351	-1197.07217	-2303.53719	827.28733	1
159	C	71.81330	67.88665	70.83110	-378.01186	-556.17301	-413.96481	1
160	O	72.39049	66.83732	71.01624	-409.44433	-307.55053	-453.30833	1
161	N	70.57309	68.25169	71.09695	-429.02477	524.70884	274.08502	1
162	H	70.28470	69.22193	70.85798	1706.34263	-1425.96036	1574.38926	1
163	C	69.68813	67.38479	71.79332	-45.25864	-626.22952	478.93267	1
164	H	68.69597	67.88359	71.71145	1988.63164	570.90773	1772.87287	1
165	C	69.74647	65.97695	71.06252	551.77128	-20.49526	-564.54996	1
166	H	69.61713	66.11096	69.96502	1434.61535	-1753.10253	1513.99471	1
167	H	70.76034	65.51933	71.18974	-714.67738	1819.09770	1898.36494	1
168	C	68.64512	65.02976	71.63801	446.99263	-555.77305	338.97221	1
169	H	68.81901	64.83969	72.72537	1953.68466	1892.25957	-161.67766	1
170	H	67.63443	65.49008	71.56144	-403.03785	2688.07032	-188.43591	1
171	C	68.72405	63.68735	70.80355	567.86262	335.74681	434.04421	1
172	H	68.46150	63.86851	69.73587	-1080.02275	1568.26081	-1948.78900	1
173	H	69.76459	63.28856	70.79552	-919.54108	2111.34692	1456.13463	1
174	C	67.75764	62.66549	71.44461	195.81897	173.33862	-745.11536	1

175	H	68.05495	62.32300	72.45595	1405.67949	-2301.21089	-390.08113	1
176	H	66.69292	62.97286	71.44643	-940.37328	-1118.32446	2299.72133	1
177	N	67.79628	61.37373	70.55929	319.26422	656.36007	-42.02424	1
178	H	67.19407	60.56773	70.89486	1961.03633	619.91968	1787.09422	1
179	H	67.47404	61.46903	69.55240	854.14343	-2156.80752	1429.08711	1
180	H	68.73759	60.89705	70.44394	1237.02905	-1378.50857	-1998.28500	1
181	C	70.16449	67.21755	73.34941	532.53319	-268.57236	517.55729	1
182	O	69.64429	66.37289	74.03694	266.16714	-290.73804	-558.88002	1
183	N	71.03037	68.15566	73.70321	-226.25352	640.49678	-270.32839	1
184	H	71.33376	68.90367	73.06291	2007.69063	-1035.27229	1523.50231	1
185	C	71.86429	67.95972	74.84400	-540.76542	-573.33303	49.50000	1
186	H	71.29000	67.39333	75.61186	-2374.20950	-1036.76023	843.75774	1
187	C	73.16614	67.18144	74.33134	-77.09082	666.87422	-415.84136	1
188	H	73.60780	67.78038	73.48563	-985.81834	617.19825	2463.91927	1
189	O	72.94586	65.87879	73.76419	293.29899	-391.65602	-477.80926	1
190	H	72.85480	66.09612	72.80334	2528.72714	-681.76262	-751.27122	1
191	C	74.11104	67.22698	75.58292	252.47363	-605.14473	440.05134	1
192	H	75.08379	66.72275	75.37757	-2052.65063	1456.49051	-1043.51830	1
193	H	74.34280	68.27346	75.89393	-2152.98800	-1661.97574	-161.70652	1
194	H	73.65419	66.70870	76.45933	-473.12726	-1584.27339	2165.61725	1
195	C	72.20687	69.52354	75.16137	360.36307	488.46713	505.10056	1
196	O	72.06164	70.33207	74.26114	-200.08817	-528.03552	-385.82850	1
197	N	72.64060	69.69867	76.40146	-597.54095	-226.44775	355.20479	1
198	H	72.69810	68.90019	77.03388	2179.23655	-1300.70981	-991.33835	1
199	C	73.19485	70.95639	76.75380	-687.68921	297.39807	-249.45179	1
200	H	72.68276	71.62915	76.02203	-349.16256	-2467.37713	-1101.72831	1
201	C	72.87874	71.25482	78.29084	672.47345	361.54328	-201.62880	1
202	H	73.51558	70.61729	78.94937	1541.41502	582.18425	2169.97026	1
203	H	73.13815	72.32215	78.49724	-2534.67717	60.25153	997.72295	1
204	C	71.39943	70.99660	78.61097	574.26774	-389.43119	-377.02542	1
205	C	70.43446	71.99387	78.28020	688.82679	-287.33580	-257.96133	1
206	H	70.75120	72.92794	77.76309	331.14182	1470.38163	2269.80013	1
207	C	71.00643	69.77868	79.24446	-383.52382	-675.04808	144.24917	1
208	H	71.75325	68.99928	79.48278	4.09847	1517.59662	2262.86397	1
209	C	69.10183	71.76355	78.62515	-134.76730	428.45285	-649.50303	1
210	H	68.35107	72.53605	78.38390	-903.23433	1600.49020	2011.53387	1
211	C	69.65921	69.59538	79.56351	-335.53281	-615.00040	-364.39058	1
212	H	69.36412	68.65321	80.05809	1596.45398	-1369.33862	1732.02659	1
213	C	68.66271	70.57460	79.27774	585.48547	-340.24194	-406.23938	1
214	O	67.29434	70.39784	79.61198	-419.15649	-173.04408	-511.94141	1
215	H	67.33878	69.50436	80.02799	-1071.84350	1559.71507	-1960.13012	1
216	C	74.80615	70.88590	76.47604	291.41878	-183.13091	710.72246	1
217	O	75.22609	70.71728	75.35435	379.87695	523.47396	-222.23622	1
218	N	75.50958	71.00997	77.59790	564.30591	373.09380	277.24371	1
219	H	75.04776	71.18030	78.49102	-120.59931	-2436.07824	-1214.35098	1
220	C	76.91590	71.20062	77.45774	404.07514	-299.37480	608.84009	1
221	H	77.16229	70.70862	76.48815	-1071.07882	-841.69025	2359.66467	1
222	C	77.14939	72.76920	77.44793	-683.12807	68.71770	-390.13096	1
223	H	76.35253	73.28798	76.87136	2068.88918	1596.58590	770.89603	1
224	H	77.09302	73.18051	78.48154	1379.86429	2342.49779	-179.85638	1
225	C	78.55379	73.01374	76.81656	-176.39967	537.49466	550.97268	1
226	H	79.34883	72.54373	77.43764	-396.28051	1942.22168	1869.33314	1
227	H	78.62812	72.53391	75.81537	-94.44700	586.00678	-2659.20016	1
228	C	78.76644	74.59276	76.70479	-291.69381	-718.18079	-150.72929	1
229	H	78.09461	75.13416	75.98782	-2303.38776	1089.76242	964.62032	1
230	H	78.75326	75.15525	77.67334	884.16729	2568.80533	-207.74283	1
231	N	80.07562	74.62819	76.20138	-594.49522	-252.81478	342.29276	1
232	H	80.53815	73.74180	76.07379	-1735.17426	2084.05705	-263.71605	1
233	C	80.71629	75.69439	75.92120	595.23177	-271.52487	442.22352	1
234	N	80.06748	76.90962	76.10254	585.53813	-424.79750	-105.81303	1
235	H	79.06955	77.03703	76.39071	959.88797	1327.56823	-2177.11905	1
236	H	80.48030	77.85225	75.89621	1578.48647	16.27378	-2220.76233	1

237	N	82.01604	75.41683	75.46178	-452.17763	-390.33541	-421.51853	1
238	H	82.50604	74.53192	75.34736	470.26107	1974.25629	-1817.92087	1
239	H	82.68581	76.14489	75.21369	1856.67307	-1573.97321	-1224.35416	1
240	C	77.64904	70.57445	78.78838	-531.47271	-581.45780	-55.06206	1
241	O	77.77105	71.21851	79.80853	-243.00837	192.73507	609.52485	1
242	N	77.99498	69.31307	78.55472	343.49288	-644.25607	38.09164	1
243	H	77.76984	68.99589	77.61129	-1691.16043	-1535.97525	-1484.73099	1
244	C	78.94363	68.57831	79.38818	542.66492	350.14337	454.42563	1
245	H	79.06102	67.60662	78.85123	1209.57979	-2396.95920	463.86744	1
246	C	80.24498	69.36269	79.44627	-737.14309	145.93010	242.71942	1
247	H	80.00932	70.36575	79.87024	-1050.18303	159.36419	-2509.06125	1
248	C	81.27541	68.69143	80.33333	-706.77696	-252.88343	-245.16230	1
249	H	82.22465	69.29125	80.40174	-1624.64039	-1665.49085	1417.86935	1
250	H	80.88278	68.55084	81.38815	2566.10521	598.51109	693.22305	1
251	H	81.55369	67.67246	79.94605	-1972.69758	107.10018	-1876.34312	1
252	C	80.83093	69.56789	78.06012	412.85148	672.58832	-27.69222	1
253	H	81.77829	70.17233	78.09151	1447.02277	1762.76533	-1490.78944	1
254	H	81.07981	68.58659	77.57016	1320.77379	-145.20455	2378.68491	1
255	H	80.11135	70.10353	77.38240	-1512.10848	1470.52031	1724.75147	1
256	C	78.24165	68.37474	80.87604	-607.11113	499.56689	73.73769	1
257	O	78.91433	68.25082	81.87990	357.97126	460.81534	356.68785	1
258	N	76.93043	68.26977	80.75244	536.55407	-368.62270	332.76306	1
259	H	76.55578	68.40764	79.81609	524.38866	2297.69985	1367.20941	1
260	C	76.13352	68.02979	81.89489	46.50277	-774.29190	-147.97904	1
261	H	76.84730	67.69395	82.68191	1676.51875	1883.29066	1032.55549	1
262	C	75.34250	69.38375	82.28682	-559.41456	-34.19198	-556.30433	1
263	H	74.60659	69.62177	81.48225	-64.66664	395.18769	2695.05373	1
264	H	74.73963	69.21835	83.21151	-2703.44278	-60.40056	333.79418	1
265	C	76.29912	70.53132	82.46717	-519.76435	377.31045	459.42366	1
266	H	76.88518	70.66946	81.51186	-1746.74323	1667.50644	-1261.73691	1
267	C	75.52148	71.81142	82.74648	570.95554	16.46261	-545.27700	1
268	H	76.20464	72.69006	82.87590	2391.58273	28.05277	-1305.07271	1
269	H	74.81878	72.05745	81.90869	175.75588	917.63458	2559.43867	1
270	H	74.90792	71.72655	83.68040	-1063.97851	-2155.34650	1283.00462	1
271	C	77.28118	70.26389	83.59710	193.76014	2.62946	-765.53141	1
272	H	77.89964	71.16932	83.83023	507.39394	-846.55087	2539.60089	1
273	H	76.75820	69.96593	84.54293	1337.57841	1818.19054	1526.01994	1
274	H	77.99761	69.43341	83.32282	1100.88635	-1172.91350	-2199.08909	1
275	C	74.99554	66.96562	81.47070	-549.21115	475.64486	-309.38218	1
276	O	74.58609	66.84934	80.34517	556.06106	-390.37755	-78.24250	1
277	O	74.37125	66.28032	82.53978	-572.27940	-310.19032	-209.75862	1
278	H	74.93887	66.61410	83.28909	-1380.08193	2212.14486	790.85944	1

Listing 11: C00011.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.8412	3365
		0.2500	300.00	0.00	0.00	0.00	-1294.1729	0.0000	300.0000
3	H	77.10411	73.37372	81.69057	-2043.14101	-1757.64893	399.89339		1
4	N	77.99704	73.74902	82.00846	426.75047	490.45733	-334.42467		1
5	H	78.51201	72.90672	82.29087	442.25559	-1110.30854	-2448.52907		1
6	C	78.70723	74.46890	81.02212	415.32972	-666.39213	83.73172		1
7	H	77.98589	74.76090	80.22733	879.32219	2491.00447	667.35213		1
8	C	79.40510	75.74283	81.72733	31.35357	477.41777	628.23362		1
9	H	79.87051	75.42510	82.69046	1168.38489	2240.25337	-1019.71136		1
10	H	80.23343	76.14703	81.09544	-360.43770	2534.90498	931.67112		1
11	C	78.34191	76.78379	81.95649	463.18208	512.70242	-382.34388		1
12	H	77.41065	76.26478	82.27868	1725.29117	1863.52247	-987.07854		1
13	C	78.75812	77.74318	83.06444	710.42801	-144.27427	-313.15367		1
14	H	77.97008	78.51533	83.26077	364.20195	-1033.13725	2494.72524		1
15	H	78.94251	77.20435	84.02969	2567.61904	335.80679	847.48802		1
16	H	79.70096	78.28967	82.80415	-2587.99029	680.92867	-512.16411		1

17	C	78.06022	77.56451	80.67947	268.17616	741.64379	-40.42634	1
18	H	77.24461	78.31837	80.82793	1283.54314	-1945.37420	-1411.27812	1
19	H	78.96683	78.12325	80.33102	-1258.57796	1317.15249	-2026.02085	1
20	H	77.74431	76.89334	79.84012	-2502.84526	909.80597	575.92391	1
21	C	79.85352	73.42632	80.53399	619.36578	-458.64843	-172.09273	1
22	O	80.09312	72.38269	81.10689	-81.40433	433.87611	522.34594	1
23	N	80.40253	73.92333	79.42258	175.23996	-622.20190	341.55523	1
24	H	80.12009	74.86623	79.15553	-876.57256	-303.22879	-2561.90213	1
25	C	81.67119	73.42021	79.01681	-571.88214	-534.10783	-106.15033	1
26	H	81.76847	72.43964	79.53740	-2713.20841	-16.25800	-248.80809	1
27	C	81.54513	73.31316	77.42037	166.60354	288.16399	-716.09568	1
28	H	81.15004	74.29995	77.05835	-2097.85574	1636.78449	-586.18044	1
29	O	80.58234	72.33737	76.96377	-317.80580	-363.38227	484.43082	1
30	H	79.85704	72.92347	76.67959	1863.74748	-1451.84923	1357.29467	1
31	C	82.99440	73.11972	76.85182	503.80731	517.99032	318.51606	1
32	H	82.99663	73.17148	75.73732	640.61020	-2157.10410	-1536.29104	1
33	H	83.71568	73.91484	77.21859	1687.88455	465.60692	2087.56452	1
34	H	83.41741	72.12683	77.13061	-1293.07895	-1899.88581	-1463.57452	1
35	C	82.75179	74.54008	79.49014	-153.07550	-733.68902	248.70981	1
36	O	82.38847	75.67119	79.68462	186.15459	-480.78787	-449.34387	1
37	N	83.98370	74.02546	79.56261	-487.53139	543.18517	42.03850	1
38	C	85.13340	74.87927	79.71822	-699.35871	69.34393	360.10701	1
39	H	84.91803	75.52578	80.59943	2.81126	-221.99807	-2715.58072	1
40	C	86.31873	73.84559	79.93435	-507.46439	-592.59194	122.07761	1
41	H	87.27838	74.20266	79.49733	-1975.08116	525.87560	-1801.71556	1
42	H	86.51631	73.68093	81.01701	1588.27743	-1913.22100	1113.83566	1
43	C	85.78846	72.54436	79.25817	-613.62442	-457.55993	-194.14490	1
44	H	85.89844	72.59189	78.15150	1707.54637	-721.27992	1996.92523	1
45	H	86.30678	71.61880	79.59593	758.23357	2100.81767	1560.55011	1
46	C	84.25788	72.60438	79.69340	-352.41524	704.96076	49.21465	1
47	H	83.55674	72.01582	79.05923	1714.76886	-2070.42778	443.35792	1
48	H	84.07443	72.35979	80.76735	1224.15040	1801.50881	1636.97633	1
49	C	85.35710	75.75612	78.36934	566.85117	537.05831	117.62814	1
50	O	85.02902	75.34406	77.25470	-550.26779	-406.08867	4.21666	1
51	N	85.98648	76.85518	78.70378	566.34832	-425.77725	180.18749	1
52	H	86.17002	76.97368	79.69947	644.44502	2646.80550	-52.73430	1
53	C	86.51274	77.78594	77.77421	612.34801	-281.48662	411.56221	1
54	H	87.09742	78.48491	78.41142	1667.23498	-1490.75142	1556.16753	1
55	C	87.43919	76.97646	76.74742	-714.45746	-175.43074	286.98927	1
56	H	86.83489	76.15502	76.26758	-787.09484	1763.03619	-1922.46060	1
57	O	88.58044	76.33217	77.34280	-429.46514	516.51932	-128.40526	1
58	H	88.39020	75.39363	77.14225	1981.82785	436.16847	-1818.18182	1
59	C	87.75797	78.06864	75.66394	630.79189	-468.94448	76.03230	1
60	H	88.42243	77.66369	74.86525	-1775.71861	2062.30353	131.89849	1
61	H	86.82959	78.43500	75.16176	-1855.14608	88.94118	1993.53760	1
62	H	88.27241	78.95255	76.10877	-1504.82350	-780.94249	-2132.90992	1
63	C	85.29392	78.57253	77.01063	288.57638	618.62814	-397.00270	1
64	O	85.24900	79.77469	77.10527	321.70495	-185.26452	574.37218	1
65	N	84.49383	77.76775	76.31998	-447.05792	-446.53431	367.76425	1
66	H	84.63182	76.72578	76.29800	350.31316	1975.63644	-1843.31522	1
67	C	83.62867	78.43194	75.39330	-511.23061	374.03917	-471.51480	1
68	H	83.20232	79.30260	75.94210	2234.79579	-898.70890	-1273.45190	1
69	C	84.55203	78.90286	74.17409	529.53781	-159.34528	563.72604	1
70	H	83.86202	79.39235	73.43802	654.59388	2347.94251	1217.51488	1
71	H	85.24363	79.71775	74.51596	-1526.55661	2103.42026	817.87394	1
72	O	85.35322	77.86989	73.52862	-554.84278	14.12789	399.58769	1
73	H	84.67619	77.16646	73.46509	1297.06236	2061.84854	1220.68812	1
74	C	82.55031	77.34166	74.84917	-662.15484	-412.13544	123.62687	1
75	O	82.86602	76.23352	74.48378	-540.01537	-317.05804	274.91456	1
76	N	81.35401	77.93776	74.75887	-202.76299	-690.00100	-131.49145	1
77	H	81.27151	78.89951	75.09040	-702.62132	-2617.37191	281.70413	1
78	C	80.21287	77.08170	74.86510	-491.73914	576.34187	222.73509	1

79	H	80.58431	76.11239	74.46075	1977.17978	-1823.58850	-434.68928	1
80	C	79.80832	76.97316	76.39702	-649.50797	-328.66843	306.11224	1
81	H	79.20421	77.85260	76.70710	2075.07803	1452.16490	-1004.45904	1
82	C	78.99009	75.65058	76.59190	-615.18735	-489.99689	-70.96352	1
83	H	78.92636	75.35650	77.66466	-1226.32661	-1724.38906	-1716.47170	1
84	H	77.94240	75.75093	76.22366	2381.64273	-969.84735	900.46860	1
85	H	79.45287	74.80072	76.03907	2122.74991	1702.23946	-141.36228	1
86	C	81.09465	76.88531	77.28826	-501.86074	-479.61276	-376.42482	1
87	H	80.84826	76.66630	78.35471	993.79261	-2246.95401	-1177.81305	1
88	H	81.79377	76.09124	76.93421	42.71279	-626.15391	-2651.37258	1
89	H	81.66911	77.84121	77.27466	-2026.39012	-1590.33709	-887.82922	1
90	C	79.02056	77.78776	73.99517	-672.89153	382.57394	-156.34072	1
91	O	79.14778	78.88784	73.50338	410.04627	221.86223	500.35950	1
92	N	77.97645	76.97310	73.96308	-378.11782	-443.79414	-441.10984	1
93	H	78.07344	76.10926	74.49140	2404.15973	-568.14894	1149.30085	1
94	C	76.86453	77.11272	73.07423	-544.54484	466.16019	331.29119	1
95	H	76.01915	76.91399	73.76822	-1409.80988	-170.17955	2325.32679	1
96	C	76.82253	78.57659	72.47541	-184.48284	116.78282	-758.89137	1
97	H	76.97499	79.32912	73.28558	1893.78641	1861.14652	611.04528	1
98	H	77.67437	78.71714	71.76893	-2170.79665	-974.19311	1327.50117	1
99	C	75.46455	78.83235	71.74660	389.51668	672.81878	-138.49152	1
100	H	75.27859	78.04674	70.97757	510.64577	1933.03327	1851.02484	1
101	H	74.61282	78.71841	72.45409	-2302.30869	-1105.72939	-948.89774	1
102	C	75.42055	80.25766	71.07573	-559.93427	-126.34590	542.30857	1
103	O	74.43804	80.60223	70.47048	-670.36003	-111.83166	76.36448	1
104	N	76.54484	80.98692	71.24837	-216.06729	-537.07037	446.51379	1
105	H	77.40821	80.76525	71.75775	-1251.96487	1074.12894	-2168.52500	1
106	H	76.67299	81.93417	70.87692	-2451.83023	-720.73851	944.84612	1
107	C	76.83225	76.01112	71.87361	546.24052	-563.88337	-85.11809	1
108	O	75.73191	75.84706	71.39960	71.70702	-307.40463	606.69673	1
109	N	77.97205	75.40884	71.50812	479.90863	-504.50129	222.86849	1
110	C	78.04379	74.65223	70.29003	75.51268	-600.91904	506.73700	1
111	H	77.38314	75.16835	69.55506	-2033.61562	1795.30103	254.89480	1
112	C	79.59860	74.68663	69.95040	523.79067	517.99274	284.45581	1
113	H	79.90952	73.85990	69.27292	1599.61665	-1127.00911	1895.98173	1
114	H	79.88846	75.63739	69.45027	-1881.83093	1275.82488	-1501.55016	1
115	C	80.22267	74.58606	71.37541	-600.05639	-404.05026	316.64485	1
116	H	80.18236	73.54248	71.76135	-2597.05260	496.36221	657.73249	1
117	H	81.28900	74.90324	71.42346	-1666.24518	1294.38985	-1723.90591	1
118	C	79.24988	75.54498	72.19121	493.57570	-129.95376	-602.56394	1
119	H	79.10598	75.25840	73.25751	-1469.08415	-637.84797	2204.22581	1
120	H	79.50471	76.63030	72.13170	-1038.97840	1068.88701	-2280.71789	1
121	C	77.60303	73.10316	70.51637	188.88100	241.05089	-727.87821	1
122	O	77.66610	72.31131	69.58434	531.88613	-49.19943	427.07960	1
123	N	77.18755	72.87036	71.75290	708.14833	26.93417	-179.73509	1
124	H	77.27112	73.70365	72.33040	-2232.69501	-1179.09831	1023.94816	1
125	C	77.15621	71.50700	72.31324	-738.32412	259.92548	104.42456	1
126	H	78.03803	71.02571	71.82679	2028.89123	1260.02983	1311.33324	1
127	C	77.22831	71.58923	73.82371	-258.65678	-345.52513	661.28459	1
128	H	76.29525	72.10323	74.17661	-1826.06090	-1801.46097	-918.64554	1
129	C	77.27493	70.20704	74.45051	-541.23400	531.92970	-218.41428	1
130	H	77.30394	70.25936	75.57341	1311.73218	-2219.18200	882.19023	1
131	H	76.37075	69.59748	74.16599	-1048.71298	1223.58118	-2196.97971	1
132	H	78.18388	69.63234	74.12196	419.06414	1903.92898	1903.44670	1
133	C	78.40617	72.40901	74.31909	-423.86431	152.66566	-648.55262	1
134	H	78.43295	72.44279	75.44173	105.68386	-2342.50080	1387.51238	1
135	H	79.38750	71.98126	73.97478	-1695.63603	-1484.73621	-1531.02793	1
136	H	78.35987	73.47124	73.95672	-1853.57121	-487.39031	1936.59343	1
137	C	75.72958	70.82487	71.84336	539.71428	-510.58232	267.58633	1
138	O	74.89667	70.51189	72.67946	-15.93758	-278.34085	-624.49402	1
139	N	75.73117	70.64884	70.54931	-676.81886	12.05292	276.17960	1
140	H	76.53658	71.02302	69.99382	-1694.44250	-373.84189	-2100.66098	1

141	C	74.62758	70.09479	69.84875	412.33078	-664.70360	108.35451	1
142	H	75.03453	69.94573	68.82308	1765.77476	1294.44366	1621.76594	1
143	C	74.17529	68.75008	70.55810	-179.66635	-721.95667	-264.73915	1
144	H	75.04746	68.08275	70.73753	-607.34922	2587.87032	-598.10018	1
145	H	73.74729	68.95869	71.56679	-359.69332	-1479.13954	-2259.74260	1
146	C	73.11774	68.06833	69.62987	-240.01076	616.02425	431.85322	1
147	H	72.27271	68.76287	69.42240	-1359.17131	782.54425	2227.99181	1
148	H	73.56322	67.82588	68.63924	-820.36667	85.81767	-2596.78715	1
149	C	72.59856	66.75620	70.34548	-513.07015	236.18570	-551.87280	1
150	H	73.44608	66.07781	70.59642	1816.11944	-1183.11722	-1650.94321	1
151	H	72.10776	66.99964	71.31582	-1800.04429	-1361.53473	1526.34643	1
152	C	71.60694	66.06256	69.38298	726.08972	-253.19732	-179.64713	1
153	H	70.68393	66.63997	69.17605	1224.27271	-456.51798	-2390.90304	1
154	H	72.05619	65.71539	68.43115	1206.40339	-1150.93514	-2154.90344	1
155	N	71.10610	64.75085	70.07746	329.70796	-633.68968	-155.67358	1
156	H	70.42769	64.16382	69.51130	1348.31305	1938.76845	1359.00643	1
157	H	71.84165	64.02892	70.33105	2096.92035	1446.54551	-966.48890	1
158	H	70.57772	64.85570	70.99205	-1197.07217	-2303.53719	827.28733	1
159	C	73.35175	71.12678	69.83682	-378.01186	-556.17301	-413.96481	1
160	O	72.83440	71.39400	68.77851	-409.44433	-307.55053	-453.30833	1
161	N	72.96976	71.50956	71.04927	-429.02477	524.70884	274.08502	1
162	H	73.44836	71.16681	71.91049	1706.34263	-1425.96036	1574.38926	1
163	C	71.80832	72.36356	71.05679	-45.25864	-626.22952	478.93267	1
164	H	72.07452	73.06460	70.23231	1988.63164	570.90773	1772.87287	1
165	C	70.57398	71.46261	70.64481	551.77128	-20.49526	-564.54996	1
166	H	70.82884	70.85126	69.74667	1434.61535	-1753.10253	1513.99471	1
167	H	70.31270	70.74161	71.45191	-714.67738	1819.09770	1898.36494	1
168	C	69.39133	72.44229	70.35067	446.99263	-555.77305	338.97221	1
169	H	69.15246	73.02424	71.26890	1953.68466	1892.25957	-161.67766	1
170	H	69.68313	73.18975	69.57931	-403.03785	2688.07032	-188.43591	1
171	C	68.12904	71.62058	69.86846	567.86262	335.74681	434.04421	1
172	H	68.35702	71.04290	68.94335	-1080.02275	1568.26081	-1948.78900	1
173	H	67.81988	70.86909	70.63046	-919.54108	2111.34692	1456.13463	1
174	C	67.00710	72.65497	69.61638	195.81897	173.33862	-745.11536	1
175	H	66.66830	73.19500	70.52149	1405.67949	-2301.21089	-390.08113	1
176	H	67.22209	73.37876	68.80498	-940.37328	-1118.32446	2299.72133	1
177	N	65.74097	71.87782	69.12328	319.26422	656.36007	-42.02424	1
178	H	64.88891	72.47600	68.91904	1961.03633	619.91968	1787.09422	1
179	H	65.83466	71.33572	68.21543	854.14343	-2156.80752	1429.08711	1
180	H	65.33256	71.14682	69.77558	1237.02905	-1378.50857	-1998.28500	1
181	C	71.63775	73.07288	72.51308	532.53319	-268.57236	517.55729	1
182	O	70.62757	72.90077	73.19114	266.16714	-290.73804	-558.88002	1
183	N	72.65675	73.86913	72.73588	-226.25352	640.49678	-270.32839	1
184	H	73.40012	73.86156	72.03961	2007.69063	-1035.27229	1523.50231	1
185	C	72.82641	74.47609	74.02126	-540.76542	-573.33303	49.50000	1
186	H	72.52987	73.66002	74.71760	-2374.20950	-1036.76023	843.75774	1
187	C	74.34373	74.93251	74.11103	-77.09082	666.87422	-415.84136	1
188	H	74.50395	75.71681	73.31963	-985.81834	617.19825	2463.91927	1
189	O	75.32539	73.89955	73.83997	293.29899	-391.65602	-477.80926	1
190	H	75.64768	74.18447	72.95920	2528.72714	-681.76262	-751.27122	1
191	C	74.45487	75.57134	75.54284	252.47363	-605.14473	440.05134	1
192	H	75.46571	76.00880	75.71577	-2052.65063	1456.49051	-1043.51830	1
193	H	73.71018	76.38909	75.69970	-2152.98800	-1661.97574	-161.70652	1
194	H	74.28511	74.80961	76.33917	-473.12726	-1584.27339	2165.61725	1
195	C	71.81497	75.75691	74.12742	360.36307	488.46713	505.10056	1
196	O	72.23376	76.89092	74.13150	-200.08817	-528.03552	-385.82850	1
197	N	70.56036	75.33433	74.24402	-597.54095	-226.44775	355.20479	1
198	H	70.31347	74.31731	74.16107	2179.23655	-1300.70981	-991.33835	1
199	C	69.58442	76.33187	74.46668	-687.68921	297.39807	-249.45179	1
200	H	70.12685	77.30567	74.53498	-349.16256	-2467.37713	-1101.72831	1
201	C	68.50314	76.25320	73.27981	672.47345	361.54328	-201.62880	1
202	H	68.07921	75.22627	73.24233	1541.41502	582.18425	2169.97026	1

203	H	67.65674	76.94623	73.48846	-2534.67717	60.25153	997.72295	1
204	C	69.17281	76.60016	71.94511	574.26774	-389.43119	-377.02542	1
205	C	69.01294	77.88977	71.35343	688.82679	-287.33580	-257.96133	1
206	H	68.41302	78.67069	71.85422	331.14182	1470.38163	2269.80013	1
207	C	69.98014	75.61392	71.30144	-383.52382	-675.04808	144.24917	1
208	H	70.14460	74.63381	71.78454	4.09847	1517.59662	2262.86397	1
209	C	69.62953	78.14228	70.12845	-134.76730	428.45285	-649.50303	1
210	H	69.50861	79.14077	69.67290	-903.23433	1600.49020	2011.53387	1
211	C	70.57543	75.91034	70.07369	-335.53281	-615.00040	-364.39058	1
212	H	71.19499	75.13468	69.59009	1596.45398	-1369.33862	1732.02659	1
213	C	70.41640	77.17574	69.43646	585.48547	-340.24194	-406.23938	1
214	O	70.99712	77.48537	68.17920	-419.15649	-173.04408	-511.94141	1
215	H	71.52053	76.66260	68.02946	-1071.84350	1559.71507	-1960.13012	1
216	C	68.73430	75.89346	75.79657	291.41878	-183.13091	710.72246	1
217	O	68.24351	74.78141	75.91536	379.87695	523.47396	-222.23622	1
218	N	68.58796	76.94637	76.58142	564.30591	373.09380	277.24371	1
219	H	69.03899	77.80889	76.28167	-120.59931	-2436.07824	-1214.35098	1
220	C	68.19878	76.75682	77.94753	404.07514	-299.37480	608.84009	1
221	H	68.55958	75.72934	78.18035	-1071.07882	-841.69025	2359.66467	1
222	C	68.88630	77.91020	78.78105	-683.12807	68.71770	-390.13096	1
223	H	69.98617	77.92013	78.60737	2068.88918	1596.58590	770.89603	1
224	H	68.52081	78.90389	78.43670	1379.86429	2342.49779	-179.85638	1
225	C	68.56559	77.70564	80.29521	-176.39967	537.49466	550.97268	1
226	H	67.45924	77.63334	80.45422	-396.28051	1942.22168	1869.33314	1
227	H	68.99230	76.75029	80.67501	-94.44700	586.00678	-2659.20016	1
228	C	69.17079	78.96228	81.07317	-291.69381	-718.18079	-150.72929	1
229	H	70.28596	79.06257	81.05612	-2303.38776	1089.76242	964.62032	1
230	H	68.73082	79.95200	80.78825	884.16729	2568.80533	-207.74283	1
231	N	68.77355	78.68768	82.39031	-594.49522	-252.81478	342.29276	1
232	H	68.13720	77.91634	82.52085	-1735.17426	2084.05705	-263.71605	1
233	C	69.14334	79.34721	83.41243	595.23177	-271.52487	442.22352	1
234	N	70.01730	80.42189	83.21642	585.53813	-424.79750	-105.81303	1
235	H	70.40962	80.78661	82.34939	959.88797	1327.56823	-2177.11905	1
236	H	70.37302	81.02836	83.95610	1578.48647	16.27378	-2220.76233	1
237	N	68.56446	78.83003	84.57998	-452.17763	-390.33541	-421.51853	1
238	H	67.92276	78.05074	84.71785	470.26107	1974.25629	-1817.92087	1
239	H	68.73106	79.22173	85.50760	1856.67307	-1573.97321	-1224.35416	1
240	C	66.57319	76.84388	78.04372	-531.47271	-581.45780	-55.06206	1
241	O	66.00416	77.37763	78.97152	-243.00837	192.73507	609.52485	1
242	N	66.04308	76.18281	77.02409	343.49288	-644.25607	38.09164	1
243	H	66.67571	75.73908	76.33669	-1691.16043	-1535.97525	-1484.73099	1
244	C	64.63788	76.33521	76.78808	542.66492	350.14337	454.42563	1
245	H	64.21938	76.21571	77.81272	1209.57979	-2396.95920	463.86744	1
246	C	64.31668	77.77757	76.21134	-737.14309	145.93010	242.71942	1
247	H	64.80660	77.92134	75.22446	-1050.18303	159.36419	-2509.06125	1
248	C	62.75846	77.89422	76.09289	-706.77696	-252.88343	-245.16230	1
249	H	62.44658	78.89765	75.71911	-1624.64039	-1665.49085	1417.86935	1
250	H	62.34796	77.13146	75.38548	2566.10521	598.51109	693.22305	1
251	H	62.25887	77.73797	77.07785	-1972.69758	107.10018	-1876.34312	1
252	C	64.76494	78.89729	77.21591	412.85148	672.58832	-27.69222	1
253	H	64.41902	79.90678	76.88835	1447.02277	1762.76533	-1490.78944	1
254	H	64.35077	78.71891	78.23850	1320.77379	-145.20455	2378.68491	1
255	H	65.87653	78.94292	77.31133	-1512.10848	1470.52031	1724.75147	1
256	C	64.24437	75.15941	75.73194	-607.11113	499.56689	73.73769	1
257	O	63.57421	75.36641	74.74158	357.97126	460.81534	356.68785	1
258	N	64.75507	74.00952	76.16233	536.55407	-368.62270	332.76306	1
259	H	65.30597	74.00724	77.02110	524.38866	2297.69985	1367.20941	1
260	C	64.44422	72.82006	75.46448	46.50277	-774.29190	-147.97904	1
261	H	63.66514	73.11131	74.72282	1676.51875	1883.29066	1032.55549	1
262	C	65.79411	72.24920	74.77810	-559.41456	-34.19198	-556.30433	1
263	H	66.52819	71.97381	75.57292	-64.66664	395.18769	2695.05373	1
264	H	65.57527	71.30678	74.22218	-2703.44278	-60.40056	333.79418	1

265	C	66.38268	73.28828	73.86528	-519.76435	377.31045	459.42366	1
266	H	66.62378	74.19003	74.47729	-1746.74323	1667.50644	-1261.73691	1
267	C	67.66618	72.77031	73.22844	570.95554	16.46261	-545.27700	1
268	H	68.03932	73.46710	72.43416	2391.58273	28.05277	-1305.07271	1
269	H	68.49580	72.66003	73.97836	175.75588	917.63458	2559.43867	1
270	H	67.51638	71.76999	72.74670	-1063.97851	-2155.34650	1283.00462	1
271	C	65.40501	73.70793	72.77676	193.76014	2.62946	-765.53141	1
272	H	65.87546	74.42234	72.05338	507.39394	-846.55087	2539.60089	1
273	H	65.03573	72.83007	72.18584	1337.57841	1818.19054	1526.01994	1
274	H	64.50734	74.23060	73.21739	1100.88635	-1172.91350	-2199.08909	1
275	C	63.97463	71.71445	76.54246	-549.21115	475.64486	-309.38218	1
276	O	64.13322	71.82615	77.72961	556.06106	-390.37755	-78.24250	1
277	O	63.43517	70.52467	75.99603	-572.27940	-310.19032	-209.75862	1
278	H	63.45086	70.77816	75.03216	-1380.08193	2212.14486	790.85944	1

Listing 12: C00012.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1294.1313	0.0000	300.0000
3	H	72.22800	83.22922	77.91478	-2043.14101	-1757.64893	399.89339		1
4	N	73.05475	82.87942	77.42850	426.75047	490.45733	-334.42467		1
5	H	72.67606	82.41107	76.58675	442.25559	-1110.30854	-2448.52907		1
6	C	73.97302	83.89811	77.09135	415.32972	-666.39213	83.73172		1
7	H	73.69882	84.81006	77.66589	879.32219	2491.00447	667.35213		1
8	C	75.47375	83.39081	77.39992	31.35357	477.41777	628.23362		1
9	H	75.68965	82.47917	76.79403	1168.38489	2240.25337	-1019.71136		1
10	H	76.22244	84.15419	77.07955	-360.43770	2534.90498	931.67112		1
11	C	75.59409	83.09545	78.87074	463.18208	512.70242	-382.34388		1
12	H	74.70517	82.50045	79.18068	1725.29117	1863.52247	-987.07854		1
13	C	76.84718	82.27629	79.15420	710.42801	-144.27427	-313.15367		1
14	H	76.94981	82.04341	80.24530	364.20195	-1033.13725	2494.72524		1
15	H	76.84252	81.29693	78.60868	2567.61904	335.80679	847.48802		1
16	H	77.77459	82.82326	78.84455	-2587.99029	680.92867	-512.16411		1
17	C	75.62802	84.37814	79.69148	268.17616	741.64379	-40.42634		1
18	H	75.72659	84.16476	80.78704	1283.54314	-1945.37420	-1411.27812		1
19	H	76.49204	85.03021	79.40260	-1258.57796	1317.15249	-2026.02085		1
20	H	74.69546	84.98355	79.55549	-2502.84526	909.80597	575.92391		1
21	C	73.74348	84.00209	75.49012	619.36578	-458.64843	-172.09273		1
22	O	73.02744	83.18213	74.92449	-81.40433	433.87611	522.34594		1
23	N	74.44879	84.99947	74.97420	175.23996	-622.20190	341.55523		1
24	H	75.00105	85.57891	75.60693	-876.57256	-303.22879	-2561.90213		1
25	C	74.57326	85.12414	73.56866	-571.88214	-534.10783	-106.15033		1
26	H	73.89865	84.33417	73.16119	-2713.20841	-16.25800	-248.80809		1
27	C	74.19591	86.62868	73.15513	166.60354	288.16399	-716.09568		1
28	H	75.00031	87.30755	73.55269	-2097.85574	1636.78449	-586.18044		1
29	O	72.94525	87.12348	73.65827	-317.80580	-363.38227	484.43082		1
30	H	73.24546	87.86134	74.22717	1863.74748	-1451.84923	1357.29467		1
31	C	74.30611	86.55874	71.58789	503.80731	517.99032	318.51606		1
32	H	74.14849	87.56059	71.12477	640.61020	-2157.10410	-1536.29104		1
33	H	75.30825	86.19249	71.25688	1687.88455	465.60692	2087.56452		1
34	H	73.54150	85.87100	71.15676	-1293.07895	-1899.88581	-1463.57452		1
35	C	76.16688	84.94766	73.22910	-153.07550	-733.68902	248.70981		1
36	O	76.80036	85.93891	72.96930	186.15459	-480.78787	-449.34387		1
37	N	76.58479	83.67738	73.31952	-487.53139	543.18517	42.03850		1
38	C	77.95999	83.32215	73.15354	-699.35871	69.34393	360.10701		1
39	H	78.55698	84.20482	73.47950	2.81126	-221.99807	-2715.58072		1
40	C	78.03494	82.02109	74.06018	-507.46439	-592.59194	122.07761		1
41	H	78.93561	81.40090	73.85609	-1975.08116	525.87560	-1801.71556		1
42	H	78.05462	82.27760	75.14272	1588.27743	-1913.22100	1113.83566		1
43	C	76.69729	81.31589	73.66485	-613.62442	-457.55993	-194.14490		1
44	H	76.80557	80.78712	72.68752	1707.54637	-721.27992	1996.92523		1

45	H	76.36159	80.55308	74.40530	758.23357	2100.81767	1560.55011	1
46	C	75.69694	82.54270	73.53177	-352.41524	704.96076	49.21465	1
47	H	75.01758	82.50561	72.63245	1714.76886	-2070.42778	443.35792	1
48	H	75.10177	82.77314	74.45036	1224.15040	1801.50881	1636.97633	1
49	C	78.16001	82.94289	71.56645	566.85117	537.05831	117.62814	1
50	O	78.26157	81.76756	71.22646	-550.26779	-406.08867	4.21666	1
51	N	78.17274	84.04515	70.85978	566.34832	-425.77725	180.18749	1
52	H	78.00728	84.89367	71.40940	644.44502	2646.80550	-52.73430	1
53	C	78.37813	84.12521	69.46200	612.34801	-281.48662	411.56221	1
54	H	78.52380	85.21293	69.27815	1667.23498	-1490.75142	1556.16753	1
55	C	79.65293	83.23767	69.06333	-714.45746	-175.43074	286.98927	1
56	H	79.49984	82.18955	69.45024	-787.09484	1763.03619	-1922.46060	1
57	O	80.91561	83.67607	69.58896	-429.46514	516.51932	-128.40526	1
58	H	81.15435	82.91881	70.16208	1981.82785	436.16847	-1818.18182	1
59	C	79.50237	83.23566	67.49842	630.79189	-468.94448	76.03230	1
60	H	80.19984	82.51093	67.01728	-1775.71861	2062.30353	131.89849	1
61	H	78.45893	82.96281	67.19332	-1855.14608	88.94118	1993.53760	1
62	H	79.71912	84.24098	67.06771	-1504.82350	-780.94249	-2132.90992	1
63	C	77.07122	83.55448	68.65057	288.57638	618.62814	-397.00270	1
64	O	76.62722	84.21528	67.74082	321.70495	-185.26452	574.37218	1
65	N	76.74108	82.32247	69.02689	-447.05792	-446.53431	367.76425	1
66	H	77.25417	81.85775	69.81417	350.31316	1975.63644	-1843.31522	1
67	C	75.44684	81.87392	68.62746	-511.23061	374.03917	-471.51480	1
68	H	75.10881	82.69587	67.95046	2234.79579	-898.70890	-1273.45190	1
69	C	75.69232	80.49666	67.85014	529.53781	-159.34528	563.72604	1
70	H	74.74838	80.24712	67.29511	654.59388	2347.94251	1217.51488	1
71	H	76.47903	80.70230	67.07765	-1526.55661	2103.42026	817.87394	1
72	O	76.05463	79.33640	68.65469	-554.84278	14.12789	399.58769	1
73	H	76.99558	79.54083	68.80566	1297.06236	2061.84854	1220.68812	1
74	C	74.53913	81.77244	69.97365	-662.15484	-412.13544	123.62687	1
75	O	74.42420	82.71802	70.72747	-540.01537	-317.05804	274.91456	1
76	N	73.85783	80.62272	70.00418	-202.76299	-690.00100	-131.49145	1
77	H	74.14645	79.91801	69.31929	-702.62132	-2617.37191	281.70413	1
78	C	73.38157	80.22113	71.29083	-491.73914	576.34187	222.73509	1
79	H	73.26547	81.15899	71.88106	1977.17978	-1823.58850	-434.68928	1
80	C	72.03786	79.41007	71.06251	-649.50797	-328.66843	306.11224	1
81	H	72.17537	78.62805	70.28491	2075.07803	1452.16490	-1004.45904	1
82	C	71.58855	78.76585	72.41860	-615.18735	-489.99689	-70.96352	1
83	H	70.61182	78.23603	72.31723	-1226.32661	-1724.38906	-1716.47170	1
84	H	72.33517	78.01227	72.77545	2381.64273	-969.84735	900.46860	1
85	H	71.47433	79.53064	73.22238	2122.74991	1702.23946	-141.36228	1
86	C	70.92912	80.42685	70.62170	-501.86074	-479.61276	-376.42482	1
87	H	69.95823	79.91651	70.41955	993.79261	-2246.95401	-1177.81305	1
88	H	70.74530	81.19669	71.40745	42.71279	-626.15391	-2651.37258	1
89	H	71.22451	80.96741	69.69180	-2026.39012	-1590.33709	-887.82922	1
90	C	74.51102	79.20374	71.91741	-672.89153	382.57394	-156.34072	1
91	O	74.99328	79.43213	73.00412	410.04627	221.86223	500.35950	1
92	N	74.74223	78.20232	71.08517	-378.11782	-443.79414	-441.10984	1
93	H	74.24051	78.20483	70.20000	2404.15973	-568.14894	1149.30085	1
94	C	75.54029	77.07462	71.47260	-544.54484	466.16019	331.29119	1
95	H	75.53670	76.48741	70.52513	-1409.80988	-170.17955	2325.32679	1
96	C	76.97724	77.70490	71.77078	-184.48284	116.78282	-758.89137	1
97	H	77.00597	78.74241	71.36871	1893.78641	1861.14652	611.04528	1
98	H	77.16618	77.80346	72.86411	-2170.79665	-974.19311	1327.50117	1
99	C	78.05524	76.83031	71.06300	389.51668	672.81878	-138.49152	1
100	H	78.04025	75.78362	71.43539	510.64577	1933.03327	1851.02484	1
101	H	77.80512	76.72932	69.98364	-2302.30869	-1105.72939	-948.89774	1
102	C	79.51300	77.41087	71.20821	-559.93427	-126.34590	542.30857	1
103	O	80.45203	76.73731	70.87251	-670.36003	-111.83166	76.36448	1
104	N	79.56450	78.67701	71.67777	-216.06729	-537.07037	446.51379	1
105	H	78.81015	79.33869	71.89659	-1251.96487	1074.12894	-2168.52500	1
106	H	80.43432	79.21547	71.75056	-2451.83023	-720.73851	944.84612	1

107	C	74.68598	76.33309	72.60660	546.24052	-563.88337	-85.11809	1
108	O	73.47401	76.18807	72.41280	71.70702	-307.40463	606.69673	1
109	N	75.39569	75.78947	73.58347	479.90863	-504.50129	222.86849	1
110	C	74.70043	75.21822	74.70701	75.51268	-600.91904	506.73700	1
111	H	73.66086	75.00909	74.36051	-2033.61562	1795.30103	254.89480	1
112	C	75.58863	73.94395	75.02254	523.79067	517.99274	284.45581	1
113	H	75.44927	73.56948	76.06310	1599.61665	-1127.00911	1895.98173	1
114	H	75.34191	73.10016	74.33943	-1881.83093	1275.82488	-1501.55016	1
115	C	77.02120	74.51404	74.75351	-600.05639	-404.05026	316.64485	1
116	H	77.33360	75.20784	75.56998	-2597.05260	496.36221	657.73249	1
117	H	77.82494	73.73981	74.65779	-1666.24518	1294.38985	-1723.90591	1
118	C	76.76629	75.30450	73.40510	493.57570	-129.95376	-602.56394	1
119	H	77.44196	76.17736	73.25422	-1469.08415	-637.84797	2204.22581	1
120	H	76.75029	74.67367	72.48594	-1038.97840	1068.88701	-2280.71789	1
121	C	74.74472	76.14642	76.05211	188.88100	241.05089	-727.87821	1
122	O	74.04638	75.80970	77.01225	531.88613	-49.19943	427.07960	1
123	N	75.64811	77.10419	76.00018	708.14833	26.93417	-179.73509	1
124	H	76.06016	77.09303	75.06734	-2232.69501	-1179.09831	1023.94816	1
125	C	75.71511	78.26701	76.86691	-738.32412	259.92548	104.42456	1
126	H	76.42089	78.94158	76.32616	2028.89123	1260.02983	1311.33324	1
127	C	74.31574	78.85250	76.99152	-258.65678	-345.52513	661.28459	1
128	H	73.63702	78.02954	77.31486	-1826.06090	-1801.46097	-918.64554	1
129	C	74.25605	79.95690	78.02996	-541.23400	531.92970	-218.41428	1
130	H	73.21004	80.34816	78.16655	1311.73218	-2219.18200	882.19023	1
131	H	74.61969	79.60469	79.03521	-1048.71298	1223.58118	-2196.97971	1
132	H	74.89465	80.83236	77.73356	419.06414	1903.92898	1903.44670	1
133	C	73.80844	79.37280	75.65908	-423.86431	152.66566	-648.55262	1
134	H	72.72217	79.66002	75.70616	105.68386	-2342.50080	1387.51238	1
135	H	74.37486	80.28546	75.32429	-1695.63603	-1484.73621	-1531.02793	1
136	H	73.92037	78.60183	74.84441	-1853.57121	-487.39031	1936.59343	1
137	C	76.32240	77.85194	78.36607	539.71428	-510.58232	267.58633	1
138	O	77.16319	78.56792	78.84143	-15.93758	-278.34085	-624.49402	1
139	N	75.74025	76.78949	78.88514	-676.81886	12.05292	276.17960	1
140	H	74.96214	76.30404	78.36981	-1694.44250	-373.84189	-2100.66098	1
141	C	76.14471	76.36884	80.17998	412.33078	-664.70360	108.35451	1
142	H	76.99397	77.03947	80.45777	1765.77476	1294.44366	1621.76594	1
143	C	74.88180	76.53163	81.13328	-179.66635	-721.95667	-264.73915	1
144	H	74.39476	77.52072	80.98500	-607.34922	2587.87032	-598.10018	1
145	H	74.10842	75.77651	80.86911	-359.69332	-1479.13954	-2259.74260	1
146	C	75.34599	76.35090	82.61399	-240.01076	616.02425	431.85322	1
147	H	76.01690	75.45472	82.69829	-1359.17131	782.54425	2227.99181	1
148	H	75.95099	77.22170	82.95392	-820.36667	85.81767	-2596.78715	1
149	C	74.07395	76.14801	83.53319	-513.07015	236.18570	-551.87280	1
150	H	73.45722	77.07462	83.57842	1816.11944	-1183.11722	-1650.94321	1
151	H	73.40703	75.35825	83.11721	-1800.04429	-1361.53473	1526.34643	1
152	C	74.58283	75.74042	84.93535	726.08972	-253.19732	-179.64713	1
153	H	75.13909	74.78187	84.96136	1224.27271	-456.51798	-2390.90304	1
154	H	75.15864	76.52517	85.46513	1206.40339	-1150.93514	-2154.90344	1
155	N	73.33286	75.48261	85.84294	329.70796	-633.68968	-155.67358	1
156	H	73.54570	75.17379	86.83525	1348.31305	1938.76845	1359.00643	1
157	H	72.68023	76.30163	86.01524	2096.92035	1446.54551	-966.48890	1
158	H	72.65829	74.72473	85.53104	-1197.07217	-2303.53719	827.28733	1
159	C	76.50774	74.77604	80.19456	-378.01186	-556.17301	-413.96481	1
160	O	76.66871	74.18743	81.24692	-409.44433	-307.55053	-453.30833	1
161	N	76.53011	74.21285	78.96134	-429.02477	524.70884	274.08502	1
162	H	76.59556	74.98613	78.29949	1706.34263	-1425.96036	1574.38926	1
163	C	77.34451	73.00201	78.91075	-45.25864	-626.22952	478.93267	1
164	H	78.17289	73.29196	79.59501	1988.63164	570.90773	1772.87287	1
165	C	76.47858	71.83300	79.51645	551.77128	-20.49526	-564.54996	1
166	H	75.92375	72.19315	80.41473	1434.61535	-1753.10253	1513.99471	1
167	H	75.69663	71.51020	78.79135	-714.67738	1819.09770	1898.36494	1
168	C	77.42317	70.64066	79.89425	446.99263	-555.77305	338.97221	1

169	H	78.09785	70.37520	79.05034	1953.68466	1892.25957	-161.67766	1
170	H	78.09126	70.90946	80.74274	-403.03785	2688.07032	-188.43591	1
171	C	76.48532	69.42356	80.26417	567.86262	335.74681	434.04421	1
172	H	75.94032	69.62044	81.21605	-1080.02275	1568.26081	-1948.78900	1
173	H	75.69864	69.28456	79.48624	-919.54108	2111.34692	1456.13463	1
174	C	77.35492	68.14898	80.37442	195.81897	173.33862	-745.11536	1
175	H	77.74649	67.77731	79.40668	1405.67949	-2301.21089	-390.08113	1
176	H	78.17524	68.20668	81.11764	-940.37328	-1118.32446	2299.72133	1
177	N	76.41907	67.01374	80.90924	319.26422	656.36007	-42.02424	1
178	H	76.84054	66.04789	81.03968	1961.03633	619.91968	1787.09422	1
179	H	75.99145	67.17910	81.86497	854.14343	-2156.80752	1429.08711	1
180	H	75.55951	66.80013	80.32535	1237.02905	-1378.50857	-1998.28500	1
181	C	77.82392	72.80819	77.38518	532.53319	-268.57236	517.55729	1
182	O	78.38482	73.73172	76.85118	266.16714	-290.73804	-558.88002	1
183	N	77.64880	71.55531	76.93265	-226.25352	640.49678	-270.32839	1
184	H	77.13997	70.85088	77.51793	2007.69063	-1035.27229	1523.50231	1
185	C	77.31433	71.40887	75.53623	-540.76542	-573.33303	49.50000	1
186	H	76.98745	72.40321	75.16344	-2374.20950	-1036.76023	843.75774	1
187	C	78.63547	70.93352	74.77558	-77.09082	666.87422	-415.84136	1
188	H	79.20533	70.26918	75.47816	-985.81834	617.19825	2463.91927	1
189	O	79.51301	72.02063	74.41521	293.29899	-391.65602	-477.80926	1
190	H	80.24633	71.88768	75.04455	2528.72714	-681.76262	-751.27122	1
191	C	78.14156	70.07734	73.55401	252.47363	-605.14473	440.05134	1
192	H	78.99997	69.62554	73.00471	-2052.65063	1456.49051	-1043.51830	1
193	H	77.46808	69.23831	73.86446	-2152.98800	-1661.97574	-161.70652	1
194	H	77.58202	70.70295	72.82056	-473.12726	-1584.27339	2165.61725	1
195	C	76.12039	70.32280	75.66118	360.36307	488.46713	505.10056	1
196	O	75.93292	69.77984	76.74592	-200.08817	-528.03552	-385.82850	1
197	N	75.46317	70.19500	74.52457	-597.54095	-226.44775	355.20479	1
198	H	75.77223	70.73659	73.71888	2179.23655	-1300.70981	-991.33835	1
199	C	74.40538	69.24583	74.39537	-687.68921	297.39807	-249.45179	1
200	H	73.72066	69.41987	75.25506	-349.16256	-2467.37713	-1101.72831	1
201	C	73.75664	69.45291	72.94891	672.47345	361.54328	-201.62880	1
202	H	74.53800	69.35195	72.16092	1541.41502	582.18425	2169.97026	1
203	H	72.99685	68.65947	72.76222	-2534.67717	60.25153	997.72295	1
204	C	73.11464	70.84624	72.90073	574.26774	-389.43119	-377.02542	1
205	C	71.82584	71.03733	73.47702	688.82679	-287.33580	-257.96133	1
206	H	71.27987	70.19306	73.93641	331.14182	1470.38163	2269.80013	1
207	C	73.81305	71.94254	72.31421	-383.52382	-675.04808	144.24917	1
208	H	74.81206	71.80228	71.86272	4.09847	1517.59662	2262.86397	1
209	C	71.27921	72.31602	73.45642	-134.76730	428.45285	-649.50303	1
210	H	70.28118	72.46034	73.90508	-903.23433	1600.49020	2011.53387	1
211	C	73.20697	73.19826	72.32722	-335.53281	-615.00040	-364.39058	1
212	H	73.76070	74.03517	71.86411	1596.45398	-1369.33862	1732.02659	1
213	C	71.92930	73.44576	72.89739	585.48547	-340.24194	-406.23938	1
214	O	71.32595	74.69979	72.92911	-419.15649	-173.04408	-511.94141	1
215	H	72.14642	75.32283	72.70952	-1071.84350	1559.71507	-1960.13012	1
216	C	75.03338	67.74869	74.39419	291.41878	-183.13091	710.72246	1
217	O	76.06640	67.45271	73.84053	379.87695	523.47396	-222.23622	1
218	N	74.11215	66.92284	74.92282	564.30591	373.09380	277.24371	1
219	H	73.30686	67.34168	75.39405	-120.59931	-2436.07824	-1214.35098	1
220	C	74.64901	65.68802	75.42708	404.07514	-299.37480	608.84009	1
221	H	75.38693	65.41941	74.63564	-1071.07882	-841.69025	2359.66467	1
222	C	75.35607	65.98184	76.81150	-683.12807	68.71770	-390.13096	1
223	H	75.99717	66.89162	76.75218	2068.88918	1596.58590	770.89603	1
224	H	74.60173	66.19208	77.60365	1379.86429	2342.49779	-179.85638	1
225	C	76.19318	64.70867	77.14955	-176.39967	537.49466	550.97268	1
226	H	75.54682	63.79833	77.11141	-396.28051	1942.22168	1869.33314	1
227	H	76.99722	64.54366	76.39792	-94.44700	586.00678	-2659.20016	1
228	C	76.80221	64.90519	78.61335	-291.69381	-718.18079	-150.72929	1
229	H	77.48640	65.77857	78.75413	-2303.38776	1089.76242	964.62032	1
230	H	76.02563	64.91469	79.42003	884.16729	2568.80533	-207.74283	1

231	N	77.54179	63.72325	78.75263	-594.49522	-252.81478	342.29276	1
232	H	77.23468	62.93529	78.20229	-1735.17426	2084.05705	-263.71605	1
233	C	78.53211	63.56434	79.53551	595.23177	-271.52487	442.22352	1
234	N	78.93864	64.65027	80.31641	585.53813	-424.79750	-105.81303	1
235	H	78.56513	65.59703	80.36519	959.88797	1327.56823	-2177.11905	1
236	H	79.71331	64.63010	80.98045	1578.48647	16.27378	-2220.76233	1
237	N	79.02462	62.25530	79.44485	-452.17763	-390.33541	-421.51853	1
238	H	78.72611	61.46647	78.87303	470.26107	1974.25629	-1817.92087	1
239	H	79.81732	61.91680	79.99136	1856.67307	-1573.97321	-1224.35416	1
240	C	73.42630	64.62170	75.62482	-531.47271	-581.45780	-55.06206	1
241	O	73.45859	63.81934	76.53797	-243.00837	192.73507	609.52485	1
242	N	72.58121	64.69588	74.60997	343.49288	-644.25607	38.09164	1
243	H	72.79159	65.42873	73.93348	-1691.16043	-1535.97525	-1484.73099	1
244	C	71.39225	63.91994	74.54729	542.66492	350.14337	454.42563	1
245	H	71.18553	63.89565	73.45465	1209.57979	-2396.95920	463.86744	1
246	C	71.62924	62.49301	75.19549	-737.14309	145.93010	242.71942	1
247	H	71.85684	62.59014	76.28974	-1050.18303	159.36419	-2509.06125	1
248	C	70.35080	61.61023	74.97734	-706.77696	-252.88343	-245.16230	1
249	H	70.49357	60.57827	75.37570	-1624.64039	-1665.49085	1417.86935	1
250	H	69.46346	62.04669	75.49800	2566.10521	598.51109	693.22305	1
251	H	70.09285	61.51727	73.89661	-1972.69758	107.10018	-1876.34312	1
252	C	72.81035	61.78473	74.44281	412.85148	672.58832	-27.69222	1
253	H	73.00508	60.76439	74.84779	1447.02277	1762.76533	-1490.78944	1
254	H	72.59929	61.67852	73.35326	1320.77379	-145.20455	2378.68491	1
255	H	73.75467	62.36955	74.54530	-1512.10848	1470.52031	1724.75147	1
256	C	70.19981	64.72130	75.34635	-607.11113	499.56689	73.73769	1
257	O	69.57324	64.18946	76.23629	357.97126	460.81534	356.68785	1
258	N	69.98819	65.88193	74.74151	536.55407	-368.62270	332.76306	1
259	H	70.65464	66.12137	74.00906	524.38866	2297.69985	1367.20941	1
260	C	69.10900	66.86251	75.27424	46.50277	-774.29190	-147.97904	1
261	H	68.99694	67.58159	74.43435	1676.51875	1883.29066	1032.55549	1
262	C	67.71036	66.17226	75.68836	-559.41456	-34.19198	-556.30433	1
263	H	67.89960	65.39236	76.47577	-64.66664	395.18769	2695.05373	1
264	H	67.00551	66.91067	76.13963	-2703.44278	-60.40056	333.79418	1
265	C	67.10464	65.54325	74.46378	-519.76435	377.31045	459.42366	1
266	H	67.90087	64.96125	73.94639	-1746.74323	1667.50644	-1261.73691	1
267	C	65.98340	64.58408	74.84494	570.95554	16.46261	-545.27700	1
268	H	65.53716	64.09083	73.94309	2391.58273	28.05277	-1305.07271	1
269	H	66.34887	63.76999	75.52271	175.75588	917.63458	2559.43867	1
270	H	65.15156	65.11228	75.37797	-1063.97851	-2155.34650	1283.00462	1
271	C	66.56313	66.59717	73.50651	193.76014	2.62946	-765.53141	1
272	H	66.11245	66.13196	72.59232	507.39394	-846.55087	2539.60089	1
273	H	65.76535	67.21926	73.98784	1337.57841	1818.19054	1526.01994	1
274	H	67.36540	67.29724	73.15974	1100.88635	-1172.91350	-2199.08909	1
275	C	69.86677	67.57342	76.49781	-549.21115	475.64486	-309.38218	1
276	O	71.06449	67.69703	76.53389	556.06106	-390.37755	-78.24250	1
277	O	69.05637	68.24238	77.44940	-572.27940	-310.19032	-209.75862	1
278	H	68.16266	67.98597	77.10201	-1380.08193	2212.14486	790.85944	1

Listing 13: C00013.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1294.1210	0.0000	300.0000
3	H	78.97967	60.06429	80.19138	-2043.14101	-1757.64893	399.89339		1
4	N	78.94044	60.45535	79.25218	426.75047	490.45733	-334.42467		1
5	H	77.96928	60.75758	79.20454	442.25559	-1110.30854	-2448.52907		1
6	C	79.87231	61.49996	79.04045	415.32972	-666.39213	83.73172		1
7	H	80.80267	61.05332	79.45327	879.32219	2491.00447	667.35213		1
8	C	79.98498	61.80571	77.46127	31.35357	477.41777	628.23362		1
9	H	79.04109	62.28645	77.10945	1168.38489	2240.25337	-1019.71136		1
10	H	80.79998	62.54143	77.25902	-360.43770	2534.90498	931.67112		1

11	C	80.23276	60.52630	76.70743	463.18208	512.70242	-382.34388	1
12	H	79.47307	59.77898	77.03061	1725.29117	1863.52247	-987.07854	1
13	C	80.08424	60.75677	75.20835	710.42801	-144.27427	-313.15367	1
14	H	80.23931	59.81164	74.62686	364.20195	-1033.13725	2494.72524	1
15	H	79.06627	61.14480	74.94679	2567.61904	335.80679	847.48802	1
16	H	80.83021	61.50304	74.83140	-2587.99029	680.92867	-512.16411	1
17	C	81.61929	59.96718	76.99749	268.17616	741.64379	-40.42634	1
18	H	81.81686	59.03024	76.41537	1283.54314	-1945.37420	-1411.27812	1
19	H	82.42375	60.69988	76.72983	-1258.57796	1317.15249	-2026.02085	1
20	H	81.74579	59.71552	78.08173	-2502.84526	909.80597	575.92391	1
21	C	79.35164	62.73416	79.94253	619.36578	-458.64843	-172.09273	1
22	O	78.86953	62.53698	81.06439	-81.40433	433.87611	522.34594	1
23	N	79.65823	63.87832	79.38590	175.23996	-622.20190	341.55523	1
24	H	80.10378	63.84312	78.47196	-876.57256	-303.22879	-2561.90213	1
25	C	79.00696	65.11101	79.74412	-571.88214	-534.10783	-106.15033	1
26	H	77.96523	65.03215	79.36703	-2713.20841	-16.25800	-248.80809	1
27	C	79.04559	65.22908	81.33677	166.60354	288.16399	-716.09568	1
28	H	79.91890	64.59636	81.66811	-2097.85574	1636.78449	-586.18044	1
29	O	77.91740	64.68153	82.01395	-317.80580	-363.38227	484.43082	1
30	H	78.16100	63.67180	81.95805	1863.74748	-1451.84923	1357.29467	1
31	C	79.34646	66.75049	81.58857	503.80731	517.99032	318.51606	1
32	H	79.52970	66.95904	82.66844	640.61020	-2157.10410	-1536.29104	1
33	H	80.24809	67.09215	81.02210	1687.88455	465.60692	2087.56452	1
34	H	78.49831	67.40171	81.26465	-1293.07895	-1899.88581	-1463.57452	1
35	C	79.87921	66.25359	78.99869	-153.07550	-733.68902	248.70981	1
36	O	81.08209	66.22715	79.07728	186.15459	-480.78787	-449.34387	1
37	N	79.09608	67.18520	78.43360	-487.53139	543.18517	42.03850	1
38	C	79.66531	68.39356	77.91406	-699.35871	69.34393	360.10701	1
39	H	80.65951	68.13554	77.47896	2.81126	-221.99807	-2715.58072	1
40	C	78.54402	68.81557	76.86290	-507.46439	-592.59194	122.07761	1
41	H	78.59488	69.89616	76.56993	-1975.08116	525.87560	-1801.71556	1
42	H	78.63179	68.22775	75.92171	1588.27743	-1913.22100	1113.83566	1
43	C	77.24078	68.45205	77.63469	-613.62442	-457.55993	-194.14490	1
44	H	77.00793	69.21902	78.40644	1707.54637	-721.27992	1996.92523	1
45	H	76.34389	68.37600	76.98005	758.23357	2100.81767	1560.55011	1
46	C	77.65266	67.06773	78.30169	-352.41524	704.96076	49.21465	1
47	H	77.22324	66.88972	79.31581	1714.76886	-2070.42778	443.35792	1
48	H	77.47418	66.17074	77.66240	1224.15040	1801.50881	1636.97633	1
49	C	79.77729	69.45423	79.13581	566.85117	537.05831	117.62814	1
50	O	79.10281	69.38851	80.15252	-550.26779	-406.08867	4.21666	1
51	N	80.70988	70.42629	78.85387	566.34832	-425.77725	180.18749	1
52	H	80.82108	70.24354	77.83702	644.44502	2646.80550	-52.73430	1
53	C	81.97980	70.21605	79.54978	612.34801	-281.48662	411.56221	1
54	H	82.23679	69.15294	79.34835	1667.23498	-1490.75142	1556.16753	1
55	C	82.97810	71.21863	78.83815	-714.45746	-175.43074	286.98927	1
56	H	82.73971	72.26174	79.18249	-787.09484	1763.03619	-1922.46060	1
57	O	82.91244	71.26954	77.39320	-429.46514	516.51932	-128.40526	1
58	H	82.65836	72.20454	77.24969	1981.82785	436.16847	-1818.18182	1
59	C	84.36870	70.77685	79.42872	630.79189	-468.94448	76.03230	1
60	H	85.18143	71.47777	79.12666	-1775.71861	2062.30353	131.89849	1
61	H	84.35601	70.73611	80.54774	-1855.14608	88.94118	1993.53760	1
62	H	84.65733	69.76307	79.06516	-1504.82350	-780.94249	-2132.90992	1
63	C	81.85272	70.52837	81.12444	288.57638	618.62814	-397.00270	1
64	O	82.76301	70.22180	81.86809	321.70495	-185.26452	574.37218	1
65	N	80.76454	71.24328	81.43771	-447.05792	-446.53431	367.76425	1
66	H	80.08366	71.38403	80.68919	350.31316	1975.63644	-1843.31522	1
67	C	80.47010	71.35148	82.84746	-511.23061	374.03917	-471.51480	1
68	H	80.73694	70.34452	83.24275	2234.79579	-898.70890	-1273.45190	1
69	C	81.49330	72.45760	83.40188	529.53781	-159.34528	563.72604	1
70	H	81.34099	72.57300	84.50773	654.59388	2347.94251	1217.51488	1
71	H	82.51782	72.01207	83.26441	-1526.55661	2103.42026	817.87394	1
72	O	81.44251	73.76353	82.77173	-554.84278	14.12789	399.58769	1

73	H	81.59775	73.49231	81.84548	1297.06236	2061.84854	1220.68812	1
74	C	78.92749	71.72515	83.03929	-662.15484	-412.13544	123.62687	1
75	O	78.57277	72.33081	84.01275	-540.01537	-317.05804	274.91456	1
76	N	78.15881	71.09816	82.11425	-202.76299	-690.00100	-131.49145	1
77	H	78.65290	70.46492	81.42800	-702.62132	-2617.37191	281.70413	1
78	C	76.97694	71.79747	81.55576	-491.73914	576.34187	222.73509	1
79	H	76.39197	70.95535	81.12121	1977.17978	-1823.58850	-434.68928	1
80	C	76.22924	72.59546	82.58878	-649.50797	-328.66843	306.11224	1
81	H	76.93169	73.35489	83.01420	2075.07803	1452.16490	-1004.45904	1
82	C	75.05943	73.33850	81.96308	-615.18735	-489.99689	-70.96352	1
83	H	74.51046	73.96252	82.71929	-1226.32661	-1724.38906	-1716.47170	1
84	H	75.40410	74.03049	81.14636	2381.64273	-969.84735	900.46860	1
85	H	74.31395	72.63169	81.50767	2122.74991	1702.23946	-141.36228	1
86	C	75.73262	71.73073	83.73489	-501.86074	-479.61276	-376.42482	1
87	H	75.19193	72.33790	84.51125	993.79261	-2246.95401	-1177.81305	1
88	H	75.02551	70.93266	83.37903	42.71279	-626.15391	-2651.37258	1
89	H	76.59147	71.21512	84.24957	-2026.39012	-1590.33709	-887.82922	1
90	C	77.55108	72.82138	80.38904	-672.89153	382.57394	-156.34072	1
91	O	78.01406	73.90488	80.65590	410.04627	221.86223	500.35950	1
92	N	77.38717	72.27735	79.19457	-378.11782	-443.79414	-441.10984	1
93	H	77.03011	71.32740	79.12245	2404.15973	-568.14894	1149.30085	1
94	C	77.76953	73.07067	78.05558	-544.54484	466.16019	331.29119	1
95	H	77.29935	74.05528	78.27303	-1409.80988	-170.17955	2325.32679	1
96	C	79.35028	73.17751	78.12042	-184.48284	116.78282	-758.89137	1
97	H	79.64584	73.68294	79.07039	1893.78641	1861.14652	611.04528	1
98	H	79.81164	72.16619	78.16039	-2170.79665	-974.19311	1327.50117	1
99	C	79.84631	73.95928	76.86416	389.51668	672.81878	-138.49152	1
100	H	79.53646	73.42677	75.93520	510.64577	1933.03327	1851.02484	1
101	H	79.33757	74.94694	76.80633	-2302.30869	-1105.72939	-948.89774	1
102	C	81.41318	74.15523	76.85347	-559.93427	-126.34590	542.30857	1
103	O	81.98860	74.34088	75.81345	-670.36003	-111.83166	76.36448	1
104	N	81.97764	74.13321	78.08524	-216.06729	-537.07037	446.51379	1
105	H	81.49090	74.13739	78.98736	-1251.96487	1074.12894	-2168.52500	1
106	H	82.93793	74.44095	78.27144	-2451.83023	-720.73851	944.84612	1
107	C	77.20168	72.32228	76.73565	546.24052	-563.88337	-85.11809	1
108	O	77.98145	71.75498	75.99536	71.70702	-307.40463	606.69673	1
109	N	75.88208	72.46733	76.60799	479.90863	-504.50129	222.86849	1
110	C	75.09680	71.60096	75.77512	75.51268	-600.91904	506.73700	1
111	H	75.48192	70.56532	75.91416	-2033.61562	1795.30103	254.89480	1
112	C	73.62664	71.86620	76.31487	523.79067	517.99274	284.45581	1
113	H	72.83886	71.58583	75.57958	1599.61665	-1127.00911	1895.98173	1
114	H	73.41529	71.29720	77.24743	-1881.83093	1275.82488	-1501.55016	1
115	C	73.70912	73.40080	76.58468	-600.05639	-404.05026	316.64485	1
116	H	73.72639	73.96927	75.62109	-2597.05260	496.36221	657.73249	1
117	H	72.86414	73.80572	77.18971	-1666.24518	1294.38985	-1723.90591	1
118	C	75.11718	73.48683	77.31691	493.57570	-129.95376	-602.56394	1
119	H	75.64455	74.46435	77.21946	-1469.08415	-637.84797	2204.22581	1
120	H	75.10789	73.17499	78.38843	-1038.97840	1068.88701	-2280.71789	1
121	C	75.14504	72.06886	74.21238	188.88100	241.05089	-727.87821	1
122	O	74.64077	71.33406	73.36107	531.88613	-49.19943	427.07960	1
123	N	75.62209	73.29066	74.06098	708.14833	26.93417	-179.73509	1
124	H	75.91394	73.62937	74.97737	-2232.69501	-1179.09831	1023.94816	1
125	C	76.19633	73.83769	72.84262	-738.32412	259.92548	104.42456	1
126	H	76.79116	74.71248	73.20009	2028.89123	1260.02983	1311.33324	1
127	C	77.04723	72.76666	72.17412	-258.65678	-345.52513	661.28459	1
128	H	76.41967	71.85074	72.07244	-1826.06090	-1801.46097	-918.64554	1
129	C	77.48831	73.19926	70.78778	-541.23400	531.92970	-218.41428	1
130	H	78.08591	72.39888	70.27085	1311.73218	-2219.18200	882.19023	1
131	H	76.60740	73.43910	70.12997	-1048.71298	1223.58118	-2196.97971	1
132	H	78.13120	74.12143	70.82848	419.06414	1903.92898	1903.44670	1
133	C	78.25943	72.40376	73.00793	-423.86431	152.66566	-648.55262	1
134	H	78.83711	71.55281	72.55255	105.68386	-2342.50080	1387.51238	1

135	H	78.97017	73.27084	73.10216	-1695.63603	-1484.73621	-1531.02793	1
136	H	77.97343	72.09060	74.07104	-1853.57121	-487.39031	1936.59343	1
137	C	74.96373	74.31567	71.82845	539.71428	-510.58232	267.58633	1
138	O	75.00723	75.41394	71.33666	-15.93758	-278.34085	-624.49402	1
139	N	74.08328	73.35511	71.64064	-676.81886	12.05292	276.17960	1
140	H	74.17856	72.43164	72.13435	-1694.44250	-373.84189	-2100.66098	1
141	C	73.00295	73.63041	70.74763	412.33078	-664.70360	108.35451	1
142	H	73.44492	74.30052	69.97422	1765.77476	1294.44366	1621.76594	1
143	C	72.48496	72.23002	70.22029	-179.66635	-721.95667	-264.73915	1
144	H	73.32867	71.60807	69.84582	-607.34922	2587.87032	-598.10018	1
145	H	72.04094	71.64942	71.05998	-359.69332	-1479.13954	-2259.74260	1
146	C	71.42441	72.47087	69.09635	-240.01076	616.02425	431.85322	1
147	H	70.68137	73.24020	69.41485	-1359.17131	782.54425	2227.99181	1
148	H	71.90180	72.86871	68.17286	-820.36667	85.81767	-2596.78715	1
149	C	70.70782	71.08730	68.82228	-513.07015	236.18570	-551.87280	1
150	H	71.44354	70.31545	68.49909	1816.11944	-1183.11722	-1650.94321	1
151	H	70.24576	70.69168	69.75586	-1800.04429	-1361.53473	1526.34643	1
152	C	69.63048	71.31171	67.73629	726.08972	-253.19732	-179.64713	1
153	H	68.84441	72.04356	68.00997	1224.27271	-456.51798	-2390.90304	1
154	H	70.03036	71.54487	66.72937	1206.40339	-1150.93514	-2154.90344	1
155	N	68.85935	69.95981	67.55949	329.70796	-633.68968	-155.67358	1
156	H	68.09020	69.96205	66.82913	1348.31305	1938.76845	1359.00643	1
157	H	69.42646	69.11294	67.26332	2096.92035	1446.54551	-966.48890	1
158	H	68.33892	69.58937	68.40726	-1197.07217	-2303.53719	827.28733	1
159	C	71.78218	74.37622	71.54502	-378.01186	-556.17301	-413.96481	1
160	O	70.89650	74.88997	70.89561	-409.44433	-307.55053	-453.30833	1
161	N	71.85865	74.25181	72.86566	-429.02477	524.70884	274.08502	1
162	H	72.68173	73.78940	73.25058	1706.34263	-1425.96036	1574.38926	1
163	C	70.95023	75.04099	73.63145	-45.25864	-626.22952	478.93267	1
164	H	70.41871	75.64850	72.85853	1988.63164	570.90773	1772.87287	1
165	C	69.99529	74.06247	74.43023	551.77128	-20.49526	-564.54996	1
166	H	69.61263	73.25539	73.76614	1434.61535	-1753.10253	1513.99471	1
167	H	70.53800	73.54943	75.25575	-714.67738	1819.09770	1898.36494	1
168	C	68.82963	74.95392	74.97264	446.99263	-555.77305	338.97221	1
169	H	69.21181	75.67916	75.72585	1953.68466	1892.25957	-161.67766	1
170	H	68.39920	75.56783	74.14989	-403.03785	2688.07032	-188.43591	1
171	C	67.71028	74.02924	75.59946	567.86262	335.74681	434.04421	1
172	H	67.35707	73.27336	74.86086	-1080.02275	1568.26081	-1948.78900	1
173	H	68.10587	73.44885	76.46441	-919.54108	2111.34692	1456.13463	1
174	C	66.55137	74.95788	76.03198	195.81897	173.33862	-745.11536	1
175	H	66.79978	75.64936	76.86165	1405.67949	-2301.21089	-390.08113	1
176	H	66.07795	75.51949	75.20192	-940.37328	-1118.32446	2299.72133	1
177	N	65.40007	74.05923	76.59612	319.26422	656.36007	-42.02424	1
178	H	64.53555	74.57791	76.92641	1961.03633	619.91968	1787.09422	1
179	H	64.97393	73.34729	75.93404	854.14343	-2156.80752	1429.08711	1
180	H	65.62279	73.46383	77.44603	1237.02905	-1378.50857	-1998.28500	1
181	C	71.82837	75.91579	74.71823	532.53319	-268.57236	517.55729	1
182	O	72.22117	75.44920	75.75870	266.16714	-290.73804	-558.88002	1
183	N	71.92728	77.13687	74.23225	-226.25352	640.49678	-270.32839	1
184	H	71.45790	77.44312	73.36396	2007.69063	-1035.27229	1523.50231	1
185	C	72.84864	78.08097	74.75968	-540.76542	-573.33303	49.50000	1
186	H	72.97951	77.89808	75.84933	-2374.20950	-1036.76023	843.75774	1
187	C	74.21083	77.89262	73.93130	-77.09082	666.87422	-415.84136	1
188	H	73.94682	77.80551	72.84014	-985.81834	617.19825	2463.91927	1
189	O	74.95879	76.70005	74.22467	293.29899	-391.65602	-477.80926	1
190	H	74.92153	76.23748	73.35775	2528.72714	-681.76262	-751.27122	1
191	C	74.97983	79.24038	74.17304	252.47363	-605.14473	440.05134	1
192	H	75.94929	79.25165	73.62208	-2052.65063	1456.49051	-1043.51830	1
193	H	74.39649	80.14472	73.82795	-2152.98800	-1661.97574	-161.70652	1
194	H	75.21571	79.38619	75.25290	-473.12726	-1584.27339	2165.61725	1
195	C	72.06004	79.44336	74.32091	360.36307	488.46713	505.10056	1
196	O	71.25871	79.36683	73.40414	-200.08817	-528.03552	-385.82850	1

197	N	72.44451	80.49282	75.02738	-597.54095	-226.44775	355.20479	1
198	H	73.16245	80.37552	75.74171	2179.23655	-1300.70981	-991.33835	1
199	C	71.96161	81.78656	74.67115	-687.68921	297.39807	-249.45179	1
200	H	70.86760	81.66816	74.50228	-349.16256	-2467.37713	-1101.72831	1
201	C	72.36603	82.81248	75.82720	672.47345	361.54328	-201.62880	1
202	H	73.46558	82.98890	75.80151	1541.41502	582.18425	2169.97026	1
203	H	71.88091	83.79575	75.62731	-2534.67717	60.25153	997.72295	1
204	C	71.96053	82.28066	77.20959	574.26774	-389.43119	-377.02542	1
205	C	70.59051	82.26868	77.60886	688.82679	-287.33580	-257.96133	1
206	H	69.80008	82.62796	76.92516	331.14182	1470.38163	2269.80013	1
207	C	72.97565	81.80441	78.09368	-383.52382	-675.04808	144.24917	1
208	H	74.03661	81.80589	77.78474	4.09847	1517.59662	2262.86397	1
209	C	70.27234	81.79622	78.88226	-134.76730	428.45285	-649.50303	1
210	H	69.21353	81.79029	79.19450	-903.23433	1600.49020	2011.53387	1
211	C	72.60639	81.34336	79.35941	-335.53281	-615.00040	-364.39058	1
212	H	73.40089	80.98442	80.03685	1596.45398	-1369.33862	1732.02659	1
213	C	71.25169	81.32281	79.80300	585.48547	-340.24194	-406.23938	1
214	O	70.86697	80.85781	81.08763	-419.15649	-173.04408	-511.94141	1
215	H	71.75417	80.63659	81.45739	-1071.84350	1559.71507	-1960.13012	1
216	C	72.74586	82.27255	73.33209	291.41878	-183.13091	710.72246	1
217	O	73.87501	81.94083	73.05007	379.87695	523.47396	-222.23622	1
218	N	71.96060	83.15055	72.72700	564.30591	373.09380	277.24371	1
219	H	70.98963	83.39060	73.00193	-120.59931	-2436.07824	-1214.35098	1
220	C	72.37664	83.68676	71.45683	404.07514	-299.37480	608.84009	1
221	H	73.37173	84.16582	71.59352	-1071.07882	-841.69025	2359.66467	1
222	C	72.45754	82.44166	70.47578	-683.12807	68.71770	-390.13096	1
223	H	73.15723	81.67934	70.89546	2068.88918	1596.58590	770.89603	1
224	H	71.46626	81.93752	70.41835	1379.86429	2342.49779	-179.85638	1
225	C	72.92458	82.90643	69.06832	-176.39967	537.49466	550.97268	1
226	H	72.28717	83.75066	68.68216	-396.28051	1942.22168	1869.33314	1
227	H	73.96715	83.29403	69.09250	-94.44700	586.00678	-2659.20016	1
228	C	72.79386	81.64349	68.07408	-291.69381	-718.18079	-150.72929	1
229	H	73.46363	80.77640	68.30604	-2303.38776	1089.76242	964.62032	1
230	H	71.72841	81.32945	67.91830	884.16729	2568.80533	-207.74283	1
231	N	73.25142	82.34852	66.96008	-594.49522	-252.81478	342.29276	1
232	H	72.62558	83.06096	66.60294	-1735.17426	2084.05705	-263.71605	1
233	C	74.36835	82.16825	66.35599	595.23177	-271.52487	442.22352	1
234	N	75.23016	81.18612	66.83737	585.53813	-424.79750	-105.81303	1
235	H	75.10833	80.56170	67.63459	959.88797	1327.56823	-2177.11905	1
236	H	76.13860	80.94473	66.43848	1578.48647	16.27378	-2220.76233	1
237	N	74.48129	83.04936	65.27942	-452.17763	-390.33541	-421.51853	1
238	H	73.83900	83.76806	64.94653	470.26107	1974.25629	-1817.92087	1
239	H	75.28628	83.08415	64.65224	1856.67307	-1573.97321	-1224.35416	1
240	C	71.14006	84.69390	71.19178	-531.47271	-581.45780	-55.06206	1
241	O	70.13761	84.59369	71.88360	-243.00837	192.73507	609.52485	1
242	N	71.40319	85.59130	70.24218	343.49288	-644.25607	38.09164	1
243	H	72.30631	85.47292	69.77957	-1691.16043	-1535.97525	-1484.73099	1
244	C	70.31045	86.26750	69.54650	542.66492	350.14337	454.42563	1
245	H	69.42427	86.12717	70.21180	1209.57979	-2396.95920	463.86744	1
246	C	70.72350	87.71976	69.36201	-737.14309	145.93010	242.71942	1
247	H	71.63933	87.73524	68.73003	-1050.18303	159.36419	-2509.06125	1
248	C	69.65721	88.54155	68.66724	-706.77696	-252.88343	-245.16230	1
249	H	69.94864	89.62624	68.60104	-1624.64039	-1665.49085	1417.86935	1
250	H	69.47037	88.18059	67.59631	2566.10521	598.51109	693.22305	1
251	H	68.67530	88.49593	69.21477	-1972.69758	107.10018	-1876.34312	1
252	C	71.07336	88.36550	70.69165	412.85148	672.58832	-27.69222	1
253	H	71.44937	89.41728	70.56098	1447.02277	1762.76533	-1490.78944	1
254	H	70.18037	88.41212	71.37379	1320.77379	-145.20455	2378.68491	1
255	H	71.87070	87.78519	71.23231	-1512.10848	1470.52031	1724.75147	1
256	C	70.16233	85.50452	68.07838	-607.11113	499.56689	73.73769	1
257	O	71.06275	84.85630	67.58698	357.97126	460.81534	356.68785	1
258	N	68.95198	85.72497	67.59601	536.55407	-368.62270	332.76306	1

259	H	68.34965	86.33776	68.14075	524.38866	2297.69985	1367.20941	1
260	C	68.68617	85.35868	66.24875	46.50277	-774.29190	-147.97904	1
261	H	69.40650	84.53357	66.04477	1676.51875	1883.29066	1032.55549	1
262	C	67.12935	84.95480	66.10079	-559.41456	-34.19198	-556.30433	1
263	H	66.49829	85.86040	66.26597	-64.66664	395.18769	2695.05373	1
264	H	66.91008	84.61994	65.05894	-2703.44278	-60.40056	333.79418	1
265	C	66.77149	83.88246	67.09449	-519.76435	377.31045	459.42366	1
266	H	67.06576	84.23297	68.10966	-1746.74323	1667.50644	-1261.73691	1
267	C	65.26790	83.63490	67.08147	570.95554	16.46261	-545.27700	1
268	H	64.96874	82.86095	67.83435	2391.58273	28.05277	-1305.07271	1
269	H	64.69217	84.56718	67.31600	175.75588	917.63458	2559.43867	1
270	H	64.91902	83.27444	66.07954	-1063.97851	-2155.34650	1283.00462	1
271	C	67.50844	82.58249	66.80226	193.76014	2.62946	-765.53141	1
272	H	67.21673	81.77277	67.52000	507.39394	-846.55087	2539.60089	1
273	H	67.28883	82.20638	65.76979	1337.57841	1818.19054	1526.01994	1
274	H	68.61891	82.71099	66.88218	1100.88635	-1172.91350	-2199.08909	1
275	C	68.93544	86.63649	65.30528	-549.21115	475.64486	-309.38218	1
276	O	69.18329	87.74519	65.72062	556.06106	-390.37755	-78.24250	1
277	O	68.79059	86.41014	63.91983	-572.27940	-310.19032	-209.75862	1
278	H	68.61287	85.42634	63.94544	-1380.08193	2212.14486	790.85944	1

Listing 14: C00014.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1294.1102	0.0000	300.0000
3	H	67.49412	74.41689	73.80266	-2043.14101	-1757.64893	399.89339		1
4	N	67.69003	75.20669	74.41096	426.75047	490.45733	-334.42467		1
5	H	67.80482	74.72324	75.30205	442.25559	-1110.30854	-2448.52907		1
6	C	68.85057	75.92805	74.02451	415.32972	-666.39213	83.73172		1
7	H	69.63080	75.15281	73.86769	879.32219	2491.00447	667.35213		1
8	C	68.53017	76.74960	72.67794	31.35357	477.41777	628.23362		1
9	H	67.67588	77.44286	72.87121	1168.38489	2240.25337	-1019.71136		1
10	H	69.39932	77.39947	72.41287	-360.43770	2534.90498	931.67112		1
11	C	68.20199	75.81146	71.54360	463.18208	512.70242	-382.34388		1
12	H	67.38354	75.13160	71.86934	1725.29117	1863.52247	-987.07854		1
13	C	67.71070	76.60002	70.33608	710.42801	-144.27427	-313.15367		1
14	H	67.44024	75.92525	69.48317	364.20195	-1033.13725	2494.72524		1
15	H	66.80116	77.20735	70.58150	2567.61904	335.80679	847.48802		1
16	H	68.49259	77.31049	69.96256	-2587.99029	680.92867	-512.16411		1
17	C	69.40891	74.97111	71.15067	268.17616	741.64379	-40.42634		1
18	H	69.18138	74.30531	70.27842	1283.54314	-1945.37420	-1411.27812		1
19	H	70.28055	75.61281	70.86019	-1258.57796	1317.15249	-2026.02085		1
20	H	69.74865	74.31096	71.98963	-2502.84526	909.80597	575.92391		1
21	C	69.26887	76.99094	75.17871	619.36578	-458.64843	-172.09273		1
22	O	70.47092	77.32732	75.25766	-81.40433	433.87611	522.34594		1
23	N	68.23271	77.39720	75.84662	175.23996	-622.20190	341.55523		1
24	H	67.38893	76.91970	75.52599	-876.57256	-303.22879	-2561.90213		1
25	C	68.14706	78.31939	76.94759	-571.88214	-534.10783	-106.15033		1
26	H	67.73624	77.71339	77.78583	-2713.20841	-16.25800	-248.80809		1
27	C	69.54212	78.92206	77.28372	166.60354	288.16399	-716.09568		1
28	H	70.04855	79.28101	76.35593	-2097.85574	1636.78449	-586.18044		1
29	O	70.55290	77.79674	77.81991	-317.80580	-363.38227	484.43082		1
30	H	70.86381	77.54051	76.92581	1863.74748	-1451.84923	1357.29467		1
31	C	69.37388	80.06072	78.31010	503.80731	517.99032	318.51606		1
32	H	70.37699	80.47385	78.59194	640.61020	-2157.10410	-1536.29104		1
33	H	68.75258	80.90261	77.91053	1687.88455	465.60692	2087.56452		1
34	H	68.88867	79.70401	79.25145	-1293.07895	-1899.88581	-1463.57452		1
35	C	67.07815	79.47429	76.46922	-153.07550	-733.68902	248.70981		1
36	O	67.06344	79.87683	75.33659	186.15459	-480.78787	-449.34387		1
37	N	66.35144	79.89229	77.51903	-487.53139	543.18517	42.03850		1
38	C	65.50223	81.03472	77.39609	-699.35871	69.34393	360.10701		1

39	H	65.22438	81.09119	76.31760	2.81126	-221.99807	-2715.58072	1
40	C	64.33906	80.72939	78.43258	-507.46439	-592.59194	122.07761	1
41	H	63.83264	81.65815	78.78608	-1975.08116	525.87560	-1801.71556	1
42	H	63.55307	80.07509	77.99279	1588.27743	-1913.22100	1113.83566	1
43	C	65.12829	79.99578	79.56283	-613.62442	-457.55993	-194.14490	1
44	H	65.68010	80.72746	80.19457	1707.54637	-721.27992	1996.92523	1
45	H	64.48057	79.40646	80.25031	758.23357	2100.81767	1560.55011	1
46	C	66.12715	79.09490	78.71858	-352.41524	704.96076	49.21465	1
47	H	67.10651	78.89775	79.21130	1714.76886	-2070.42778	443.35792	1
48	H	65.69563	78.12946	78.36291	1224.15040	1801.50881	1636.97633	1
49	C	66.24110	82.39589	77.95068	566.85117	537.05831	117.62814	1
50	O	65.66286	83.02191	78.84685	-550.26779	-406.08867	4.21666	1
51	N	67.35909	82.64069	77.33926	566.34832	-425.77725	180.18749	1
52	H	67.55331	81.96277	76.60164	644.44502	2646.80550	-52.73430	1
53	C	68.18165	83.80393	77.50206	612.34801	-281.48662	411.56221	1
54	H	68.02624	84.38509	76.56795	1667.23498	-1490.75142	1556.16753	1
55	C	67.78113	84.60679	78.81568	-714.45746	-175.43074	286.98927	1
56	H	67.63917	83.84021	79.63004	-787.09484	1763.03619	-1922.46060	1
57	O	66.56407	85.34642	78.73506	-429.46514	516.51932	-128.40526	1
58	H	65.90717	84.61004	79.04045	1981.82785	436.16847	-1818.18182	1
59	C	69.06592	85.46060	79.12315	630.79189	-468.94448	76.03230	1
60	H	68.94418	86.05066	80.06109	-1775.71861	2062.30353	131.89849	1
61	H	69.97204	84.82193	79.25154	-1855.14608	88.94118	1993.53760	1
62	H	69.28099	86.18469	78.30364	-1504.82350	-780.94249	-2132.90992	1
63	C	69.70254	83.23164	77.60766	288.57638	618.62814	-397.00270	1
64	O	70.06944	82.62844	78.62220	321.70495	-185.26452	574.37218	1
65	N	70.39387	83.63081	76.57070	-447.05792	-446.53431	367.76425	1
66	H	69.86126	84.16286	75.88148	350.31316	1975.63644	-1843.31522	1
67	C	71.62626	83.05672	76.15225	-511.23061	374.03917	-471.51480	1
68	H	71.94354	83.78912	75.37613	2234.79579	-898.70890	-1273.45190	1
69	C	72.64572	82.99331	77.38299	529.53781	-159.34528	563.72604	1
70	H	73.69754	82.99962	76.98301	654.59388	2347.94251	1217.51488	1
71	H	72.50274	83.95975	77.93741	-1526.55661	2103.42026	817.87394	1
72	O	72.53540	81.87749	78.27113	-554.84278	14.12789	399.58769	1
73	H	71.58026	82.05841	78.62527	1297.06236	2061.84854	1220.68812	1
74	C	71.32910	81.61118	75.47557	-662.15484	-412.13544	123.62687	1
75	O	70.21507	81.23249	75.18293	-540.01537	-317.05804	274.91456	1
76	N	72.48128	81.00558	75.19651	-202.76299	-690.00100	-131.49145	1
77	H	73.36317	81.43671	75.46620	-702.62132	-2617.37191	281.70413	1
78	C	72.43572	79.85283	74.35930	-491.73914	576.34187	222.73509	1
79	H	71.41878	79.41114	74.49896	1977.17978	-1823.58850	-434.68928	1
80	C	72.67979	80.38520	72.87356	-649.50797	-328.66843	306.11224	1
81	H	73.48437	81.15127	72.87086	2075.07803	1452.16490	-1004.45904	1
82	C	73.03138	79.21029	71.90151	-615.18735	-489.99689	-70.96352	1
83	H	73.05275	79.54809	70.83870	-1226.32661	-1724.38906	-1716.47170	1
84	H	74.03672	78.78544	72.12847	2381.64273	-969.84735	900.46860	1
85	H	72.28952	78.38010	71.97235	2122.74991	1702.23946	-141.36228	1
86	C	71.32968	80.99057	72.36205	-501.86074	-479.61276	-376.42482	1
87	H	71.44694	81.48105	71.36670	993.79261	-2246.95401	-1177.81305	1
88	H	70.54409	80.20563	72.25730	42.71279	-626.15391	-2651.37258	1
89	H	70.93232	81.75422	73.07530	-2026.39012	-1590.33709	-887.82922	1
90	C	73.69098	78.91843	74.81156	-672.89153	382.57394	-156.34072	1
91	O	74.83353	79.29792	74.76763	410.04627	221.86223	500.35950	1
92	N	73.22501	77.68954	75.07896	-378.11782	-443.79414	-441.10984	1
93	H	72.18940	77.51113	75.06390	2404.15973	-568.14894	1149.30085	1
94	C	74.05981	76.92558	75.98452	-544.54484	466.16019	331.29119	1
95	H	74.81565	77.66252	76.34719	-1409.80988	-170.17955	2325.32679	1
96	C	73.04872	76.45385	77.11599	-184.48284	116.78282	-758.89137	1
97	H	72.75269	77.34856	77.71286	1893.78641	1861.14652	611.04528	1
98	H	72.10854	76.07205	76.65691	-2170.79665	-974.19311	1327.50117	1
99	C	73.64179	75.35964	78.05303	389.51668	672.81878	-138.49152	1
100	H	73.64875	74.36705	77.53819	510.64577	1933.03327	1851.02484	1

101	H	74.71912	75.55707	78.23791	-2302.30869	-1105.72939	-948.89774	1
102	C	72.85918	75.25434	79.42456	-559.93427	-126.34590	542.30857	1
103	O	73.26436	74.52913	80.30113	-670.36003	-111.83166	76.36448	1
104	N	71.76819	76.03194	79.49490	-216.06729	-537.07037	446.51379	1
105	H	71.33217	76.68876	78.76822	-1251.96487	1074.12894	-2168.52500	1
106	H	71.17867	76.02517	80.33851	-2451.83023	-720.73851	944.84612	1
107	C	74.77252	75.64422	75.33915	546.24052	-563.88337	-85.11809	1
108	O	75.36884	74.91504	76.13657	71.70702	-307.40463	606.69673	1
109	N	74.77584	75.54689	74.01335	479.90863	-504.50129	222.86849	1
110	C	74.88983	74.30129	73.31293	75.51268	-600.91904	506.73700	1
111	H	74.33152	73.54268	73.90626	-2033.61562	1795.30103	254.89480	1
112	C	74.26688	74.65920	71.90223	523.79067	517.99274	284.45581	1
113	H	74.57354	73.94774	71.10228	1599.61665	-1127.00911	1895.98173	1
114	H	73.15414	74.65510	71.92984	-1881.83093	1275.82488	-1501.55016	1
115	C	74.82079	76.10299	71.68261	-600.05639	-404.05026	316.64485	1
116	H	75.89483	76.08082	71.39141	-2597.05260	496.36221	657.73249	1
117	H	74.28783	76.67386	70.88889	-1666.24518	1294.38985	-1723.90591	1
118	C	74.61145	76.70500	73.13574	493.57570	-129.95376	-602.56394	1
119	H	75.33609	77.49458	73.45538	-1469.08415	-637.84797	2204.22581	1
120	H	73.57218	77.05842	73.34098	-1038.97840	1068.88701	-2280.71789	1
121	C	76.44336	73.85005	73.03755	188.88100	241.05089	-727.87821	1
122	O	76.65677	72.84445	72.40001	531.88613	-49.19943	427.07960	1
123	N	77.31367	74.74536	73.49261	708.14833	26.93417	-179.73509	1
124	H	76.90465	75.49621	74.04677	-2232.69501	-1179.09831	1023.94816	1
125	C	78.70964	74.43175	73.51682	-738.32412	259.92548	104.42456	1
126	H	78.77957	73.78205	72.61345	2028.89123	1260.02983	1311.33324	1
127	C	79.47571	75.81640	73.38953	-258.65678	-345.52513	661.28459	1
128	H	79.24588	76.44198	74.27875	-1826.06090	-1801.46097	-918.64554	1
129	C	81.02179	75.79583	73.13192	-541.23400	531.92970	-218.41428	1
130	H	81.40501	76.82813	72.95160	1311.73218	-2219.18200	882.19023	1
131	H	81.60520	75.39097	73.99472	-1048.71298	1223.58118	-2196.97971	1
132	H	81.29549	75.18931	72.22383	419.06414	1903.92898	1903.44670	1
133	C	78.94281	76.48921	72.07714	-423.86431	152.66566	-648.55262	1
134	H	79.37957	77.50413	71.92502	105.68386	-2342.50080	1387.51238	1
135	H	79.19408	75.87976	71.17605	-1695.63603	-1484.73621	-1531.02793	1
136	H	77.83429	76.60269	72.09795	-1853.57121	-487.39031	1936.59343	1
137	C	78.92795	73.57102	74.87607	539.71428	-510.58232	267.58633	1
138	O	78.10570	72.72354	75.23113	-15.93758	-278.34085	-624.49402	1
139	N	80.05157	73.87745	75.48311	-676.81886	12.05292	276.17960	1
140	H	80.63309	74.60759	75.08100	-1694.44250	-373.84189	-2100.66098	1
141	C	80.57765	72.98918	76.48637	412.33078	-664.70360	108.35451	1
142	H	80.53522	71.97602	76.02555	1765.77476	1294.44366	1621.76594	1
143	C	82.03616	73.49321	76.81891	-179.66635	-721.95667	-264.73915	1
144	H	82.63887	73.67271	75.90095	-607.34922	2587.87032	-598.10018	1
145	H	81.97995	74.47980	77.33127	-359.69332	-1479.13954	-2259.74260	1
146	C	82.70928	72.42751	77.74808	-240.01076	616.02425	431.85322	1
147	H	81.95715	72.04406	78.49351	-1359.17131	782.54425	2227.99181	1
148	H	83.05467	71.53939	77.17212	-820.36667	85.81767	-2596.78715	1
149	C	83.90441	73.12877	78.50819	-513.07015	236.18570	-551.87280	1
150	H	84.77818	73.28040	77.83394	1816.11944	-1183.11722	-1650.94321	1
151	H	83.60908	74.14478	78.85777	-1800.04429	-1361.53473	1526.34643	1
152	C	84.26499	72.23525	79.71839	726.08972	-253.19732	-179.64713	1
153	H	83.46545	72.15282	80.48216	1224.27271	-456.51798	-2390.90304	1
154	H	84.64076	71.22673	79.45484	1206.40339	-1150.93514	-2154.90344	1
155	N	85.45227	72.92395	80.47059	329.70796	-633.68968	-155.67358	1
156	H	85.79074	72.42833	81.34523	1348.31305	1938.76845	1359.00643	1
157	H	86.35969	73.04370	79.93320	2096.92035	1446.54551	-966.48890	1
158	H	85.28419	73.90504	80.83956	-1197.07217	-2303.53719	827.28733	1
159	C	79.70142	73.04897	77.85293	-378.01186	-556.17301	-413.96481	1
160	O	80.03478	72.40894	78.83159	-409.44433	-307.55053	-453.30833	1
161	N	78.69551	73.91714	77.76409	-429.02477	524.70884	274.08502	1
162	H	78.50120	74.30166	76.83733	1706.34263	-1425.96036	1574.38926	1

163	C	77.80003	73.97939	78.87848	-45.25864	-626.22952	478.93267	1
164	H	78.44390	73.76144	79.76280	1988.63164	570.90773	1772.87287	1
165	C	77.17691	75.43522	78.85900	551.77128	-20.49526	-564.54996	1
166	H	77.97906	76.20585	78.82231	1434.61535	-1753.10253	1513.99471	1
167	H	76.57943	75.58425	77.92884	-714.67738	1819.09770	1898.36494	1
168	C	76.29797	75.60611	80.14134	446.99263	-555.77305	338.97221	1
169	H	75.49088	74.83047	80.17268	1953.68466	1892.25957	-161.67766	1
170	H	76.90011	75.45238	81.06494	-403.03785	2688.07032	-188.43591	1
171	C	75.70350	77.07151	80.09290	567.86262	335.74681	434.04421	1
172	H	76.51893	77.82844	80.15357	-1080.02275	1568.26081	-1948.78900	1
173	H	75.19261	77.26362	79.12204	-919.54108	2111.34692	1456.13463	1
174	C	74.70656	77.24553	81.26227	195.81897	173.33862	-745.11536	1
175	H	73.89791	76.48603	81.29802	1405.67949	-2301.21089	-390.08113	1
176	H	75.17323	77.34984	82.26260	-940.37328	-1118.32446	2299.72133	1
177	N	73.94436	78.58920	81.01101	319.26422	656.36007	-42.02424	1
178	H	73.22700	78.86144	81.74314	1961.03633	619.91968	1787.09422	1
179	H	74.51969	79.47807	80.93641	854.14343	-2156.80752	1429.08711	1
180	H	73.36037	78.63282	80.12615	1237.02905	-1378.50857	-1998.28500	1
181	C	76.63407	72.84599	78.71244	532.53319	-268.57236	517.55729	1
182	O	75.90719	72.64116	79.65438	266.16714	-290.73804	-558.88002	1
183	N	76.58964	72.32515	77.49238	-226.25352	640.49678	-270.32839	1
184	H	77.28383	72.58105	76.75001	2007.69063	-1035.27229	1523.50231	1
185	C	75.76829	71.17314	77.31469	-540.76542	-573.33303	49.50000	1
186	H	75.20643	71.06311	78.27552	-2374.20950	-1036.76023	843.75774	1
187	C	74.84829	71.51417	76.06281	-77.09082	666.87422	-415.84136	1
188	H	75.52011	71.85267	75.21887	-985.81834	617.19825	2463.91927	1
189	O	73.97940	72.65438	76.21075	293.29899	-391.65602	-477.80926	1
190	H	74.67328	73.40165	76.17992	2528.72714	-681.76262	-751.27122	1
191	C	74.14590	70.15432	75.72444	252.47363	-605.14473	440.05134	1
192	H	73.54470	70.22686	74.78825	-2052.65063	1456.49051	-1043.51830	1
193	H	74.88169	69.32974	75.58328	-2152.98800	-1661.97574	-161.70652	1
194	H	73.45240	69.84417	76.54081	-473.12726	-1584.27339	2165.61725	1
195	C	76.82054	69.94174	77.03759	360.36307	488.46713	505.10056	1
196	O	77.27796	69.33625	77.97628	-200.08817	-528.03552	-385.82850	1
197	N	77.09115	69.77713	75.74830	-597.54095	-226.44775	355.20479	1
198	H	76.65603	70.38151	75.05286	2179.23655	-1300.70981	-991.33835	1
199	C	77.66165	68.52378	75.36456	-687.68921	297.39807	-249.45179	1
200	H	78.54388	68.43111	76.03484	-349.16256	-2467.37713	-1101.72831	1
201	C	76.61821	67.32690	75.54395	672.47345	361.54328	-201.62880	1
202	H	75.72194	67.50980	74.90964	1541.41502	582.18425	2169.97026	1
203	H	77.08768	66.39428	75.15480	-2534.67717	60.25153	997.72295	1
204	C	76.19994	67.12414	77.01275	574.26774	-389.43119	-377.02542	1
205	C	77.15914	66.69699	77.98211	688.82679	-287.33580	-257.96133	1
206	H	78.22005	66.56373	77.70278	331.14182	1470.38163	2269.80013	1
207	C	74.83372	67.29991	77.39069	-383.52382	-675.04808	144.24917	1
208	H	74.07999	67.61554	76.64724	4.09847	1517.59662	2262.86397	1
209	C	76.73562	66.46156	79.29176	-134.76730	428.45285	-649.50303	1
210	H	77.48151	66.14064	80.03984	-903.23433	1600.49020	2011.53387	1
211	C	74.45774	67.05531	78.71432	-335.53281	-615.00040	-364.39058	1
212	H	73.39864	67.19890	78.99117	1596.45398	-1369.33862	1732.02659	1
213	C	75.38338	66.62571	79.71036	585.48547	-340.24194	-406.23938	1
214	O	75.00648	66.35626	81.05249	-419.15649	-173.04408	-511.94141	1
215	H	74.05507	66.61159	81.01322	-1071.84350	1559.71507	-1960.13012	1
216	C	77.95896	68.54480	73.76728	291.41878	-183.13091	710.72246	1
217	O	77.39221	67.72651	73.07205	379.87695	523.47396	-222.23622	1
218	N	78.80996	69.49747	73.37929	564.30591	373.09380	277.24371	1
219	H	79.20082	70.12289	74.08459	-120.59931	-2436.07824	-1214.35098	1
220	C	79.30167	69.35882	72.03313	404.07514	-299.37480	608.84009	1
221	H	79.55236	68.27938	71.93333	-1071.07882	-841.69025	2359.66467	1
222	C	78.11365	69.76998	71.07669	-683.12807	68.71770	-390.13096	1
223	H	77.17495	69.24715	71.37944	2068.88918	1596.58590	770.89603	1
224	H	77.89529	70.86077	71.15895	1379.86429	2342.49779	-179.85638	1

225	C	78.53824	69.38403	69.62455	-176.39967	537.49466	550.97268	1
226	H	79.50715	69.85428	69.34276	-396.28051	1942.22168	1869.33314	1
227	H	78.70004	68.28706	69.53071	-94.44700	586.00678	-2659.20016	1
228	C	77.34839	69.88529	68.68558	-291.69381	-718.18079	-150.72929	1
229	H	76.34734	69.44106	68.91337	-2303.38776	1089.76242	964.62032	1
230	H	77.22229	70.99554	68.60566	884.16729	2568.80533	-207.74283	1
231	N	77.72508	69.38595	67.43176	-594.49522	-252.81478	342.29276	1
232	H	78.52969	68.77931	67.40770	-1735.17426	2084.05705	-263.71605	1
233	C	77.10746	69.63123	66.34754	595.23177	-271.52487	442.22352	1
234	N	75.98421	70.46221	66.42206	585.53813	-424.79750	-105.81303	1
235	H	75.57416	70.92106	67.23465	959.88797	1327.56823	-2177.11905	1
236	H	75.40093	70.73378	65.63030	1578.48647	16.27378	-2220.76233	1
237	N	77.70876	68.98226	65.26059	-452.17763	-390.33541	-421.51853	1
238	H	78.51492	68.36103	65.20949	470.26107	1974.25629	-1817.92087	1
239	H	77.34733	69.04361	64.30777	1856.67307	-1573.97321	-1224.35416	1
240	C	80.54507	70.37827	71.73666	-531.47271	-581.45780	-55.06206	1
241	O	81.44093	70.01543	71.00761	-243.00837	192.73507	609.52485	1
242	N	80.30636	71.57746	72.25524	343.49288	-644.25607	38.09164	1
243	H	79.45799	71.65663	72.81680	-1691.16043	-1535.97525	-1484.73099	1
244	C	81.25472	72.62937	72.19922	542.66492	350.14337	454.42563	1
245	H	80.89004	73.35492	72.95837	1209.57979	-2396.95920	463.86744	1
246	C	82.69090	72.04533	72.56282	-737.14309	145.93010	242.71942	1
247	H	82.98846	71.26902	71.81765	-1050.18303	159.36419	-2509.06125	1
248	C	83.74415	73.20242	72.62123	-706.77696	-252.88343	-245.16230	1
249	H	84.74562	72.83047	72.94266	-1624.64039	-1665.49085	1417.86935	1
250	H	83.87476	73.68720	71.62280	2566.10521	598.51109	693.22305	1
251	H	83.43888	73.99942	73.33897	-1972.69758	107.10018	-1876.34312	1
252	C	82.60999	71.42614	73.99988	412.85148	672.58832	-27.69222	1
253	H	83.59967	71.04495	74.34452	1447.02277	1762.76533	-1490.78944	1
254	H	82.26369	72.17850	74.74329	1320.77379	-145.20455	2378.68491	1
255	H	81.89108	70.57416	74.03370	-1512.10848	1470.52031	1724.75147	1
256	C	81.30058	73.27416	70.69662	-607.11113	499.56689	73.73769	1
257	O	81.97749	74.26651	70.51107	357.97126	460.81534	356.68785	1
258	N	80.58007	72.60507	69.80395	536.55407	-368.62270	332.76306	1
259	H	80.04402	71.81315	70.15644	524.38866	2297.69985	1367.20941	1
260	C	80.38530	73.20214	68.53148	46.50277	-774.29190	-147.97904	1
261	H	81.30109	73.81591	68.37650	1676.51875	1883.29066	1032.55549	1
262	C	80.10784	72.08549	67.40250	-559.41456	-34.19198	-556.30433	1
263	H	79.19040	71.50692	67.66772	-64.66664	395.18769	2695.05373	1
264	H	79.87584	72.58814	66.43275	-2703.44278	-60.40056	333.79418	1
265	C	81.27755	71.15076	67.23845	-519.76435	377.31045	459.42366	1
266	H	81.45540	70.63519	68.20949	-1746.74323	1667.50644	-1261.73691	1
267	C	80.96015	70.11010	66.17049	570.95554	16.46261	-545.27700	1
268	H	81.77681	69.34905	66.07381	2391.58273	28.05277	-1305.07271	1
269	H	80.01389	69.55844	66.39889	175.75588	917.63458	2559.43867	1
270	H	80.82651	70.58210	65.16281	-1063.97851	-2155.34650	1283.00462	1
271	C	82.54696	71.89342	66.84495	193.76014	2.62946	-765.53141	1
272	H	83.39650	71.18642	66.65762	507.39394	-846.55087	2539.60089	1
273	H	82.40174	72.49218	65.90849	1337.57841	1818.19054	1526.01994	1
274	H	82.87774	72.60199	67.64775	1100.88635	-1172.91350	-2199.08909	1
275	C	79.04982	74.10850	68.60316	-549.21115	475.64486	-309.38218	1
276	O	78.10012	73.84405	69.29207	556.06106	-390.37755	-78.24250	1
277	O	78.98758	75.17320	67.7203	-572.27940	-310.19032	-209.75862	1
278	H	79.89584	75.08040	67.27135	-1380.08193	2212.14486	790.85944	1

Listing 15: C00015.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	1.0837	4335
		0.2500	300.00	0.00	0.00	0.00	-1294.0898	0.0000	300.0000
3	H	74.40700	81.18762	86.05284	-2043.14101	-1757.64893	399.89339		1
4	N	74.98250	80.68799	85.37747	426.75047	490.45733	-334.42467		1

5	H	75.22072	79.83376	85.87685	442.25559	-1110.30854	-2448.52907	1
6	C	76.09979	81.40186	84.89445	415.32972	-666.39213	83.73172	1
7	H	75.72219	82.41201	84.63075	879.32219	2491.00447	667.35213	1
8	C	77.24028	81.42918	86.03071	31.35357	477.41777	628.23362	1
9	H	77.56681	80.38413	86.24957	1168.38489	2240.25337	-1019.71136	1
10	H	78.14366	81.95520	85.63853	-360.43770	2534.90498	931.67112	1
11	C	76.74319	82.09630	87.28837	463.18208	512.70242	-382.34388	1
12	H	75.84311	81.54977	87.64821	1725.29117	1863.52247	-987.07854	1
13	C	77.80853	82.03151	88.37572	710.42801	-144.27427	-313.15367	1
14	H	77.45117	82.49168	89.33309	364.20195	-1033.13725	2494.72524	1
15	H	78.10444	80.97502	88.60425	2567.61904	335.80679	847.48802	1
16	H	78.73886	82.57820	88.07308	-2587.99029	680.92867	-512.16411	1
17	C	76.36138	83.54870	87.03919	268.17616	741.64379	-40.42634	1
18	H	76.02677	84.05492	87.98152	1283.54314	-1945.37420	-1411.27812	1
19	H	77.22494	84.13775	86.63503	-1258.57796	1317.15249	-2026.02085	1
20	H	75.52325	83.63836	86.30112	-2502.84526	909.80597	575.92391	1
21	C	76.68700	80.54253	83.62682	619.36578	-458.64843	-172.09273	1
22	O	77.00451	79.37981	83.71900	-81.40433	433.87611	522.34594	1
23	N	76.78765	81.37044	82.59242	175.23996	-622.20190	341.55523	1
24	H	76.56728	82.35498	82.74035	-876.57256	-303.22879	-2561.90213	1
25	C	77.19255	80.91318	81.30922	-571.88214	-534.10783	-106.15033	1
26	H	77.14485	81.83007	80.67912	-2713.20841	-16.25800	-248.80809	1
27	C	78.70022	80.39291	81.50756	166.60354	288.16399	-716.09568	1
28	H	78.64050	79.45474	82.12845	-2097.85574	1636.78449	-586.18044	1
29	O	79.57270	81.29633	82.21061	-317.80580	-363.38227	484.43082	1
30	H	79.72381	80.79429	83.03681	1863.74748	-1451.84923	1357.29467	1
31	C	79.18904	80.04094	80.05654	503.80731	517.99032	318.51606	1
32	H	80.22140	79.61921	80.06956	640.61020	-2157.10410	-1536.29104	1
33	H	78.52498	79.28160	79.55197	1687.88455	465.60692	2087.56452	1
34	H	79.21476	80.94703	79.40696	-1293.07895	-1899.88581	-1463.57452	1
35	C	76.18938	79.74503	80.79682	-153.07550	-733.68902	248.70981	1
36	O	76.63741	78.94030	80.01202	186.15459	-480.78787	-449.34387	1
37	N	74.91444	79.88459	81.17888	-487.53139	543.18517	42.03850	1
38	C	74.01559	78.77145	81.24464	-699.35871	69.34393	360.10701	1
39	H	74.62238	77.87838	81.52245	2.81126	-221.99807	-2715.58072	1
40	C	72.99376	79.28942	82.35003	-507.46439	-592.59194	122.07761	1
41	H	72.04986	78.69989	82.37975	-1975.08116	525.87560	-1801.71556	1
42	H	73.43817	79.25266	83.37049	1588.27743	-1913.22100	1113.83566	1
43	C	72.79868	80.76041	81.87165	-613.62442	-457.55993	-194.14490	1
44	H	72.14845	80.80644	80.96905	1707.54637	-721.27992	1996.92523	1
45	H	72.33124	81.42199	82.63531	758.23357	2100.81767	1560.55011	1
46	C	74.29901	81.15874	81.53202	-352.41524	704.96076	49.21465	1
47	H	74.43042	81.84821	80.66099	1714.76886	-2070.42778	443.35792	1
48	H	74.87625	81.54310	82.40377	1224.15040	1801.50881	1636.97633	1
49	C	73.19793	78.57658	79.84916	566.85117	537.05831	117.62814	1
50	O	72.16366	77.90693	79.84049	-550.26779	-406.08867	4.21666	1
51	N	73.79453	79.12645	78.77809	566.34832	-425.77725	180.18749	1
52	H	74.61723	79.59264	79.18050	644.44502	2646.80550	-52.73430	1
53	C	72.93122	79.90863	77.90894	612.34801	-281.48662	411.56221	1
54	H	72.06722	80.19870	78.54621	1667.23498	-1490.75142	1556.16753	1
55	C	73.80540	81.14949	77.44930	-714.45746	-175.43074	286.98927	1
56	H	74.60848	80.78690	76.75177	-787.09484	1763.03619	-1922.46060	1
57	O	74.50797	81.85870	78.50487	-429.46514	516.51932	-128.40526	1
58	H	75.43312	81.73194	78.22455	1981.82785	436.16847	-1818.18182	1
59	C	72.77205	82.02416	76.65086	630.79189	-468.94448	76.03230	1
60	H	73.25438	82.93417	76.22435	-1775.71861	2062.30353	131.89849	1
61	H	72.31114	81.46346	75.80059	-1855.14608	88.94118	1993.53760	1
62	H	71.94100	82.36918	77.30912	-1504.82350	-780.94249	-2132.90992	1
63	C	72.48352	79.01939	76.64277	288.57638	618.62814	-397.00270	1
64	O	71.59151	79.43141	75.89244	321.70495	-185.26452	574.37218	1
65	N	73.28936	77.96313	76.43229	-447.05792	-446.53431	367.76425	1
66	H	73.98642	78.04791	77.18363	350.31316	1975.63644	-1843.31522	1

67	C	72.78350	76.62493	76.23683	-511.23061	374.03917	-471.51480	1
68	H	73.73701	76.06283	76.12514	2234.79579	-898.70890	-1273.45190	1
69	C	72.07122	76.11712	77.57549	529.53781	-159.34528	563.72604	1
70	H	71.91639	75.01298	77.42216	654.59388	2347.94251	1217.51488	1
71	H	72.80470	76.23859	78.42245	-1526.55661	2103.42026	817.87394	1
72	O	70.81915	76.70490	77.94554	-554.84278	14.12789	399.58769	1
73	H	71.13992	77.25779	78.75670	1297.06236	2061.84854	1220.68812	1
74	C	71.80883	76.40689	74.99303	-662.15484	-412.13544	123.62687	1
75	O	71.35235	75.31010	74.80971	-540.01537	-317.05804	274.91456	1
76	N	71.66634	77.50034	74.20077	-202.76299	-690.00100	-131.49145	1
77	H	72.06674	78.38676	74.59273	-702.62132	-2617.37191	281.70413	1
78	C	70.37072	77.60841	73.45815	-491.73914	576.34187	222.73509	1
79	H	70.28164	76.61729	72.94649	1977.17978	-1823.58850	-434.68928	1
80	C	69.24248	77.91242	74.43185	-649.50797	-328.66843	306.11224	1
81	H	69.57022	78.77724	75.05619	2075.07803	1452.16490	-1004.45904	1
82	C	67.97623	78.30673	73.69271	-615.18735	-489.99689	-70.96352	1
83	H	67.15765	78.61502	74.39981	-1226.32661	-1724.38906	-1716.47170	1
84	H	68.15464	79.16830	72.99093	2381.64273	-969.84735	900.46860	1
85	H	67.57889	77.45687	73.07237	2122.74991	1702.23946	-141.36228	1
86	C	68.93924	76.76759	75.37826	-501.86074	-479.61276	-376.42482	1
87	H	68.09181	77.01710	76.07617	993.79261	-2246.95401	-1177.81305	1
88	H	68.65485	75.83159	74.82184	42.71279	-626.15391	-2651.37258	1
89	H	69.83518	76.51418	76.02049	-2026.39012	-1590.33709	-887.82922	1
90	C	70.48505	78.85871	72.46014	-672.89153	382.57394	-156.34072	1
91	O	70.07010	78.79623	71.25027	410.04627	221.86223	500.35950	1
92	N	70.97453	79.94055	72.99680	-378.11782	-443.79414	-441.10984	1
93	H	71.19765	79.93716	74.00180	2404.15973	-568.14894	1149.30085	1
94	C	70.56021	81.09491	72.24641	-544.54484	466.16019	331.29119	1
95	H	69.50720	81.20399	72.57731	-1409.80988	-170.17955	2325.32679	1
96	C	71.39800	82.34769	72.65378	-184.48284	116.78282	-758.89137	1
97	H	70.98236	82.83271	73.56764	1893.78641	1861.14652	611.04528	1
98	H	72.44463	82.06940	72.92052	-2170.79665	-974.19311	1327.50117	1
99	C	71.34589	83.32753	71.42898	389.51668	672.81878	-138.49152	1
100	H	71.56712	82.77895	70.48677	510.64577	1933.03327	1851.02484	1
101	H	70.30679	83.69298	71.27569	-2302.30869	-1105.72939	-948.89774	1
102	C	72.33288	84.54543	71.54757	-559.93427	-126.34590	542.30857	1
103	O	72.48575	85.28414	70.60725	-670.36003	-111.83166	76.36448	1
104	N	72.93640	84.65382	72.75237	-216.06729	-537.07037	446.51379	1
105	H	72.81357	84.08453	73.59748	-1251.96487	1074.12894	-2168.52500	1
106	H	73.57566	85.41520	73.00435	-2451.83023	-720.73851	944.84612	1
107	C	70.53465	80.60501	70.61402	546.24052	-563.88337	-85.11809	1
108	O	69.62876	81.08327	69.92147	71.70702	-307.40463	606.69673	1
109	N	71.81283	80.42461	70.11943	479.90863	-504.50129	222.86849	1
110	C	72.03249	80.26554	68.73724	75.51268	-600.91904	506.73700	1
111	H	71.19798	80.80302	68.22249	-2033.61562	1795.30103	254.89480	1
112	C	73.50488	80.88175	68.59192	523.79067	517.99274	284.45581	1
113	H	74.00491	80.58689	67.64314	1599.61665	-1127.00911	1895.98173	1
114	H	73.48756	81.99381	68.61742	-1881.83093	1275.82488	-1501.55016	1
115	C	74.18500	80.29505	69.86101	-600.05639	-404.05026	316.64485	1
116	H	74.45824	79.22532	69.72461	-2597.05260	496.36221	657.73249	1
117	H	75.11868	80.82460	70.15317	-1666.24518	1294.38985	-1723.90591	1
118	C	73.00860	80.46149	70.93076	493.57570	-129.95376	-602.56394	1
119	H	72.93331	79.65186	71.69657	-1469.08415	-637.84797	2204.22581	1
120	H	73.00169	81.45161	71.44420	-1038.97840	1068.88701	-2280.71789	1
121	C	72.19607	78.70002	68.23516	188.88100	241.05089	-727.87821	1
122	O	72.45506	78.49464	67.07492	531.88613	-49.19943	427.07960	1
123	N	72.04423	77.80733	69.20689	708.14833	26.93417	-179.73509	1
124	H	71.82197	78.20869	70.11916	-2232.69501	-1179.09831	1023.94816	1
125	C	72.50775	76.43041	69.04723	-738.32412	259.92548	104.42456	1
126	H	72.33048	76.20054	67.96978	2028.89123	1260.02983	1311.33324	1
127	C	73.98145	76.40845	69.41939	-258.65678	-345.52513	661.28459	1
128	H	74.13808	77.14067	70.25578	-1826.06090	-1801.46097	-918.64554	1

129	C	74.43565	75.05048	69.91761	-541.23400	531.92970	-218.41428	1
130	H	75.55141	75.01356	70.06297	1311.73218	-2219.18200	882.19023	1
131	H	73.96794	74.79902	70.91200	-1048.71298	1223.58118	-2196.97971	1
132	H	74.16044	74.22820	69.19955	419.06414	1903.92898	1903.44670	1
133	C	74.84441	76.84398	68.25005	-423.86431	152.66566	-648.55262	1
134	H	75.92596	76.94808	68.54311	105.68386	-2342.50080	1387.51238	1
135	H	74.79688	76.10395	67.40325	-1695.63603	-1484.73621	-1531.02793	1
136	H	74.50816	77.83735	67.83555	-1853.57121	-487.39031	1936.59343	1
137	C	71.61716	75.50557	70.09921	539.71428	-510.58232	267.58633	1
138	O	71.58644	75.74182	71.28587	-15.93758	-278.34085	-624.49402	1
139	N	71.07927	74.48584	69.45551	-676.81886	12.05292	276.17960	1
140	H	71.24717	74.40930	68.45500	-1694.44250	-373.84189	-2100.66098	1
141	C	70.17876	73.63708	70.16437	412.33078	-664.70360	108.35451	1
142	H	69.84609	74.28519	71.00906	1765.77476	1294.44366	1621.76594	1
143	C	69.05193	73.20948	69.14295	-179.66635	-721.95667	-264.73915	1
144	H	68.62774	74.10524	68.63556	-607.34922	2587.87032	-598.10018	1
145	H	69.48447	72.58307	68.33074	-359.69332	-1479.13954	-2259.74260	1
146	C	67.93221	72.42040	69.89988	-240.01076	616.02425	431.85322	1
147	H	68.36184	71.51743	70.39485	-1359.17131	782.54425	2227.99181	1
148	H	67.48479	73.03854	70.71019	-820.36667	85.81767	-2596.78715	1
149	C	66.84115	72.01979	68.82617	-513.07015	236.18570	-551.87280	1
150	H	66.46552	72.92271	68.29209	1816.11944	-1183.11722	-1650.94321	1
151	H	67.28719	71.36896	68.03936	-1800.04429	-1361.53473	1526.34643	1
152	C	65.67688	71.29128	69.53537	726.08972	-253.19732	-179.64713	1
153	H	65.95037	70.32016	69.99386	1224.27271	-456.51798	-2390.90304	1
154	H	65.11877	71.91136	70.26491	1206.40339	-1150.93514	-2154.90344	1
155	N	64.61560	70.92369	68.44182	329.70796	-633.68968	-155.67358	1
156	H	63.75788	70.40625	68.79067	1348.31305	1938.76845	1359.00643	1
157	H	64.17064	71.72608	67.90811	2096.92035	1446.54551	-966.48890	1
158	H	64.93533	70.28757	67.65471	-1197.07217	-2303.53719	827.28733	1
159	C	71.01906	72.32900	70.69777	-378.01186	-556.17301	-413.96481	1
160	O	70.62398	71.20363	70.50268	-409.44433	-307.55053	-453.30833	1
161	N	72.08470	72.72481	71.38193	-429.02477	524.70884	274.08502	1
162	H	72.25034	73.73074	71.47745	1706.34263	-1425.96036	1574.38926	1
163	C	72.96575	71.73197	71.89685	-45.25864	-626.22952	478.93267	1
164	H	72.33731	70.82847	72.07844	1988.63164	570.90773	1772.87287	1
165	C	74.09329	71.48313	70.80503	551.77128	-20.49526	-564.54996	1
166	H	73.64617	71.34240	69.79622	1434.61535	-1753.10253	1513.99471	1
167	H	74.74558	72.38053	70.71947	-714.67738	1819.09770	1898.36494	1
168	C	74.91901	70.22935	71.23927	446.99263	-555.77305	338.97221	1
169	H	74.60699	69.88618	72.25046	1953.68466	1892.25957	-161.67766	1
170	H	74.72822	69.36953	70.55896	-403.03785	2688.07032	-188.43591	1
171	C	76.45400	70.60630	71.25859	567.86262	335.74681	434.04421	1
172	H	76.81468	70.86770	70.23789	-1080.02275	1568.26081	-1948.78900	1
173	H	76.63019	71.51249	71.87982	-919.54108	2111.34692	1456.13463	1
174	C	77.22348	69.38461	71.82507	195.81897	173.33862	-745.11536	1
175	H	76.92149	69.07632	72.84756	1405.67949	-2301.21089	-390.08113	1
176	H	77.22251	68.50303	71.15231	-940.37328	-1118.32446	2299.72133	1
177	N	78.71766	69.77201	71.95110	319.26422	656.36007	-42.02424	1
178	H	79.43618	68.91429	71.97014	1961.03633	619.91968	1787.09422	1
179	H	79.09610	70.39846	71.18458	854.14343	-2156.80752	1429.08711	1
180	H	78.97402	70.33808	72.81134	1237.02905	-1378.50857	-1998.28500	1
181	C	73.77089	72.35464	73.17713	532.53319	-268.57236	517.55729	1
182	O	74.19509	73.48107	73.16062	266.16714	-290.73804	-558.88002	1
183	N	74.07226	71.35075	74.02492	-226.25352	640.49678	-270.32839	1
184	H	73.50745	70.50967	73.88734	2007.69063	-1035.27229	1523.50231	1
185	C	74.33939	71.72363	75.39628	-540.76542	-573.33303	49.50000	1
186	H	73.56583	72.48466	75.63991	-2374.20950	-1036.76023	843.75774	1
187	C	74.19071	70.38186	76.22664	-77.09082	666.87422	-415.84136	1
188	H	75.08697	69.73123	76.03147	-985.81834	617.19825	2463.91927	1
189	O	73.03847	69.56581	75.90403	293.29899	-391.65602	-477.80926	1
190	H	73.46540	68.72334	75.65993	2528.72714	-681.76262	-751.27122	1

191	C	74.24576	70.91470	77.70582	252.47363	-605.14473	440.05134	1
192	H	74.23954	70.07661	78.44081	-2052.65063	1456.49051	-1043.51830	1
193	H	75.16372	71.52312	77.89765	-2152.98800	-1661.97574	-161.70652	1
194	H	73.36578	71.55966	77.93553	-473.12726	-1584.27339	2165.61725	1
195	C	75.85060	72.31790	75.52118	360.36307	488.46713	505.10056	1
196	O	76.15661	72.92313	76.52947	-200.08817	-528.03552	-385.82850	1
197	N	76.62385	71.92353	74.51151	-597.54095	-226.44775	355.20479	1
198	H	76.09014	71.44728	73.78478	2179.23655	-1300.70981	-991.33835	1
199	C	77.88124	72.51117	74.21257	-687.68921	297.39807	-249.45179	1
200	H	77.92902	72.47161	73.10238	-349.16256	-2467.37713	-1101.72831	1
201	C	78.04263	73.99339	74.78905	672.47345	361.54328	-201.62880	1
202	H	77.76587	74.00462	75.87803	1541.41502	582.18425	2169.97026	1
203	H	79.11801	74.28343	74.72229	-2534.67717	60.25153	997.72295	1
204	C	77.17629	74.99563	74.00830	574.26774	-389.43119	-377.02542	1
205	C	77.64223	75.60480	72.80396	688.82679	-287.33580	-257.96133	1
206	H	78.63123	75.33954	72.38892	331.14182	1470.38163	2269.80013	1
207	C	75.89012	75.33064	74.52443	-383.52382	-675.04808	144.24917	1
208	H	75.51280	74.83062	75.43840	4.09847	1517.59662	2262.86397	1
209	C	76.83375	76.55353	72.16750	-134.76730	428.45285	-649.50303	1
210	H	77.20510	77.02473	71.24059	-903.23433	1600.49020	2011.53387	1
211	C	75.11832	76.28259	73.84808	-335.53281	-615.00040	-364.39058	1
212	H	74.11975	76.53412	74.24363	1596.45398	-1369.33862	1732.02659	1
213	C	75.55361	76.93778	72.66269	585.48547	-340.24194	-406.23938	1
214	O	74.75162	77.93145	72.01136	-419.15649	-173.04408	-511.94141	1
215	H	73.92747	77.83977	72.54909	-1071.84350	1559.71507	-1960.13012	1
216	C	79.08410	71.65510	74.88623	291.41878	-183.13091	710.72246	1
217	O	80.18906	72.14761	74.96038	379.87695	523.47396	-222.23622	1
218	N	78.73867	70.38725	75.16412	564.30591	373.09380	277.24371	1
219	H	77.74057	70.19171	75.08421	-120.59931	-2436.07824	-1214.35098	1
220	C	79.59142	69.67717	76.07251	404.07514	-299.37480	608.84009	1
221	H	80.55294	70.24569	76.06549	-1071.07882	-841.69025	2359.66467	1
222	C	78.88482	69.68575	77.49664	-683.12807	68.71770	-390.13096	1
223	H	78.55816	70.71414	77.76864	2068.88918	1596.58590	770.89603	1
224	H	77.95545	69.07387	77.47036	1379.86429	2342.49779	-179.85638	1
225	C	79.88949	69.11758	78.54512	-176.39967	537.49466	550.97268	1
226	H	80.23950	68.09555	78.24285	-396.28051	1942.22168	1869.33314	1
227	H	80.80873	69.74363	78.59112	-94.44700	586.00678	-2659.20016	1
228	C	79.17173	69.05532	79.97005	-291.69381	-718.18079	-150.72929	1
229	H	78.97366	70.04334	80.45811	-2303.38776	1089.76242	964.62032	1
230	H	78.23208	68.44812	80.01981	884.16729	2568.80533	-207.74283	1
231	N	80.15613	68.38265	80.71288	-594.49522	-252.81478	342.29276	1
232	H	81.01508	68.15646	80.23532	-1735.17426	2084.05705	-263.71605	1
233	C	80.03876	68.04211	81.93219	595.23177	-271.52487	442.22352	1
234	N	78.84339	68.36313	82.58445	585.53813	-424.79750	-105.81303	1
235	H	78.02112	68.84520	82.22376	959.88797	1327.56823	-2177.11905	1
236	H	78.63106	68.14481	83.55836	1578.48647	16.27378	-2220.76233	1
237	N	81.19147	67.38582	82.38699	-452.17763	-390.33541	-421.51853	1
238	H	82.05564	67.14346	81.90466	470.26107	1974.25629	-1817.92087	1
239	H	81.29319	67.02650	83.33684	1856.67307	-1573.97321	-1224.35416	1
240	C	79.73670	68.12372	75.64735	-531.47271	-581.45780	-55.06206	1
241	O	80.35423	67.34570	76.34310	-243.00837	192.73507	609.52485	1
242	N	79.02858	67.81020	74.54913	343.49288	-644.25607	38.09164	1
243	H	78.69011	68.61804	74.02988	-1691.16043	-1535.97525	-1484.73099	1
244	C	79.27798	66.49576	73.93289	542.66492	350.14337	454.42563	1
245	H	79.58662	65.85056	74.79297	1209.57979	-2396.95920	463.86744	1
246	C	78.00553	66.05992	73.22173	-737.14309	145.93010	242.71942	1
247	H	77.76807	66.82844	72.45369	-1050.18303	159.36419	-2509.06125	1
248	C	78.20208	64.73150	72.51563	-706.77696	-252.88343	-245.16230	1
249	H	77.28341	64.42090	71.94558	-1624.64039	-1665.49085	1417.86935	1
250	H	79.05414	64.77617	71.78146	2566.10521	598.51109	693.22305	1
251	H	78.43790	63.90712	73.24442	-1972.69758	107.10018	-1876.34312	1
252	C	76.82649	65.98259	74.17301	412.85148	672.58832	-27.69222	1

253	H	75.87286	65.71897	73.63731	1447.02277	1762.76533	-1490.78944	1
254	H	76.99024	65.20246	74.96735	1320.77379	-145.20455	2378.68491	1
255	H	76.65923	66.96234	74.70094	-1512.10848	1470.52031	1724.75147	1
256	C	80.46239	66.69328	72.80626	-607.11113	499.56689	73.73769	1
257	O	80.44460	67.65924	72.03841	357.97126	460.81534	356.68785	1
258	N	81.30008	65.70082	72.86342	536.55407	-368.62270	332.76306	1
259	H	81.14627	64.98911	73.57611	524.38866	2297.69985	1367.20941	1
260	C	82.12635	65.39275	71.72790	46.50277	-774.29190	-147.97904	1
261	H	81.38475	65.12502	70.94333	1676.51875	1883.29066	1032.55549	1
262	C	82.94296	66.71833	71.31932	-559.41456	-34.19198	-556.30433	1
263	H	82.74048	67.51019	72.08339	-64.66664	395.18769	2695.05373	1
264	H	84.04515	66.53761	71.32977	-2703.44278	-60.40056	333.79418	1
265	C	82.48154	67.17342	69.95848	-519.76435	377.31045	459.42366	1
266	H	81.37049	67.27098	69.98803	-1746.74323	1667.50644	-1261.73691	1
267	C	83.07042	68.54170	69.63762	570.95554	16.46261	-545.27700	1
268	H	82.71967	68.92027	68.64309	2391.58273	28.05277	-1305.07271	1
269	H	82.77951	69.30437	70.40579	175.75588	917.63458	2559.43867	1
270	H	84.19002	68.51177	69.60580	-1063.97851	-2155.34650	1283.00462	1
271	C	82.85730	66.18325	68.86573	193.76014	2.62946	-765.53141	1
272	H	82.50448	66.52840	67.85961	507.39394	-846.55087	2539.60089	1
273	H	83.96727	66.04602	68.79681	1337.57841	1818.19054	1526.01994	1
274	H	82.40822	65.17207	69.04347	1100.88635	-1172.91350	-2199.08909	1
275	C	83.03585	64.15828	72.16682	-549.21115	475.64486	-309.38218	1
276	O	82.77863	63.46707	73.12032	556.06106	-390.37755	-78.24250	1
277	O	84.12741	63.83156	71.32007	-572.27940	-310.19032	-209.75862	1
278	H	84.01138	64.54073	70.63466	-1380.08193	2212.14486	790.85944	1

Listing 16: C00016.xmolout

1		276						
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750 11100
		0.2500	300.00	0.00	0.00	0.00	-1294.0794	0.0000 300.0000
3	H	73.51008	68.00272	85.91873	-2043.14101	-1757.64893	399.89339	1
4	N	74.37950	67.76352	85.44411	426.75047	490.45733	-334.42467	1
5	H	74.05490	67.38443	84.54964	442.25559	-1110.30854	-2448.52907	1
6	C	75.24949	68.85554	85.24031	415.32972	-666.39213	83.73172	1
7	H	75.06718	69.60390	86.04164	879.32219	2491.00447	667.35213	1
8	C	76.76091	68.28828	85.22154	31.35357	477.41777	628.23362	1
9	H	76.85394	67.54584	84.39280	1168.38489	2240.25337	-1019.71136	1
10	H	77.48320	69.10935	84.98806	-360.43770	2534.90498	931.67112	1
11	C	77.10442	67.63903	86.53644	463.18208	512.70242	-382.34388	1
12	H	76.26026	66.97419	86.82841	1725.29117	1863.52247	-987.07854	1
13	C	78.36202	66.79175	86.38525	710.42801	-144.27427	-313.15367	1
14	H	78.64021	66.28699	87.34604	364.20195	-1033.13725	2494.72524	1
15	H	78.23008	65.98938	85.61409	2567.61904	335.80679	847.48802	1
16	H	79.24036	67.41222	86.07008	-2587.99029	680.92867	-512.16411	1
17	C	77.31541	68.67821	87.62873	268.17616	741.64379	-40.42634	1
18	H	77.58415	68.20093	88.60651	1283.54314	-1945.37420	-1411.27812	1
19	H	78.14346	69.38697	87.36759	-1258.57796	1317.15249	-2026.02085	1
20	H	76.39418	69.29232	87.80044	-2502.84526	909.80597	575.92391	1
21	C	74.90008	69.36208	83.73387	619.36578	-458.64843	-172.09273	1
22	O	74.47561	68.60167	82.88531	-81.40433	433.87611	522.34594	1
23	N	75.26659	70.63353	83.59993	175.23996	-622.20190	341.55523	1
24	H	75.64141	71.12784	84.40901	-876.57256	-303.22879	-2561.90213	1
25	C	75.27334	71.20099	82.30027	-571.88214	-534.10783	-106.15033	1
26	H	74.83011	70.40809	81.65141	-2713.20841	-16.25800	-248.80809	1
27	C	74.47431	72.59246	82.33937	166.60354	288.16399	-716.09568	1
28	H	75.08064	73.32554	82.94268	-2097.85574	1636.78449	-586.18044	1
29	O	73.16870	72.55429	82.93758	-317.80580	-363.38227	484.43082	1
30	H	73.29194	73.15247	83.70297	1863.74748	-1451.84923	1357.29467	1
31	C	74.50987	73.01300	80.82388	503.80731	517.99032	318.51606	1
32	H	74.06967	74.02592	80.67223	640.61020	-2157.10410	-1536.29104	1

33	H	75.55303	73.04096	80.42533	1687.88455	465.60692	2087.56452	1
34	H	73.92927	72.30287	80.18971	-1293.07895	-1899.88581	-1463.57452	1
35	C	76.81649	71.62406	81.93992	-153.07550	-733.68902	248.70981	1
36	O	77.11848	72.78109	82.07155	186.15459	-480.78787	-449.34387	1
37	N	77.58508	70.57208	81.62892	-487.53139	543.18517	42.03850	1
38	C	78.84231	70.74302	80.96483	-699.35871	69.34393	360.10701	1
39	H	79.06304	71.83074	81.07181	2.81126	-221.99807	-2715.58072	1
40	C	79.75922	69.76556	81.82149	-507.46439	-592.59194	122.07761	1
41	H	80.71710	69.50456	81.31902	-1975.08116	525.87560	-1801.71556	1
42	H	80.03429	70.23000	82.79420	1588.27743	-1913.22100	1113.83566	1
43	C	78.81002	68.54605	82.04105	-613.62442	-457.55993	-194.14490	1
44	H	78.75585	67.89729	81.13930	1707.54637	-721.27992	1996.92523	1
45	H	79.11846	67.88681	82.88384	758.23357	2100.81767	1560.55011	1
46	C	77.43214	69.28860	82.30739	-352.41524	704.96076	49.21465	1
47	H	76.52952	68.77502	81.89638	1714.76886	-2070.42778	443.35792	1
48	H	77.24681	69.56290	83.37215	1224.15040	1801.50881	1636.97633	1
49	C	78.60270	70.30087	79.41111	566.85117	537.05831	117.62814	1
50	O	77.78181	70.92951	78.74268	-550.26779	-406.08867	4.21666	1
51	N	79.31014	69.25740	79.07295	566.34832	-425.77725	180.18749	1
52	H	79.97002	68.88358	79.75117	644.44502	2646.80550	-52.73430	1
53	C	79.38377	68.81591	77.71055	612.34801	-281.48662	411.56221	1
54	H	79.69928	69.70440	77.12081	1667.23498	-1490.75142	1556.16753	1
55	C	80.44341	67.62853	77.72468	-714.45746	-175.43074	286.98927	1
56	H	80.05523	66.80452	78.38601	-787.09484	1763.03619	-1922.46060	1
57	O	81.74594	67.95611	78.25328	-429.46514	516.51932	-128.40526	1
58	H	81.82714	67.30845	78.98026	1981.82785	436.16847	-1818.18182	1
59	C	80.39513	67.14900	76.22759	630.79189	-468.94448	76.03230	1
60	H	80.99225	66.21919	76.07880	-1775.71861	2062.30353	131.89849	1
61	H	79.34965	66.93350	75.89600	-1855.14608	88.94118	1993.53760	1
62	H	80.80921	67.92205	75.53977	-1504.82350	-780.94249	-2132.90992	1
63	C	77.90459	68.28806	77.25565	288.57638	618.62814	-397.00270	1
64	O	77.58107	68.36858	76.09340	321.70495	-185.26452	574.37218	1
65	N	77.33435	67.62602	78.26932	-447.05792	-446.53431	367.76425	1
66	H	77.88104	67.71199	79.12793	350.31316	1975.63644	-1843.31522	1
67	C	75.90723	67.55549	78.40817	-511.23061	374.03917	-471.51480	1
68	H	75.83881	66.82199	79.24191	2234.79579	-898.70890	-1273.45190	1
69	C	75.41835	68.98570	78.91009	529.53781	-159.34528	563.72604	1
70	H	74.37986	68.83498	79.31306	654.59388	2347.94251	1217.51488	1
71	H	76.07170	69.27956	79.77559	-1526.55661	2103.42026	817.87394	1
72	O	75.37679	70.07086	77.96190	-554.84278	14.12789	399.58769	1
73	H	76.28710	70.49593	78.15014	1297.06236	2061.84854	1220.68812	1
74	C	75.28544	66.95786	77.04371	-662.15484	-412.13544	123.62687	1
75	O	75.59402	65.84877	76.67748	-540.01537	-317.05804	274.91456	1
76	N	74.38241	67.79589	76.46709	-202.76299	-690.00100	-131.49145	1
77	H	74.27040	68.68310	76.98124	-702.62132	-2617.37191	281.70413	1
78	C	74.72183	68.01919	75.06511	-491.73914	576.34187	222.73509	1
79	H	75.82555	67.84320	75.01996	1977.17978	-1823.58850	-434.68928	1
80	C	73.87673	67.03280	74.17197	-649.50797	-328.66843	306.11224	1
81	H	72.80220	67.07168	74.45480	2075.07803	1452.16490	-1004.45904	1
82	C	74.07200	67.47294	72.67822	-615.18735	-489.99689	-70.96352	1
83	H	73.51930	66.80607	71.97589	-1226.32661	-1724.38906	-1716.47170	1
84	H	73.70010	68.51208	72.51003	2381.64273	-969.84735	900.46860	1
85	H	75.14635	67.45623	72.38033	2122.74991	1702.23946	-141.36228	1
86	C	74.43340	65.57334	74.33138	-501.86074	-479.61276	-376.42482	1
87	H	74.14885	64.92263	73.47090	993.79261	-2246.95401	-1177.81305	1
88	H	75.54848	65.56821	74.40915	42.71279	-626.15391	-2651.37258	1
89	H	74.04280	65.08876	75.25983	-2026.39012	-1590.33709	-887.82922	1
90	C	74.27965	69.54618	74.71837	-672.89153	382.57394	-156.34072	1
91	O	73.12239	69.91523	74.65123	410.04627	221.86223	500.35950	1
92	N	75.38464	70.25036	74.51176	-378.11782	-443.79414	-441.10984	1
93	H	76.29727	69.79953	74.59244	2404.15973	-568.14894	1149.30085	1
94	C	75.21000	71.58465	74.02384	-544.54484	466.16019	331.29119	1

95	H	74.28596	71.92448	74.54323	-1409.80988	-170.17955	2325.32679	1
96	C	76.52404	72.38244	74.38454	-184.48284	116.78282	-758.89137	1
97	H	76.74466	72.29047	75.47243	1893.78641	1861.14652	611.04528	1
98	H	77.41133	71.97020	73.85337	-2170.79665	-974.19311	1327.50117	1
99	C	76.24689	73.87585	73.98096	389.51668	672.81878	-138.49152	1
100	H	76.32275	73.99280	72.87409	510.64577	1933.03327	1851.02484	1
101	H	75.18718	74.14001	74.19492	-2302.30869	-1105.72939	-948.89774	1
102	C	77.14541	74.90865	74.69171	-559.93427	-126.34590	542.30857	1
103	O	76.76148	76.13740	74.73126	-670.36003	-111.83166	76.36448	1
104	N	78.23259	74.40058	75.19287	-216.06729	-537.07037	446.51379	1
105	H	78.46753	73.40047	75.10268	-1251.96487	1074.12894	-2168.52500	1
106	H	78.97357	74.90159	75.77677	-2451.83023	-720.73851	944.84612	1
107	C	75.03651	71.50171	72.39297	546.24052	-563.88337	-85.11809	1
108	O	75.91389	71.04020	71.71311	71.70702	-307.40463	606.69673	1
109	N	73.85856	72.02928	72.02129	479.90863	-504.50129	222.86849	1
110	C	73.52681	72.20717	70.64395	75.51268	-600.91904	506.73700	1
111	H	74.05372	71.41759	70.06025	-2033.61562	1795.30103	254.89480	1
112	C	71.93903	72.10108	70.68917	523.79067	517.99274	284.45581	1
113	H	71.44866	72.53855	69.79087	1599.61665	-1127.00911	1895.98173	1
114	H	71.59790	71.04443	70.76100	-1881.83093	1275.82488	-1501.55016	1
115	C	71.63423	72.88908	71.99938	-600.05639	-404.05026	316.64485	1
116	H	71.70675	73.98401	71.81063	-2597.05260	496.36221	657.73249	1
117	H	70.61772	72.70012	72.41284	-1666.24518	1294.38985	-1723.90591	1
118	C	72.80348	72.39852	72.95526	493.57570	-129.95376	-602.56394	1
119	H	73.20157	73.18841	73.63495	-1469.08415	-637.84797	2204.22581	1
120	H	72.59368	71.45809	73.55237	-1038.97840	1068.88701	-2280.71789	1
121	C	73.95461	73.72751	70.21443	188.88100	241.05089	-727.87821	1
122	O	74.16011	74.60664	71.01315	531.88613	-49.19943	427.07960	1
123	N	73.83096	73.87293	68.85185	708.14833	26.93417	-179.73509	1
124	H	73.77854	72.89242	68.55337	-2232.69501	-1179.09831	1023.94816	1
125	C	74.74668	74.82670	68.17829	-738.32412	259.92548	104.42456	1
126	H	75.74789	74.63469	68.62685	2028.89123	1260.02983	1311.33324	1
127	C	74.68442	74.54612	66.69776	-258.65678	-345.52513	661.28459	1
128	H	73.60992	74.48172	66.41179	-1826.06090	-1801.46097	-918.64554	1
129	C	75.32095	75.66495	65.89071	-541.23400	531.92970	-218.41428	1
130	H	75.18676	75.51187	64.78471	1311.73218	-2219.18200	882.19023	1
131	H	74.87281	76.66534	66.15332	-1048.71298	1223.58118	-2196.97971	1
132	H	76.42533	75.73886	66.08744	419.06414	1903.92898	1903.44670	1
133	C	75.33984	73.22504	66.33202	-423.86431	152.66566	-648.55262	1
134	H	75.26319	73.01441	65.23027	105.68386	-2342.50080	1387.51238	1
135	H	76.43278	73.22122	66.59584	-1695.63603	-1484.73621	-1531.02793	1
136	H	74.86717	72.35925	66.87049	-1853.57121	-487.39031	1936.59343	1
137	C	74.20831	76.34976	68.49562	539.71428	-510.58232	267.58633	1
138	O	74.95511	77.29030	68.35123	-15.93758	-278.34085	-624.49402	1
139	N	72.89595	76.36835	68.73640	-676.81886	12.05292	276.17960	1
140	H	72.48093	75.43984	68.81219	-1694.44250	-373.84189	-2100.66098	1
141	C	72.39301	77.44214	69.54198	412.33078	-664.70360	108.35451	1
142	H	73.28726	77.97938	69.94416	1765.77476	1294.44366	1621.76594	1
143	C	71.52379	78.31164	68.54615	-179.66635	-721.95667	-264.73915	1
144	H	72.13421	78.62517	67.66983	-607.34922	2587.87032	-598.10018	1
145	H	70.69491	77.69748	68.12742	-359.69332	-1479.13954	-2259.74260	1
146	C	70.96051	79.55673	69.30713	-240.01076	616.02425	431.85322	1
147	H	70.35809	79.24509	70.19003	-1359.17131	782.54425	2227.99181	1
148	H	71.78243	80.19359	69.70372	-820.36667	85.81767	-2596.78715	1
149	C	70.07316	80.34973	68.26416	-513.07015	236.18570	-551.87280	1
150	H	70.68452	80.66693	67.38837	1816.11944	-1183.11722	-1650.94321	1
151	H	69.27328	79.69342	67.85038	-1800.04429	-1361.53473	1526.34643	1
152	C	69.45362	81.57775	68.96935	726.08972	-253.19732	-179.64713	1
153	H	68.73711	81.33378	69.77892	1224.27271	-456.51798	-2390.90304	1
154	H	70.18826	82.32635	69.32767	1206.40339	-1150.93514	-2154.90344	1
155	N	68.59878	82.33848	67.89890	329.70796	-633.68968	-155.67358	1
156	H	68.10372	83.21041	68.24442	1348.31305	1938.76845	1359.00643	1

157	H	69.11153	82.71446	67.04897	2096.92035	1446.54551	-966.48890	1
158	H	67.79603	81.80616	67.45266	-1197.07217	-2303.53719	827.28733	1
159	C	71.38586	76.79954	70.65245	-378.01186	-556.17301	-413.96481	1
160	O	70.48942	76.05724	70.33375	-409.44433	-307.55053	-453.30833	1
161	N	71.71827	77.25175	71.86351	-429.02477	524.70884	274.08502	1
162	H	72.52675	77.90769	71.97232	1706.34263	-1425.96036	1574.38926	1
163	C	70.64784	77.21985	72.84002	-45.25864	-626.22952	478.93267	1
164	H	69.78123	77.71503	72.34938	1988.63164	570.90773	1772.87287	1
165	C	70.36182	75.69981	73.14880	551.77128	-20.49526	-564.54996	1
166	H	70.04090	75.17432	72.21476	1434.61535	-1753.10253	1513.99471	1
167	H	71.29778	75.19408	73.47835	-714.67738	1819.09770	1898.36494	1
168	C	69.25946	75.57514	74.25316	446.99263	-555.77305	338.97221	1
169	H	69.59554	76.04763	75.20384	1953.68466	1892.25957	-161.67766	1
170	H	68.32826	76.10731	73.95611	-403.03785	2688.07032	-188.43591	1
171	C	68.99608	74.02678	74.44218	567.86262	335.74681	434.04421	1
172	H	68.62555	73.57303	73.49433	-1080.02275	1568.26081	-1948.78900	1
173	H	69.94422	73.49238	74.68213	-919.54108	2111.34692	1456.13463	1
174	C	67.96404	73.83505	75.57703	195.81897	173.33862	-745.11536	1
175	H	68.32318	74.13154	76.58273	1405.67949	-2301.21089	-390.08113	1
176	H	66.97072	74.28574	75.38117	-940.37328	-1118.32446	2299.72133	1
177	N	67.68547	72.29747	75.69254	319.26422	656.36007	-42.02424	1
178	H	67.00473	72.00735	76.45247	1961.03633	619.91968	1787.09422	1
179	H	67.26772	71.81666	74.84342	854.14343	-2156.80752	1429.08711	1
180	H	68.51707	71.67453	75.90933	1237.02905	-1378.50857	-1998.28500	1
181	C	71.14098	77.95965	74.19348	532.53319	-268.57236	517.55729	1
182	O	70.35631	78.61849	74.87200	266.16714	-290.73804	-558.88002	1
183	N	72.38969	77.64429	74.47619	-226.25352	640.49678	-270.32839	1
184	H	72.90728	77.09093	73.79581	2007.69063	-1035.27229	1523.50231	1
185	C	72.93233	78.10745	75.71766	-540.76542	-573.33303	49.50000	1
186	H	72.04708	78.08152	76.39495	-2374.20950	-1036.76023	843.75774	1
187	C	74.10632	77.09373	76.09800	-77.09082	666.87422	-415.84136	1
188	H	74.83821	77.08989	75.24398	-985.81834	617.19825	2463.91927	1
189	O	73.67319	75.73120	76.28689	293.29899	-391.65602	-477.80926	1
190	H	74.25372	75.26961	75.64890	2528.72714	-681.76262	-751.27122	1
191	C	74.81384	77.75016	77.34006	252.47363	-605.14473	440.05134	1
192	H	75.63046	77.09275	77.72590	-2052.65063	1456.49051	-1043.51830	1
193	H	75.28811	78.72757	77.07232	-2152.98800	-1661.97574	-161.70652	1
194	H	74.10239	77.93167	78.17964	-473.12726	-1584.27339	2165.61725	1
195	C	73.41320	79.63774	75.43534	360.36307	488.46713	505.10056	1
196	O	74.59706	79.93031	75.32532	-200.08817	-528.03552	-385.82850	1
197	N	72.33539	80.38359	75.41838	-597.54095	-226.44775	355.20479	1
198	H	71.40024	79.91496	75.49180	2179.23655	-1300.70981	-991.33835	1
199	C	72.37184	81.76006	75.10046	-687.68921	297.39807	-249.45179	1
200	H	71.34531	82.10441	75.35343	-349.16256	-2467.37713	-1101.72831	1
201	C	73.52567	82.51035	75.91878	672.47345	361.54328	-201.62880	1
202	H	74.52834	82.16468	75.57281	1541.41502	582.18425	2169.97026	1
203	H	73.47287	83.60449	75.71520	-2534.67717	60.25153	997.72295	1
204	C	73.36567	82.22416	77.41839	574.26774	-389.43119	-377.02542	1
205	C	72.36773	82.89245	78.18873	688.82679	-287.33580	-257.96133	1
206	H	71.70211	83.64198	77.72348	331.14182	1470.38163	2269.80013	1
207	C	74.22161	81.25645	78.02584	-383.52382	-675.04808	144.24917	1
208	H	74.99279	80.73939	77.42343	4.09847	1517.59662	2262.86397	1
209	C	72.25001	82.57210	79.54110	-134.76730	428.45285	-649.50303	1
210	H	71.47927	83.08796	80.13964	-903.23433	1600.49020	2011.53387	1
211	C	74.06223	80.96654	79.38227	-335.53281	-615.00040	-364.39058	1
212	H	74.72692	80.21168	79.83789	1596.45398	-1369.33862	1732.02659	1
213	C	73.07707	81.60870	80.18826	585.48547	-340.24194	-406.23938	1
214	O	72.90457	81.32189	81.56745	-419.15649	-173.04408	-511.94141	1
215	H	73.62348	80.65742	81.68974	-1071.84350	1559.71507	-1960.13012	1
216	C	72.68838	81.92957	73.50165	291.41878	-183.13091	710.72246	1
217	O	71.91360	82.52639	72.79624	379.87695	523.47396	-222.23622	1
218	N	73.87698	81.41662	73.19545	564.30591	373.09380	277.24371	1

219	H	74.45228	80.92459	73.92165	-120.59931	-2436.07824	-1214.35098	1
220	C	74.11970	81.17619	71.80157	404.07514	-299.37480	608.84009	1
221	H	73.09791	81.20253	71.35902	-1071.07882	-841.69025	2359.66467	1
222	C	74.96659	82.43483	71.34436	-683.12807	68.71770	-390.13096	1
223	H	74.52211	83.35146	71.79368	2068.88918	1596.58590	770.89603	1
224	H	76.00734	82.39587	71.73592	1379.86429	2342.49779	-179.85638	1
225	C	74.95464	82.54463	69.78938	-176.39967	537.49466	550.97268	1
226	H	75.49737	81.69075	69.31130	-396.28051	1942.22168	1869.33314	1
227	H	73.91682	82.51324	69.38756	-94.44700	586.00678	-2659.20016	1
228	C	75.65313	83.94851	69.47733	-291.69381	-718.18079	-150.72929	1
229	H	75.13562	84.84735	69.89927	-2303.38776	1089.76242	964.62032	1
230	H	76.73163	84.01206	69.77173	884.16729	2568.80533	-207.74283	1
231	N	75.59243	84.05285	68.08183	-594.49522	-252.81478	342.29276	1
232	H	75.27976	83.23717	67.57909	-1735.17426	2084.05705	-263.71605	1
233	C	75.90980	85.09377	67.42525	595.23177	-271.52487	442.22352	1
234	N	76.34836	86.21125	68.14504	585.53813	-424.79750	-105.81303	1
235	H	76.46416	86.33100	69.15050	959.88797	1327.56823	-2177.11905	1
236	H	76.63205	87.09854	67.72856	1578.48647	16.27378	-2220.76233	1
237	N	75.74843	84.89576	66.04675	-452.17763	-390.33541	-421.51853	1
238	H	75.43099	84.08409	65.51898	470.26107	1974.25629	-1817.92087	1
239	H	75.95496	85.61663	65.35398	1856.67307	-1573.97321	-1224.35416	1
240	C	74.81471	79.70523	71.72642	-531.47271	-581.45780	-55.06206	1
241	O	74.08151	78.72404	71.76392	-243.00837	192.73507	609.52485	1
242	N	76.14168	79.73473	71.72342	343.49288	-644.25607	38.09164	1
243	H	76.49407	80.69177	71.72408	-1691.16043	-1535.97525	-1484.73099	1
244	C	76.90819	78.67389	71.06322	542.66492	350.14337	454.42563	1
245	H	76.12789	78.00440	70.62460	1209.57979	-2396.95920	463.86744	1
246	C	77.80331	79.33874	70.03025	-737.14309	145.93010	242.71942	1
247	H	78.14706	80.31407	70.44127	-1050.18303	159.36419	-2509.06125	1
248	C	79.04395	78.51678	69.72413	-706.77696	-252.88343	-245.16230	1
249	H	79.60888	78.91222	68.83434	-1624.64039	-1665.49085	1417.86935	1
250	H	79.75741	78.50515	70.59892	2566.10521	598.51109	693.22305	1
251	H	78.77844	77.43947	69.51748	-1972.69758	107.10018	-1876.34312	1
252	C	77.04308	79.62482	68.75066	412.85148	672.58832	-27.69222	1
253	H	77.70879	80.07369	67.96091	1447.02277	1762.76533	-1490.78944	1
254	H	76.58529	78.68154	68.32109	1320.77379	-145.20455	2378.68491	1
255	H	76.19379	80.35188	68.93081	-1512.10848	1470.52031	1724.75147	1
256	C	77.87031	77.86509	72.14075	-607.11113	499.56689	73.73769	1
257	O	78.54139	76.93919	71.73618	357.97126	460.81534	356.68785	1
258	N	77.85165	78.37684	73.36185	536.55407	-368.62270	332.76306	1
259	H	77.19078	79.13024	73.54460	524.38866	2297.69985	1367.20941	1
260	C	78.73059	77.79058	74.30125	46.50277	-774.29190	-147.97904	1
261	H	79.23105	76.96538	73.73774	1676.51875	1883.29066	1032.55549	1
262	C	79.74314	78.90872	74.88036	-559.41456	-34.19198	-556.30433	1
263	H	79.15873	79.78804	75.24253	-64.66664	395.18769	2695.05373	1
264	H	80.27141	78.49390	75.77390	-2703.44278	-60.40056	333.79418	1
265	C	80.73037	79.32218	73.82190	-519.76435	377.31045	459.42366	1
266	H	80.17133	79.56041	72.88903	-1746.74323	1667.50644	-1261.73691	1
267	C	81.48963	80.56606	74.26728	570.95554	16.46261	-545.27700	1
268	H	82.23947	80.89130	73.50084	2391.58273	28.05277	-1305.07271	1
269	H	80.80029	81.43094	74.44713	175.75588	917.63458	2559.43867	1
270	H	82.04932	80.38567	75.22127	-1063.97851	-2155.34650	1283.00462	1
271	C	81.71934	78.20143	73.53014	193.76014	2.62946	-765.53141	1
272	H	82.49605	78.51692	72.78657	507.39394	-846.55087	2539.60089	1
273	H	82.26017	77.87934	74.45768	1337.57841	1818.19054	1526.01994	1
274	H	81.20942	77.29516	73.11240	1100.88635	-1172.91350	-2199.08909	1
275	C	77.93656	77.26277	75.62103	-549.21115	475.64486	-309.38218	1
276	O	77.30984	77.90113	76.40118	556.06106	-390.37755	-78.24250	1
277	O	79.23324	76.46331	76.35169	-572.27940	-310.19032	-209.75862	1
278	H	79.10041	76.79193	77.21994	-1380.08193	2212.14486	790.85944	1

Listing 17: C00017.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1294.0761	0.0000	300.0000
3	H	68.01668	88.30775	68.92051	-2043.14101	-1757.64893	399.89339		1
4	N	68.77492	88.78997	69.39946	426.75047	490.45733	-334.42467		1
5	H	69.10167	88.05903	70.02897	442.25559	-1110.30854	-2448.52907		1
6	C	69.75801	89.32942	68.53898	415.32972	-666.39213	83.73172		1
7	H	69.37033	89.19704	67.50595	879.32219	2491.00447	667.35213		1
8	C	69.95625	90.88049	68.92487	31.35357	477.41777	628.23362		1
9	H	70.28243	90.95806	69.98956	1168.38489	2240.25337	-1019.71136		1
10	H	70.77430	91.33790	68.31727	-360.43770	2534.90498	931.67112		1
11	C	68.65113	91.60692	68.71661	463.18208	512.70242	-382.34388		1
12	H	67.82892	90.95512	69.08962	1725.29117	1863.52247	-987.07854		1
13	C	68.62674	92.90631	69.51101	710.42801	-144.27427	-313.15367		1
14	H	67.65847	93.45468	69.37729	364.20195	-1033.13725	2494.72524		1
15	H	68.75527	92.72259	70.60908	2567.61904	335.80679	847.48802		1
16	H	69.44710	93.59991	69.19215	-2587.99029	680.92867	-512.16411		1
17	C	68.41361	91.90473	67.24270	268.17616	741.64379	-40.42634		1
18	H	67.43571	92.42731	67.07887	1283.54314	-1945.37420	-1411.27812		1
19	H	69.21553	92.56522	66.82216	-1258.57796	1317.15249	-2026.02085		1
20	H	68.39800	90.96956	66.62587	-2502.84526	909.80597	575.92391		1
21	C	71.13753	88.51167	68.81918	619.36578	-458.64843	-172.09273		1
22	O	71.81314	88.06746	67.90818	-81.40433	433.87611	522.34594		1
23	N	71.40173	88.49679	70.12273	175.23996	-622.20190	341.55523		1
24	H	70.69990	88.89389	70.74589	-876.57256	-303.22879	-2561.90213		1
25	C	72.39742	87.58164	70.57843	-571.88214	-534.10783	-106.15033		1
26	H	73.13086	87.53936	69.74307	-2713.20841	-16.25800	-248.80809		1
27	C	72.97343	88.13466	71.96291	166.60354	288.16399	-716.09568		1
28	H	72.12405	88.21899	72.69434	-2097.85574	1636.78449	-586.18044		1
29	O	73.57580	89.44036	71.89506	-317.80580	-363.38227	484.43082		1
30	H	72.98504	89.95307	72.48152	1863.74748	-1451.84923	1357.29467		1
31	C	73.93199	86.97179	72.41413	503.80731	517.99032	318.51606		1
32	H	74.43941	87.21733	73.37578	640.61020	-2157.10410	-1536.29104		1
33	H	73.39261	86.00484	72.57616	1687.88455	465.60692	2087.56452		1
34	H	74.73177	86.78592	71.66029	-1293.07895	-1899.88581	-1463.57452		1
35	C	71.60797	86.17328	70.84481	-153.07550	-733.68902	248.70981		1
36	O	70.76648	86.12932	71.70155	186.15459	-480.78787	-449.34387		1
37	N	72.05555	85.19714	70.03584	-487.53139	543.18517	42.03850		1
38	C	71.49541	83.88631	70.09228	-699.35871	69.34393	360.10701		1
39	H	70.46659	83.98249	70.50946	2.81126	-221.99807	-2715.58072		1
40	C	71.59105	83.43732	68.57064	-507.46439	-592.59194	122.07761		1
41	H	71.52876	82.33364	68.44090	-1975.08116	525.87560	-1801.71556		1
42	H	70.77114	83.87963	67.96174	1588.27743	-1913.22100	1113.83566		1
43	C	72.97746	84.03090	68.16804	-613.62442	-457.55993	-194.14490		1
44	H	73.80799	83.38808	68.53972	1707.54637	-721.27992	1996.92523		1
45	H	73.11899	84.12608	67.06758	758.23357	2100.81767	1560.55011		1
46	C	72.96095	85.42965	68.91654	-352.41524	704.96076	49.21465		1
47	H	73.94793	85.74621	69.32962	1714.76886	-2070.42778	443.35792		1
48	H	72.51031	86.29019	68.33411	1224.15040	1801.50881	1636.97633		1
49	C	72.44986	82.89276	70.98700	566.85117	537.05831	117.62814		1
50	O	72.11266	81.74777	71.17755	-550.26779	-406.08867	4.21666		1
51	N	73.56588	83.49989	71.37252	566.34832	-425.77725	180.18749		1
52	H	73.67283	84.48229	71.12943	644.44502	2646.80550	-52.73430		1
53	C	74.52483	82.76522	72.11309	612.34801	-281.48662	411.56221		1
54	H	74.25508	81.69151	71.97555	1667.23498	-1490.75142	1556.16753		1
55	C	75.96081	83.20401	71.56102	-714.45746	-175.43074	286.98927		1
56	H	76.10540	84.29948	71.77224	-787.09484	1763.03619	-1922.46060		1
57	O	76.16635	83.04923	70.14504	-429.46514	516.51932	-128.40526		1
58	H	76.35086	83.97221	69.87777	1981.82785	436.16847	-1818.18182		1
59	C	76.90922	82.36293	72.49211	630.79189	-468.94448	76.03230		1

60	H	77.98137	82.60543	72.30804	-1775.71861	2062.30353	131.89849	1
61	H	76.70703	82.55174	73.57225	-1855.14608	88.94118	1993.53760	1
62	H	76.78401	81.26892	72.31777	-1504.82350	-780.94249	-2132.90992	1
63	C	74.42973	83.29639	73.66972	288.57638	618.62814	-397.00270	1
64	O	74.43679	84.47673	73.93304	321.70495	-185.26452	574.37218	1
65	N	74.36127	82.23887	74.47697	-447.05792	-446.53431	367.76425	1
66	H	74.47797	81.34548	73.99752	350.31316	1975.63644	-1843.31522	1
67	C	74.78557	82.38504	75.84355	-511.23061	374.03917	-471.51480	1
68	H	75.83267	82.75474	75.78986	2234.79579	-898.70890	-1273.45190	1
69	C	73.82421	83.45651	76.53375	529.53781	-159.34528	563.72604	1
70	H	74.21389	83.61937	77.57553	654.59388	2347.94251	1217.51488	1
71	H	73.95548	84.43006	75.97627	-1526.55661	2103.42026	817.87394	1
72	O	72.41787	83.09437	76.63735	-554.84278	14.12789	399.58769	1
73	H	72.10843	83.42293	75.77240	1297.06236	2061.84854	1220.68812	1
74	C	74.65682	80.96749	76.60558	-662.15484	-412.13544	123.62687	1
75	O	75.28903	80.73767	77.60947	-540.01537	-317.05804	274.91456	1
76	N	73.76913	80.09964	75.99200	-202.76299	-690.00100	-131.49145	1
77	H	73.34845	80.72163	75.29108	-702.62132	-2617.37191	281.70413	1
78	C	72.84261	79.35361	76.88705	-491.73914	576.34187	222.73509	1
79	H	72.61857	80.06098	77.71859	1977.17978	-1823.58850	-434.68928	1
80	C	71.64220	79.00270	76.04134	-649.50797	-328.66843	306.11224	1
81	H	72.01793	78.54890	75.09577	2075.07803	1452.16490	-1004.45904	1
82	C	70.74746	77.98841	76.73275	-615.18735	-489.99689	-70.96352	1
83	H	69.86814	77.70385	76.09190	-1226.32661	-1724.38906	-1716.47170	1
84	H	71.30673	77.04247	76.97436	2381.64273	-969.84735	900.46860	1
85	H	70.34018	78.38882	77.70173	2122.74991	1702.23946	-141.36228	1
86	C	70.82412	80.22966	75.67664	-501.86074	-479.61276	-376.42482	1
87	H	69.95108	79.96744	75.01798	993.79261	-2246.95401	-1177.81305	1
88	H	70.41191	80.73737	76.59194	42.71279	-626.15391	-2651.37258	1
89	H	71.43551	80.99668	75.12631	-2026.39012	-1590.33709	-887.82922	1
90	C	73.59319	77.98814	77.38892	-672.89153	382.57394	-156.34072	1
91	O	74.12105	77.21079	76.59507	410.04627	221.86223	500.35950	1
92	N	73.37977	77.81304	78.67237	-378.11782	-443.79414	-441.10984	1
93	H	72.89726	78.56127	79.16578	2404.15973	-568.14894	1149.30085	1
94	C	74.18091	76.85886	79.36594	-544.54484	466.16019	331.29119	1
95	H	74.51014	76.14461	78.57693	-1409.80988	-170.17955	2325.32679	1
96	C	75.37273	77.70227	79.98912	-184.48284	116.78282	-758.89137	1
97	H	75.88771	78.28881	79.19383	1893.78641	1861.14652	611.04528	1
98	H	74.98561	78.45085	80.71756	-2170.79665	-974.19311	1327.50117	1
99	C	76.34540	76.69953	80.68122	389.51668	672.81878	-138.49152	1
100	H	75.81191	76.14284	81.48389	510.64577	1933.03327	1851.02484	1
101	H	76.65836	75.90872	79.96419	-2302.30869	-1105.72939	-948.89774	1
102	C	77.62096	77.40291	81.28311	-559.93427	-126.34590	542.30857	1
103	O	78.42217	76.74470	81.89451	-670.36003	-111.83166	76.36448	1
104	N	77.69788	78.72688	81.03004	-216.06729	-537.07037	446.51379	1
105	H	77.05727	79.33838	80.51002	-1251.96487	1074.12894	-2168.52500	1
106	H	78.47337	79.32366	81.33737	-2451.83023	-720.73851	944.84612	1
107	C	73.27936	76.21722	80.57470	546.24052	-563.88337	-85.11809	1
108	O	73.17920	76.80363	81.61965	71.70702	-307.40463	606.69673	1
109	N	72.74158	75.04120	80.20602	479.90863	-504.50129	222.86849	1
110	C	71.80631	74.36273	81.04247	75.51268	-600.91904	506.73700	1
111	H	71.39472	75.11419	81.75611	-2033.61562	1795.30103	254.89480	1
112	C	70.78430	73.78032	79.96934	523.79067	517.99274	284.45581	1
113	H	70.16863	72.94520	80.37242	1599.61665	-1127.00911	1895.98173	1
114	H	70.07700	74.55960	79.60870	-1881.83093	1275.82488	-1501.55016	1
115	C	71.76943	73.33732	78.84456	-600.05639	-404.05026	316.64485	1
116	H	72.26222	72.37315	79.10088	-2597.05260	496.36221	657.73249	1
117	H	71.27754	73.19157	77.85708	-1666.24518	1294.38985	-1723.90591	1
118	C	72.82472	74.52391	78.84499	493.57570	-129.95376	-602.56394	1
119	H	73.87693	74.20267	78.65786	-1469.08415	-637.84797	2204.22581	1
120	H	72.57299	75.37957	78.17445	-1038.97840	1068.88701	-2280.71789	1
121	C	72.45184	73.05092	81.78086	188.88100	241.05089	-727.87821	1

122	O	71.70018	72.20760	82.25709	531.88613	-49.19943	427.07960	1
123	N	73.77944	73.00564	81.71370	708.14833	26.93417	-179.73509	1
124	H	74.07436	73.84788	81.21663	-2232.69501	-1179.09831	1023.94816	1
125	C	74.63866	72.38415	82.71780	-738.32412	259.92548	104.42456	1
126	H	75.62973	72.87135	82.55551	2028.89123	1260.02983	1311.33324	1
127	C	74.07477	72.64565	84.10405	-258.65678	-345.52513	661.28459	1
128	H	73.02504	72.26931	84.11606	-1826.06090	-1801.46097	-918.64554	1
129	C	74.85752	71.90239	85.17086	-541.23400	531.92970	-218.41428	1
130	H	74.38615	72.00630	86.18674	1311.73218	-2219.18200	882.19023	1
131	H	74.92489	70.80068	84.94011	-1048.71298	1223.58118	-2196.97971	1
132	H	75.91245	72.28419	85.25133	419.06414	1903.92898	1903.44670	1
133	C	74.03651	74.12742	84.43084	-423.86431	152.66566	-648.55262	1
134	H	73.55866	74.32160	85.43039	105.68386	-2342.50080	1387.51238	1
135	H	75.06991	74.57018	84.46518	-1695.63603	-1484.73621	-1531.02793	1
136	H	73.45403	74.70683	83.66183	-1853.57121	-487.39031	1936.59343	1
137	C	74.72350	70.74351	82.47283	539.71428	-510.58232	267.58633	1
138	O	75.68759	70.14781	82.88096	-15.93758	-278.34085	-624.49402	1
139	N	73.61911	70.26032	81.93270	-676.81886	12.05292	276.17960	1
140	H	72.83084	70.90703	81.73650	-1694.44250	-373.84189	-2100.66098	1
141	C	73.61296	68.88879	81.55847	412.33078	-664.70360	108.35451	1
142	H	74.44438	68.41741	82.13500	1765.77476	1294.44366	1621.76594	1
143	C	72.16068	68.34115	81.88436	-179.66635	-721.95667	-264.73915	1
144	H	71.89288	68.53146	82.94757	-607.34922	2587.87032	-598.10018	1
145	H	71.39816	68.88791	81.28533	-359.69332	-1479.13954	-2259.74260	1
146	C	72.13236	66.81275	81.55670	-240.01076	616.02425	431.85322	1
147	H	72.48036	66.63456	80.51298	-1359.17131	782.54425	2227.99181	1
148	H	72.83705	66.25340	82.21188	-820.36667	85.81767	-2596.78715	1
149	C	70.65301	66.28096	81.73270	-513.07015	236.18570	-551.87280	1
150	H	70.32237	66.35428	82.79420	1816.11944	-1183.11722	-1650.94321	1
151	H	69.93399	66.89876	81.14702	-1800.04429	-1361.53473	1526.34643	1
152	C	70.64339	64.81470	81.24089	726.08972	-253.19732	-179.64713	1
153	H	70.87656	64.68943	80.16451	1224.27271	-456.51798	-2390.90304	1
154	H	71.26311	64.12147	81.84379	1206.40339	-1150.93514	-2154.90344	1
155	N	69.18289	64.27041	81.38804	329.70796	-633.68968	-155.67358	1
156	H	69.03493	63.27013	81.06730	1348.31305	1938.76845	1359.00643	1
157	H	68.77443	64.23790	82.36714	2096.92035	1446.54551	-966.48890	1
158	H	68.42163	64.77625	80.84830	-1197.07217	-2303.53719	827.28733	1
159	C	73.79740	68.70692	79.93531	-378.01186	-556.17301	-413.96481	1
160	O	74.25452	67.66702	79.51469	-409.44433	-307.55053	-453.30833	1
161	N	73.25746	69.70217	79.23822	-429.02477	524.70884	274.08502	1
162	H	72.96085	70.52729	79.75455	1706.34263	-1425.96036	1574.38926	1
163	C	73.40088	69.63584	77.82417	-45.25864	-626.22952	478.93267	1
164	H	73.64078	68.56558	77.61685	1988.63164	570.90773	1772.87287	1
165	C	72.06940	70.15795	77.14630	551.77128	-20.49526	-564.54996	1
166	H	71.18017	69.62727	77.55396	1434.61535	-1753.10253	1513.99471	1
167	H	71.90562	71.23467	77.36647	-714.67738	1819.09770	1898.36494	1
168	C	72.21452	69.92013	75.60619	446.99263	-555.77305	338.97221	1
169	H	73.10445	70.46051	75.21409	1953.68466	1892.25957	-161.67766	1
170	H	72.39099	68.84343	75.38673	-403.03785	2688.07032	-188.43591	1
171	C	70.90130	70.42755	74.88598	567.86262	335.74681	434.04421	1
172	H	70.00924	69.85829	75.23496	-1080.02275	1568.26081	-1948.78900	1
173	H	70.69789	71.49411	75.13602	-919.54108	2111.34692	1456.13463	1
174	C	71.10988	70.25093	73.36358	195.81897	173.33862	-745.11536	1
175	H	71.92274	70.87020	72.93422	1405.67949	-2301.21089	-390.08113	1
176	H	71.22170	69.19958	73.03098	-940.37328	-1118.32446	2299.72133	1
177	N	69.81173	70.75252	72.64596	319.26422	656.36007	-42.02424	1
178	H	69.82461	70.68917	71.58716	1961.03633	619.91968	1787.09422	1
179	H	68.90698	70.24565	72.87240	854.14343	-2156.80752	1429.08711	1
180	H	69.53785	71.76779	72.79077	1237.02905	-1378.50857	-1998.28500	1
181	C	74.60806	70.67512	77.38241	532.53319	-268.57236	517.55729	1
182	O	74.61118	71.85286	77.63927	266.16714	-290.73804	-558.88002	1
183	N	75.40201	69.97654	76.57584	-226.25352	640.49678	-270.32839	1

184	H	75.20707	68.98094	76.47407	2007.69063	-1035.27229	1523.50231	1
185	C	76.71331	70.46692	76.31350	-540.76542	-573.33303	49.50000	1
186	H	76.64663	71.52988	76.64377	-2374.20950	-1036.76023	843.75774	1
187	C	77.69392	69.60300	77.23538	-77.09082	666.87422	-415.84136	1
188	H	77.66719	68.54282	76.86518	-985.81834	617.19825	2463.91927	1
189	O	77.33942	69.56087	78.63211	293.29899	-391.65602	-477.80926	1
190	H	77.00475	68.64825	78.72006	2528.72714	-681.76262	-751.27122	1
191	C	79.11127	70.21942	76.95520	252.47363	-605.14473	440.05134	1
192	H	79.91412	69.65234	77.48181	-2052.65063	1456.49051	-1043.51830	1
193	H	79.35878	70.21299	75.85916	-2152.98800	-1661.97574	-161.70652	1
194	H	79.17131	71.27580	77.30690	-473.12726	-1584.27339	2165.61725	1
195	C	76.99311	70.28872	74.71713	360.36307	488.46713	505.10056	1
196	O	78.13855	70.06045	74.27717	-200.08817	-528.03552	-385.82850	1
197	N	75.89421	70.48239	74.02763	-597.54095	-226.44775	355.20479	1
198	H	75.13785	70.64648	74.69045	2179.23655	-1300.70981	-991.33835	1
199	C	75.80210	70.77449	72.64943	-687.68921	297.39807	-249.45179	1
200	H	74.73305	71.04164	72.50345	-349.16256	-2467.37713	-1101.72831	1
201	C	76.79925	71.99473	72.36384	672.47345	361.54328	-201.62880	1
202	H	77.76403	71.83726	72.90060	1541.41502	582.18425	2169.97026	1
203	H	77.02658	72.04992	71.27469	-2534.67717	60.25153	997.72295	1
204	C	76.11527	73.28761	72.83283	574.26774	-389.43119	-377.02542	1
205	C	75.28022	73.98617	71.91239	688.82679	-287.33580	-257.96133	1
206	H	75.12122	73.59976	70.88953	331.14182	1470.38163	2269.80013	1
207	C	76.28423	73.79542	74.15539	-383.52382	-675.04808	144.24917	1
208	H	76.91391	73.25455	74.88462	4.09847	1517.59662	2262.86397	1
209	C	74.67547	75.16934	72.32580	-134.76730	428.45285	-649.50303	1
210	H	74.04058	75.70802	71.60114	-903.23433	1600.49020	2011.53387	1
211	C	75.64477	74.98624	74.51345	-335.53281	-615.00040	-364.39058	1
212	H	75.79074	75.36613	75.54058	1596.45398	-1369.33862	1732.02659	1
213	C	74.82463	75.72981	73.62163	585.48547	-340.24194	-406.23938	1
214	O	74.18315	76.92417	73.95055	-419.15649	-173.04408	-511.94141	1
215	H	74.27982	76.93480	74.99111	-1071.84350	1559.71507	-1960.13012	1
216	C	76.23747	69.48318	71.74453	291.41878	-183.13091	710.72246	1
217	O	75.42382	68.96278	71.02133	379.87695	523.47396	-222.23622	1
218	N	77.52844	69.19320	71.88205	564.30591	373.09380	277.24371	1
219	H	78.10874	69.72484	72.56793	-120.59931	-2436.07824	-1214.35098	1
220	C	77.98904	67.99651	71.21856	404.07514	-299.37480	608.84009	1
221	H	77.18213	67.25909	71.43421	-1071.07882	-841.69025	2359.66467	1
222	C	77.98568	68.34842	69.66624	-683.12807	68.71770	-390.13096	1
223	H	77.02251	68.83996	69.39197	2068.88918	1596.58590	770.89603	1
224	H	78.78011	69.09466	69.44235	1379.86429	2342.49779	-179.85638	1
225	C	78.20190	67.05186	68.83041	-176.39967	537.49466	550.97268	1
226	H	79.08081	66.47511	69.21748	-396.28051	1942.22168	1869.33314	1
227	H	77.32811	66.36729	68.91906	-94.44700	586.00678	-2659.20016	1
228	C	78.44074	67.49204	67.31235	-291.69381	-718.18079	-150.72929	1
229	H	77.56694	67.95996	66.79178	-2303.38776	1089.76242	964.62032	1
230	H	79.33380	68.14571	67.14037	884.16729	2568.80533	-207.74283	1
231	N	78.70305	66.25437	66.70527	-594.49522	-252.81478	342.29276	1
232	H	78.77694	65.45560	67.31629	-1735.17426	2084.05705	-263.71605	1
233	C	78.86480	66.07576	65.45717	595.23177	-271.52487	442.22352	1
234	N	78.76935	67.19020	64.61686	585.53813	-424.79750	-105.81303	1
235	H	78.59098	68.16538	64.85325	959.88797	1327.56823	-2177.11905	1
236	H	78.88578	67.16953	63.60316	1578.48647	16.27378	-2220.76233	1
237	N	79.11989	64.72678	65.17151	-452.17763	-390.33541	-421.51853	1
238	H	79.19851	63.91833	65.78661	470.26107	1974.25629	-1817.92087	1
239	H	79.28612	64.37660	64.22737	1856.67307	-1573.97321	-1224.35416	1
240	C	79.44400	67.54432	71.72255	-531.47271	-581.45780	-55.06206	1
241	O	80.05796	66.76394	71.03914	-243.00837	192.73507	609.52485	1
242	N	79.82296	68.01916	72.92718	343.49288	-644.25607	38.09164	1
243	H	79.19256	68.66892	73.42380	-1691.16043	-1535.97525	-1484.73099	1
244	C	81.28773	68.16378	73.13884	542.66492	350.14337	454.42563	1
245	H	81.64911	68.63214	72.19500	1209.57979	-2396.95920	463.86744	1

246	C	81.53103	69.01330	74.36250	-737.14309	145.93010	242.71942	1
247	H	80.88163	68.62775	75.18050	-1050.18303	159.36419	-2509.06125	1
248	C	82.97411	68.92986	74.82971	-706.77696	-252.88343	-245.16230	1
249	H	83.13979	69.50578	75.78148	-1624.64039	-1665.49085	1417.86935	1
250	H	83.28864	67.86448	75.01931	2566.10521	598.51109	693.22305	1
251	H	83.68008	69.34524	74.05876	-1972.69758	107.10018	-1876.34312	1
252	C	81.17083	70.46865	74.12314	412.85148	672.58832	-27.69222	1
253	H	81.36896	71.10068	75.03243	1447.02277	1762.76533	-1490.78944	1
254	H	81.76452	70.90884	73.27515	1320.77379	-145.20455	2378.68491	1
255	H	80.07437	70.58426	73.86417	-1512.10848	1470.52031	1724.75147	1
256	C	81.96156	66.67511	73.35077	-607.11113	499.56689	73.73769	1
257	O	83.15544	66.53265	73.16622	357.97126	460.81534	356.68785	1
258	N	81.09543	65.79047	73.81163	536.55407	-368.62270	332.76306	1
259	H	80.14150	66.13086	73.91701	524.38866	2297.69985	1367.20941	1
260	C	81.52193	64.45767	74.04555	46.50277	-774.29190	-147.97904	1
261	H	82.50673	64.39874	73.52612	1676.51875	1883.29066	1032.55549	1
262	C	81.64703	64.17732	75.63373	-559.41456	-34.19198	-556.30433	1
263	H	80.64324	64.28601	76.10788	-64.66664	395.18769	2695.05373	1
264	H	81.94399	63.11418	75.79651	-2703.44278	-60.40056	333.79418	1
265	C	82.63263	65.10717	76.28398	-519.76435	377.31045	459.42366	1
266	H	82.26384	66.15085	76.16099	-1746.74323	1667.50644	-1261.73691	1
267	C	82.74745	64.80040	77.77321	570.95554	16.46261	-545.27700	1
268	H	83.45200	65.50356	78.28728	2391.58273	28.05277	-1305.07271	1
269	H	81.75822	64.88194	78.29216	175.75588	917.63458	2559.43867	1
270	H	83.12997	63.76250	77.95068	-1063.97851	-2155.34650	1283.00462	1
271	C	84.01031	65.00627	75.64566	193.76014	2.62946	-765.53141	1
272	H	84.78053	65.57318	76.22977	507.39394	-846.55087	2539.60089	1
273	H	84.36127	63.94422	75.57767	1337.57841	1818.19054	1526.01994	1
274	H	84.00426	65.43673	74.59530	1100.88635	-1172.91350	-2199.08909	1
275	C	80.38920	63.48592	73.45256	-549.21115	475.64486	-309.38218	1
276	O	80.11667	62.44103	73.98531	556.06106	-390.37755	-78.24250	1
277	O	79.79403	63.84460	72.22163	-572.27940	-310.19032	-209.75862	1
278	H	80.19481	64.75251	72.10358	-1380.08193	2212.14486	790.85944	1

Listing 18: C00018.xmolout

	276								
	150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100	
	0.2500	300.00	0.00	0.00	0.00	-1294.0746	0.0000	300.0000	
3	H	82.46862	61.03615	72.92558	-2043.14101	-1757.64893	399.89339		1
4	N	82.53466	61.20196	71.92144	426.75047	490.45733	-334.42467		1
5	H	81.60387	61.56208	71.71056	442.25559	-1110.30854	-2448.52907		1
6	C	83.59720	62.05695	71.54210	415.32972	-666.39213	83.73172		1
7	H	84.39788	61.81344	72.27293	879.32219	2491.00447	667.35213		1
8	C	84.01145	61.70600	70.02462	31.35357	477.41777	628.23362		1
9	H	83.12890	61.82920	69.35274	1168.38489	2240.25337	-1019.71136		1
10	H	84.77573	62.43659	69.66731	-360.43770	2534.90498	931.67112		1
11	C	84.52834	60.29687	69.89541	463.18208	512.70242	-382.34388		1
12	H	83.75696	59.60359	70.30061	1725.29117	1863.52247	-987.07854		1
13	C	84.75829	59.96828	68.42444	710.42801	-144.27427	-313.15367		1
14	H	85.11436	58.91530	68.28337	364.20195	-1033.13725	2494.72524		1
15	H	83.82144	60.08639	67.82123	2567.61904	335.80679	847.48802		1
16	H	85.53009	60.64166	67.96972	-2587.99029	680.92867	-512.16411		1
17	C	85.82379	60.07982	70.66428	268.17616	741.64379	-40.42634		1
18	H	86.23775	59.05227	70.49130	1283.54314	-1945.37420	-1411.27812		1
19	H	86.61487	60.81108	70.35543	-1258.57796	1317.15249	-2026.02085		1
20	H	85.67602	60.19366	71.76904	-2502.84526	909.80597	575.92391		1
21	C	83.05603	63.59109	71.72360	619.36578	-458.64843	-172.09273		1
22	O	83.21594	64.26122	72.91384	-81.40433	433.87611	522.34594		1
23	N	82.45865	64.05993	70.74600	175.23996	-622.20190	341.55523		1
24	H	82.42773	63.40092	69.97569	-876.57256	-303.22879	-2561.90213		1
25	C	83.87059	66.28440	71.39087	-571.88214	-534.10783	-106.15033		1

26	H	84.96888	66.19500	71.54866	-2713.20841	-16.25800	-248.80809	1
27	C	80.90006	67.17024	69.91478	166.60354	288.16399	-716.09568	1
28	H	81.25383	65.31339	72.01758	-2097.85574	1636.78449	-586.18044	1
29	O	83.37747	66.37513	67.78090	-317.80580	-363.38227	484.43082	2
30	H	82.71245	66.21938	68.43937	1863.74748	-1451.84923	1357.29467	2
31	C	80.79417	68.31137	70.70769	503.80731	517.99032	318.51606	1
32	H	80.78062	69.18311	68.33914	640.61020	-2157.10410	-1536.29104	3
33	H	79.64966	69.02912	72.43645	1687.88455	465.60692	2087.56452	1
34	H	84.15078	68.04809	70.04585	-1293.07895	-1899.88581	-1463.57452	1
35	C	83.09196	65.92318	72.66878	-153.07550	-733.68902	248.70981	1
36	O	81.27348	66.17139	72.52321	186.15459	-480.78787	-449.34387	1
37	N	83.53398	66.58592	73.65935	-487.53139	543.18517	42.03850	1
38	C	82.72054	66.91384	74.81875	-699.35871	69.34393	360.10701	1
39	H	81.76899	66.34315	74.74130	2.81126	-221.99807	-2715.58072	1
40	C	83.67974	66.45600	75.98549	-507.46439	-592.59194	122.07761	1
41	H	83.39888	66.89064	76.97170	-1975.08116	525.87560	-1801.71556	1
42	H	83.66387	65.34964	76.10742	1588.27743	-1913.22100	1113.83566	1
43	C	85.07611	66.94489	75.47008	-613.62442	-457.55993	-194.14490	1
44	H	85.20225	68.04031	75.63327	1707.54637	-721.27992	1996.92523	1
45	H	85.93420	66.44899	75.97919	758.23357	2100.81767	1560.55011	1
46	C	84.99154	66.60633	73.93366	-352.41524	704.96076	49.21465	1
47	H	85.45207	67.36443	73.26053	1714.76886	-2070.42778	443.35792	1
48	H	85.34751	65.58652	73.65935	1224.15040	1801.50881	1636.97633	1
49	C	82.53148	68.52607	74.88723	566.85117	537.05831	117.62814	1
50	O	83.50779	69.26524	74.74265	-550.26779	-406.08867	4.21666	1
51	N	81.28033	68.83646	75.14169	566.34832	-425.77725	180.18749	1
52	H	80.66565	68.02467	75.20264	644.44502	2646.80550	-52.73430	1
53	C	80.82623	70.06421	75.68491	612.34801	-281.48662	411.56221	1
54	H	79.78648	69.83127	76.00296	1667.23498	-1490.75142	1556.16753	1
55	C	81.77398	70.46315	76.91048	-714.45746	-175.43074	286.98927	1
56	H	82.84026	70.48905	76.54761	-787.09484	1763.03619	-1922.46060	1
57	O	81.76229	69.56717	78.03569	-429.46514	516.51932	-128.40526	1
58	H	82.70405	69.30578	78.07884	1981.82785	436.16847	-1818.18182	1
59	C	81.27954	71.93138	77.18278	630.79189	-468.94448	76.03230	1
60	H	81.92337	72.45305	77.92844	-1775.71861	2062.30353	131.89849	1
61	H	81.28262	72.54355	76.24453	-1855.14608	88.94118	1993.53760	1
62	H	80.23740	71.94356	77.57882	-1504.82350	-780.94249	-2132.90992	1
63	C	80.85879	71.30715	74.61074	288.57638	618.62814	-397.00270	1
64	O	79.89437	72.02408	74.50553	321.70495	-185.26452	574.37218	1
65	N	82.06603	71.43848	74.07146	-447.05792	-446.53431	367.76425	1
66	H	82.81651	70.73307	74.30617	350.31316	1975.63644	-1843.31522	1
67	C	82.17027	72.20916	72.86732	-511.23061	374.03917	-471.51480	1
68	H	81.84437	73.23629	73.14123	2234.79579	-898.70890	-1273.45190	1
69	C	83.70761	72.07966	72.47696	529.53781	-159.34528	563.72604	1
70	H	83.91193	72.77147	71.61721	654.59388	2347.94251	1217.51488	1
71	H	84.29679	72.46398	73.35098	-1526.55661	2103.42026	817.87394	1
72	O	84.17200	70.74930	72.10291	-554.84278	14.12789	399.58769	1
73	H	84.13421	70.31348	72.97684	1297.06236	2061.84854	1220.68812	1
74	C	81.20951	71.59168	71.70670	-662.15484	-412.13544	123.62687	1
75	O	80.87131	72.30398	70.75424	-540.01537	-317.05804	274.91456	1
76	N	81.02929	70.30739	71.90202	-202.76299	-690.00100	-131.49145	1
77	H	81.52746	70.04048	72.75490	-702.62132	-2617.37191	281.70413	1
78	C	80.00754	69.39202	71.44201	-491.73914	576.34187	222.73509	1
79	H	81.19198	69.66624	68.75394	1977.17978	-1823.58850	-434.68928	3
80	C	82.05063	67.73178	70.49562	-649.50797	-328.66843	306.11224	1
81	H	80.31448	66.43047	72.43414	2075.07803	1452.16490	-1004.45904	1
82	C	80.19826	66.07580	69.15706	-615.18735	-489.99689	-70.96352	1
83	H	80.41701	65.07075	69.59983	-1226.32661	-1724.38906	-1716.47170	1
84	H	79.08806	66.21850	69.16457	2381.64273	-969.84735	900.46860	1
85	H	80.52865	66.03103	68.08892	2122.74991	1702.23946	-141.36228	1
86	C	83.49644	67.75361	70.89918	-501.86074	-479.61276	-376.42482	1
87	H	83.60026	65.55345	70.59089	993.79261	-2246.95401	-1177.81305	1

88	H	83.70686	67.22557	68.04038	42.71279	-626.15391	-2651.37258	2
89	H	83.67244	68.51251	71.70247	-2026.39012	-1590.33709	-887.82922	1
90	C	78.71856	69.76835	70.47107	-672.89153	382.57394	-156.34072	1
91	O	77.84486	68.93495	70.45390	410.04627	221.86223	500.35950	1
92	N	78.87838	70.83842	69.72688	-378.11782	-443.79414	-441.10984	1
93	H	79.74165	71.43460	69.85768	2404.15973	-568.14894	1149.30085	1
94	C	77.70142	71.48360	69.21807	-544.54484	466.16019	331.29119	1
95	H	78.12209	72.24015	68.51971	-1409.80988	-170.17955	2325.32679	1
96	C	76.75850	70.41382	68.52890	-184.48284	116.78282	-758.89137	1
97	H	77.31654	69.84925	67.74643	1893.78641	1861.14652	611.04528	1
98	H	76.40856	69.64830	69.27736	-2170.79665	-974.19311	1327.50117	1
99	C	75.52219	71.15055	67.92297	389.51668	672.81878	-138.49152	1
100	H	75.01849	71.75448	68.71304	510.64577	1933.03327	1851.02484	1
101	H	75.84102	71.89923	67.16501	-2302.30869	-1105.72939	-948.89774	1
102	C	74.48297	70.14937	67.29089	-559.93427	-126.34590	542.30857	1
103	O	73.45899	70.57687	66.82348	-670.36003	-111.83166	76.36448	1
104	N	74.86377	68.85378	67.33297	-216.06729	-537.07037	446.51379	1
105	H	75.70319	68.42612	67.74133	-1251.96487	1074.12894	-2168.52500	1
106	H	74.28468	68.07685	66.99664	-2451.83023	-720.73851	944.84612	1
107	C	76.92095	72.15214	70.48080	546.24052	-563.88337	-85.11809	1
108	O	75.85327	71.70231	70.83924	71.70702	-307.40463	606.69673	1
109	N	77.55145	73.24874	70.91322	479.90863	-504.50129	222.86849	1
110	C	77.32864	73.79064	72.22202	75.51268	-600.91904	506.73700	1
111	H	77.38365	72.93871	72.93787	-2033.61562	1795.30103	254.89480	1
112	C	78.50572	74.84430	72.34532	523.79067	517.99274	284.45581	1
113	H	78.31535	75.61854	73.12299	1599.61665	-1127.00911	1895.98173	1
114	H	79.46844	74.34937	72.60739	-1881.83093	1275.82488	-1501.55016	1
115	C	78.53776	75.41203	70.89193	-600.05639	-404.05026	316.64485	1
116	H	77.66933	76.08405	70.70140	-2597.05260	496.36221	657.73249	1
117	H	79.45606	75.99512	70.65508	-1666.24518	1294.38985	-1723.90591	1
118	C	78.42396	74.05717	70.07004	493.57570	-129.95376	-602.56394	1
119	H	77.96929	74.14752	69.05511	-1469.08415	-637.84797	2204.22581	1
120	H	79.38749	73.47799	70.01406	-1038.97840	1068.88701	-2280.71789	1
121	C	75.87906	74.55592	72.29069	188.88100	241.05089	-727.87821	1
122	O	75.58443	75.16255	73.29333	531.88613	-49.19943	427.07960	1
123	N	75.20030	74.40761	71.16216	708.14833	26.93417	-179.73509	1
124	H	75.63610	73.81651	70.44988	-2232.69501	-1179.09831	1023.94816	1
125	C	73.86298	74.86361	71.00748	-738.32412	259.92548	104.42456	1
126	H	73.56307	74.43279	70.02584	2028.89123	1260.02983	1311.33324	1
127	C	73.04932	74.21129	72.20993	-258.65678	-345.52513	661.28459	1
128	H	73.54324	74.45285	73.18012	-1826.06090	-1801.46097	-918.64554	1
129	C	71.52327	74.55828	72.27712	-541.23400	531.92970	-218.41428	1
130	H	70.95440	73.76902	72.82354	1311.73218	-2219.18200	882.19023	1
131	H	71.33052	75.51602	72.82275	-1048.71298	1223.58118	-2196.97971	1
132	H	71.07276	74.64281	71.25945	419.06414	1903.92898	1903.44670	1
133	C	73.12532	72.67314	71.91698	-423.86431	152.66566	-648.55262	1
134	H	72.77393	72.06908	72.78635	105.68386	-2342.50080	1387.51238	1
135	H	72.49121	72.39448	71.04228	-1695.63603	-1484.73621	-1531.02793	1
136	H	74.18564	72.34324	71.67318	-1853.57121	-487.39031	1936.59343	1
137	C	74.00962	76.48600	70.90398	539.71428	-510.58232	267.58633	1
138	O	74.96419	77.01396	70.37541	-15.93758	-278.34085	-624.49402	1
139	N	72.89314	77.06844	71.33224	-676.81886	12.05292	276.17960	1
140	H	72.13447	76.49975	71.70691	-1694.44250	-373.84189	-2100.66098	1
141	C	72.87468	78.48803	71.40544	412.33078	-664.70360	108.35451	1
142	H	73.87385	78.79780	71.01192	1765.77476	1294.44366	1621.76594	1
143	C	71.66471	78.98334	70.50570	-179.66635	-721.95667	-264.73915	1
144	H	71.67873	78.48031	69.51310	-607.34922	2587.87032	-598.10018	1
145	H	70.69269	78.70558	70.97076	-359.69332	-1479.13954	-2259.74260	1
146	C	71.78821	80.53382	70.35180	-240.01076	616.02425	431.85322	1
147	H	71.82882	81.01619	71.36278	-1359.17131	782.54425	2227.99181	1
148	H	72.73566	80.81127	69.83641	-820.36667	85.81767	-2596.78715	1
149	C	70.53227	81.04787	69.53897	-513.07015	236.18570	-551.87280	1

150	H	70.54281	80.65604	68.49591	1816.11944	-1183.11722	-1650.94321	1
151	H	69.58617	80.67514	69.99437	-1800.04429	-1361.53473	1526.34643	1
152	C	70.57276	82.59351	69.55572	726.08972	-253.19732	-179.64713	1
153	H	70.45525	83.04541	70.56097	1224.27271	-456.51798	-2390.90304	1
154	H	71.44683	83.03948	69.04065	1206.40339	-1150.93514	-2154.90344	1
155	N	69.33159	83.10238	68.74813	329.70796	-633.68968	-155.67358	1
156	H	69.21556	84.15565	68.70063	1348.31305	1938.76845	1359.00643	1
157	H	69.28357	82.84049	67.72064	2096.92035	1446.54551	-966.48890	1
158	H	68.37450	82.80290	69.09596	-1197.07217	-2303.53719	827.28733	1
159	C	72.60041	78.92956	72.96435	-378.01186	-556.17301	-413.96481	1
160	O	72.16127	80.04413	73.17417	-409.44433	-307.55053	-453.30833	1
161	N	72.98286	77.99926	73.81371	-429.02477	524.70884	274.08502	1
162	H	73.38931	77.16891	73.38586	1706.34263	-1425.96036	1574.38926	1
163	C	72.87752	78.10056	75.23374	-45.25864	-626.22952	478.93267	1
164	H	73.82448	77.66032	75.61881	1988.63164	570.90773	1772.87287	1
165	C	72.66358	79.62141	75.60540	551.77128	-20.49526	-564.54996	1
166	H	73.42438	80.23567	75.06910	1434.61535	-1753.10253	1513.99471	1
167	H	71.67251	79.96593	75.21137	-714.67738	1819.09770	1898.36494	1
168	C	72.71840	79.90937	77.14276	446.99263	-555.77305	338.97221	1
169	H	71.85241	79.44612	77.66981	1953.68466	1892.25957	-161.67766	1
170	H	73.63762	79.49535	77.61392	-403.03785	2688.07032	-188.43591	1
171	C	72.67365	81.48812	77.23295	567.86262	335.74681	434.04421	1
172	H	73.57935	81.93932	76.76664	-1080.02275	1568.26081	-1948.78900	1
173	H	71.80316	81.88383	76.65980	-919.54108	2111.34692	1456.13463	1
174	C	72.54871	81.89750	78.71987	195.81897	173.33862	-745.11536	1
175	H	71.57953	81.60838	79.18624	1405.67949	-2301.21089	-390.08113	1
176	H	73.39657	81.59491	79.36861	-940.37328	-1118.32446	2299.72133	1
177	N	72.47240	83.44596	78.82035	319.26422	656.36007	-42.02424	1
178	H	72.07639	83.76125	79.80711	1961.03633	619.91968	1787.09422	1
179	H	73.35918	84.01307	78.68262	854.14343	-2156.80752	1429.08711	1
180	H	71.81452	83.90656	78.12780	1237.02905	-1378.50857	-1998.28500	1
181	C	71.57606	77.25429	75.74585	532.53319	-268.57236	517.55729	1
182	O	70.59257	77.02306	75.06033	266.16714	-290.73804	-558.88002	1
183	N	71.76521	76.98681	77.02653	-226.25352	640.49678	-270.32839	1
184	H	72.64428	77.29276	77.43600	2007.69063	-1035.27229	1523.50231	1
185	C	70.76014	76.33763	77.80237	-540.76542	-573.33303	49.50000	1
186	H	70.23559	75.71942	77.03772	-2374.20950	-1036.76023	843.75774	1
187	C	71.48973	75.51793	78.96211	-77.09082	666.87422	-415.84136	1
188	H	71.90589	76.24921	79.70755	-985.81834	617.19825	2463.91927	1
189	O	72.59423	74.69360	78.54400	293.29899	-391.65602	-477.80926	1
190	H	73.32775	75.08168	79.06060	2528.72714	-681.76262	-751.27122	1
191	C	70.28977	74.74054	79.61784	252.47363	-605.14473	440.05134	1
192	H	70.62243	74.16289	80.51149	-2052.65063	1456.49051	-1043.51830	1
193	H	69.47738	75.43138	79.95247	-2152.98800	-1661.97574	-161.70652	1
194	H	69.83838	74.01221	78.90497	-473.12726	-1584.27339	2165.61725	1
195	C	69.79963	77.50965	78.40876	360.36307	488.46713	505.10056	1
196	O	69.51457	77.58929	79.59239	-200.08817	-528.03552	-385.82850	1
197	N	69.40255	78.24449	77.39266	-597.54095	-226.44775	355.20479	1
198	H	69.70316	77.96640	76.44130	2179.23655	-1300.70981	-991.33835	1
199	C	68.51363	79.33108	77.55981	-687.68921	297.39807	-249.45179	1
200	H	68.36361	79.68963	76.51809	-349.16256	-2467.37713	-1101.72831	1
201	C	67.16857	78.78297	78.23493	672.47345	361.54328	-201.62880	1
202	H	67.38790	78.34447	79.23583	1541.41502	582.18425	2169.97026	1
203	H	66.45959	79.62768	78.39261	-2534.67717	60.25153	997.72295	1
204	C	66.54791	77.70921	77.33090	574.26774	-389.43119	-377.02542	1
205	C	65.77989	78.07818	76.18594	688.82679	-287.33580	-257.96133	1
206	H	65.62924	79.14130	75.92497	331.14182	1470.38163	2269.80013	1
207	C	66.75601	76.33260	77.64882	-383.52382	-675.04808	144.24917	1
208	H	67.36821	76.04602	78.52326	4.09847	1517.59662	2262.86397	1
209	C	65.22157	77.06616	75.40522	-134.76730	428.45285	-649.50303	1
210	H	64.62362	77.34977	74.52168	-903.23433	1600.49020	2011.53387	1
211	C	66.17352	75.35632	76.83760	-335.53281	-615.00040	-364.39058	1

212	H	66.33496	74.29561	77.09808	1596.45398	-1369.33862	1732.02659	1
213	C	65.38504	75.68031	75.69470	585.48547	-340.24194	-406.23938	1
214	O	64.78430	74.69655	74.86667	-419.15649	-173.04408	-511.94141	1
215	H	65.08012	73.88092	75.33575	-1071.84350	1559.71507	-1960.13012	1
216	C	69.20124	80.47398	78.51612	291.41878	-183.13091	710.72246	1
217	O	69.64670	81.45324	77.97983	379.87695	523.47396	-222.23622	1
218	N	69.08196	80.17370	79.80630	564.30591	373.09380	277.24371	1
219	H	68.83210	79.18969	80.04801	-120.59931	-2436.07824	-1214.35098	1
220	C	69.69954	80.95583	80.84282	404.07514	-299.37480	608.84009	1
221	H	68.99288	80.76258	81.68116	-1071.07882	-841.69025	2359.66467	1
222	C	71.08838	80.25135	81.14865	-683.12807	68.71770	-390.13096	1
223	H	70.94373	79.15809	81.30304	2068.88918	1596.58590	770.89603	1
224	H	71.77670	80.32947	80.27798	1379.86429	2342.49779	-179.85638	1
225	C	71.71152	80.91865	82.41346	-176.39967	537.49466	550.97268	1
226	H	71.76914	82.02861	82.28578	-396.28051	1942.22168	1869.33314	1
227	H	71.07167	80.75170	83.30910	-94.44700	586.00678	-2659.20016	1
228	C	73.17221	80.30865	82.62438	-291.69381	-718.18079	-150.72929	1
229	H	73.21658	79.21115	82.84116	-2303.38776	1089.76242	964.62032	1
230	H	73.90822	80.52817	81.80929	884.16729	2568.80533	-207.74283	1
231	N	73.58903	80.99581	83.77560	-594.49522	-252.81478	342.29276	1
232	H	72.95064	81.67684	84.15707	-1735.17426	2084.05705	-263.71605	1
233	C	74.70384	80.82110	84.36058	595.23177	-271.52487	442.22352	1
234	N	75.58261	79.87580	83.82002	585.53813	-424.79750	-105.81303	1
235	H	75.47022	79.28444	82.99767	959.88797	1327.56823	-2177.11905	1
236	H	76.50285	79.65090	84.19949	1578.48647	16.27378	-2220.76233	1
237	N	74.82355	81.65504	85.48168	-452.17763	-390.33541	-421.51853	1
238	H	74.18167	82.34095	85.87630	470.26107	1974.25629	-1817.92087	1
239	H	75.64546	81.66145	86.08685	1856.67307	-1573.97321	-1224.35416	1
240	C	69.81840	82.52333	80.49854	-531.47271	-581.45780	-55.06206	1
241	O	70.87528	83.13028	80.73743	-243.00837	192.73507	609.52485	1
242	N	68.67958	83.04456	80.09610	343.49288	-644.25607	38.09164	1
243	H	67.95127	82.34527	79.94812	-1691.16043	-1535.97525	-1484.73099	1
244	C	68.63590	84.37694	79.49355	542.66492	350.14337	454.42563	1
245	H	69.60819	84.46609	78.95383	1209.57979	-2396.95920	463.86744	1
246	C	67.40740	84.48706	78.60637	-737.14309	145.93010	242.71942	1
247	H	66.52467	84.16677	79.20343	-1050.18303	159.36419	-2509.06125	1
248	C	67.17484	85.91808	78.15701	-706.77696	-252.88343	-245.16230	1
249	H	66.22502	86.02124	77.56309	-1624.64039	-1665.49085	1417.86935	1
250	H	67.10189	86.62066	79.03279	2566.10521	598.51109	693.22305	1
251	H	68.01651	86.28987	77.51015	-1972.69758	107.10018	-1876.34312	1
252	C	67.50300	83.57663	77.39618	412.85148	672.58832	-27.69222	1
253	H	66.58430	83.64008	76.74987	1447.02277	1762.76533	-1490.78944	1
254	H	68.38540	83.84338	76.75100	1320.77379	-145.20455	2378.68491	1
255	H	67.63403	82.49902	77.69681	-1512.10848	1470.52031	1724.75147	1
256	C	68.52439	85.49432	80.72063	-607.11113	499.56689	73.73769	1
257	O	69.09097	86.55947	80.61036	357.97126	460.81534	356.68785	1
258	N	67.67325	85.10499	81.65450	536.55407	-368.62270	332.76306	1
259	H	67.30995	84.15658	81.57198	524.38866	2297.69985	1367.20941	1
260	C	67.59921	85.85468	82.85594	46.50277	-774.29190	-147.97904	1
261	H	68.47261	86.54490	82.81112	1676.51875	1883.29066	1032.55549	1
262	C	66.19112	86.64580	82.92520	-559.41456	-34.19198	-556.30433	1
263	H	65.35641	85.90643	82.96081	-64.66664	395.18769	2695.05373	1
264	H	66.12536	87.22379	83.87753	-2703.44278	-60.40056	333.79418	1
265	C	66.02518	87.55646	81.73995	-519.76435	377.31045	459.42366	1
266	H	66.07971	86.93602	80.81718	-1746.74323	1667.50644	-1261.73691	1
267	C	64.66671	88.24687	81.77845	570.95554	16.46261	-545.27700	1
268	H	64.51833	88.91581	80.89193	2391.58273	28.05277	-1305.07271	1
269	H	63.82540	87.50731	81.78076	175.75588	917.63458	2559.43867	1
270	H	64.55271	88.88207	82.69402	-1063.97851	-2155.34650	1283.00462	1
271	C	67.12387	88.60745	81.67736	193.76014	2.62946	-765.53141	1
272	H	66.91227	89.38148	80.89510	507.39394	-846.55087	2539.60089	1
273	H	67.24296	89.14585	82.65292	1337.57841	1818.19054	1526.01994	1

274	H	68.12074	88.13630	81.41649	1100.88635	-1172.91350	-2199.08909	1
275	C	67.61087	84.78877	84.06491	-549.21115	475.64486	-309.38218	1
276	O	67.31776	83.62981	83.92705	556.06106	-390.37755	-78.24250	1
277	O	67.87827	85.31842	85.35012	-572.27940	-310.19032	-209.75862	1
278	H	68.05385	86.26561	85.09322	-1380.08193	2212.14486	790.85944	1

Listing 19: C00019.xmolout

1	276							
2	150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	1.5875	6350
	0.2500	300.00	0.00	0.00	0.00	-1294.0657	0.0000	300.0000
3	H	69.78210	73.61447	67.11124	-2043.14101	-1757.64893	399.89339	1
4	N	70.77008	73.85433	67.04981	426.75047	490.45733	-334.42467	1
5	H	71.01159	73.51292	66.11992	442.25559	-1110.30854	-2448.52907	1
6	C	71.06397	75.22668	67.22701	415.32972	-666.39213	83.73172	1
7	H	70.35683	75.63511	67.98304	879.32219	2491.00447	667.35213	1
8	C	72.59742	75.32217	67.63800	31.35357	477.41777	628.23362	1
9	H	73.20713	74.66050	66.98365	1168.38489	2240.25337	-1019.71136	1
10	H	72.98960	76.35342	67.48759	-360.43770	2534.90498	931.67112	1
11	C	72.73932	74.89609	69.13711	463.18208	512.70242	-382.34388	1
12	H	72.20146	73.94011	69.32339	1725.29117	1863.52247	-987.07854	1
13	C	74.27070	74.74100	69.45953	710.42801	-144.27427	-313.15367	1
14	H	74.43192	74.31757	70.47704	364.20195	-1033.13725	2494.72524	1
15	H	74.77258	74.05430	68.73913	2567.61904	335.80679	847.48802	1
16	H	74.81031	75.71905	69.41639	-2587.99029	680.92867	-512.16411	1
17	C	72.16545	76.05420	70.03144	268.17616	741.64379	-40.42634	1
18	H	72.42223	75.90076	71.10310	1283.54314	-1945.37420	-1411.27812	1
19	H	72.57743	77.04532	69.72931	-1258.57796	1317.15249	-2026.02085	1
20	H	71.05503	76.12174	69.96364	-2502.84526	909.80597	575.92391	1
21	C	70.95202	75.92236	65.73956	619.36578	-458.64843	-172.09273	1
22	O	71.42768	75.41965	64.74779	-81.40433	433.87611	522.34594	1
23	N	70.35118	77.09725	65.88204	175.23996	-622.20190	341.55523	1
24	H	69.97228	77.34230	66.79500	-876.57256	-303.22879	-2561.90213	1
25	C	70.24591	77.94617	64.74263	-571.88214	-534.10783	-106.15033	1
26	H	70.29492	77.21553	63.90078	-2713.20841	-16.25800	-248.80809	1
27	C	68.86081	78.74375	64.84773	166.60354	288.16399	-716.09568	1
28	H	68.94867	79.53770	65.63775	-2097.85574	1636.78449	-586.18044	1
29	O	67.71053	77.95544	65.19788	-317.80580	-363.38227	484.43082	1
30	H	67.41531	78.40571	66.01529	1863.74748	-1451.84923	1357.29467	1
31	C	68.79698	79.44330	63.44083	503.80731	517.99032	318.51606	1
32	H	67.90140	80.10099	63.35326	640.61020	-2157.10410	-1536.29104	1
33	H	69.69512	80.07733	63.24691	1687.88455	465.60692	2087.56452	1
34	H	68.73743	78.69318	62.61815	-1293.07895	-1899.88581	-1463.57452	1
35	C	71.49283	79.00237	64.66745	-153.07550	-733.68902	248.70981	1
36	O	71.82346	79.30726	63.54888	186.15459	-480.78787	-449.34387	1
37	N	71.93257	79.52480	65.82386	-487.53139	543.18517	42.03850	1
38	C	73.04339	80.42549	65.81497	-699.35871	69.34393	360.10701	1
39	H	73.08274	80.90071	64.80635	2.81126	-221.99807	-2715.58072	1
40	C	72.65488	81.37750	67.03364	-507.46439	-592.59194	122.07761	1
41	H	73.52441	81.94908	67.42740	-1975.08116	525.87560	-1801.71556	1
42	H	71.89278	82.12798	66.72812	1588.27743	-1913.22100	1113.83566	1
43	C	72.06740	80.37021	68.06791	-613.62442	-457.55993	-194.14490	1
44	H	72.87646	79.89165	68.66799	1707.54637	-721.27992	1996.92523	1
45	H	71.38008	80.84732	68.80220	758.23357	2100.81767	1560.55011	1
46	C	71.33964	79.30856	67.13535	-352.41524	704.96076	49.21465	1
47	H	71.55189	78.24690	67.40107	1714.76886	-2070.42778	443.35792	1
48	H	70.24090	79.45306	67.02386	1224.15040	1801.50881	1636.97633	1
49	C	74.40541	79.61807	66.21130	566.85117	537.05831	117.62814	1
50	O	74.42597	78.69779	67.02304	-550.26779	-406.08867	4.21666	1
51	N	75.41676	80.21151	65.61895	566.34832	-425.77725	180.18749	1
52	H	75.21960	80.98134	64.98381	644.44502	2646.80550	-52.73430	1
53	C	76.68878	79.55305	65.65615	612.34801	-281.48662	411.56221	1

54	H	76.39932	78.47988	65.59110	1667.23498	-1490.75142	1556.16753	1
55	C	77.58012	80.09019	64.45019	-714.45746	-175.43074	286.98927	1
56	H	77.78389	81.18401	64.60995	-787.09484	1763.03619	-1922.46060	1
57	O	76.99091	79.96795	63.14255	-429.46514	516.51932	-128.40526	1
58	H	76.96074	80.90115	62.85455	1981.82785	436.16847	-1818.18182	1
59	C	78.90870	79.27598	64.67379	630.79189	-468.94448	76.03230	1
60	H	79.69438	79.57125	63.94063	-1775.71861	2062.30353	131.89849	1
61	H	79.33078	79.43825	65.69427	-1855.14608	88.94118	1993.53760	1
62	H	78.73904	78.18098	64.55351	-1504.82350	-780.94249	-2132.90992	1
63	C	77.36045	79.91671	67.10433	288.57638	618.62814	-397.00270	1
64	O	78.23182	80.74486	67.21467	321.70495	-185.26452	574.37218	1
65	N	76.81658	79.14011	68.03868	-447.05792	-446.53431	367.76425	1
66	H	75.98803	78.53591	67.82585	350.31316	1975.63644	-1843.31522	1
67	C	77.23540	79.40357	69.37374	-511.23061	374.03917	-471.51480	1
68	H	78.16537	80.01534	69.28531	2234.79579	-898.70890	-1273.45190	1
69	C	76.02588	80.25846	69.98455	529.53781	-159.34528	563.72604	1
70	H	76.31273	80.60902	71.00916	654.59388	2347.94251	1217.51488	1
71	H	75.96041	81.18508	69.35194	-1526.55661	2103.42026	817.87394	1
72	O	74.71276	79.63181	70.00669	-554.84278	14.12789	399.58769	1
73	H	74.66016	79.36491	69.06477	1297.06236	2061.84854	1220.68812	1
74	C	77.47168	77.94807	70.07390	-662.15484	-412.13544	123.62687	1
75	O	76.70255	77.02188	70.00232	-540.01537	-317.05804	274.91456	1
76	N	78.62644	78.02030	70.75851	-202.76299	-690.00100	-131.49145	1
77	H	79.11254	78.91251	70.66587	-702.62132	-2617.37191	281.70413	1
78	C	79.35885	76.78673	71.06816	-491.73914	576.34187	222.73509	1
79	H	78.85821	76.01607	70.43513	1977.17978	-1823.58850	-434.68928	1
80	C	80.82862	76.99170	70.76284	-649.50797	-328.66843	306.11224	1
81	H	81.20329	77.82336	71.40060	2075.07803	1452.16490	-1004.45904	1
82	C	81.63933	75.75026	71.09218	-615.18735	-489.99689	-70.96352	1
83	H	82.73507	75.90492	70.89329	-1226.32661	-1724.38906	-1716.47170	1
84	H	81.53226	75.46190	72.17419	2381.64273	-969.84735	900.46860	1
85	H	81.31182	74.86600	70.48020	2122.74991	1702.23946	-141.36228	1
86	C	81.05892	77.39023	69.31549	-501.86074	-479.61276	-376.42482	1
87	H	82.14978	77.55200	69.09716	993.79261	-2246.95401	-1177.81305	1
88	H	80.69032	76.60015	68.60608	42.71279	-626.15391	-2651.37258	1
89	H	80.52074	78.34250	69.05561	-2026.39012	-1590.33709	-887.82922	1
90	C	79.14019	76.49031	72.68345	-672.89153	382.57394	-156.34072	1
91	O	78.83690	75.38410	73.06247	410.04627	221.86223	500.35950	1
92	N	79.38511	77.57930	73.49545	-378.11782	-443.79414	-441.10984	1
93	H	79.53857	78.29564	72.76672	2404.15973	-568.14894	1149.30085	1
94	C	78.24566	77.79284	74.37547	-544.54484	466.16019	331.29119	1
95	H	77.88235	76.76659	74.61096	-1409.80988	-170.17955	2325.32679	1
96	C	78.68344	78.61913	75.63924	-184.48284	116.78282	-758.89137	1
97	H	79.63985	78.23896	76.06544	1893.78641	1861.14652	611.04528	1
98	H	78.85867	79.68803	75.37831	-2170.79665	-974.19311	1327.50117	1
99	C	77.49453	78.44852	76.64426	389.51668	672.81878	-138.49152	1
100	H	76.55225	78.84493	76.18971	510.64577	1933.03327	1851.02484	1
101	H	77.27611	77.36020	76.80899	-2302.30869	-1105.72939	-948.89774	1
102	C	77.74555	79.12837	78.04048	-559.93427	-126.34590	542.30857	1
103	O	77.07571	78.81798	78.99521	-670.36003	-111.83166	76.36448	1
104	N	78.73000	80.05249	78.02324	-216.06729	-537.07037	446.51379	1
105	H	79.25195	80.41243	77.21675	-1251.96487	1074.12894	-2168.52500	1
106	H	78.95112	80.66840	78.81322	-2451.83023	-720.73851	944.84612	1
107	C	77.20378	78.72570	73.53443	546.24052	-563.88337	-85.11809	1
108	O	77.49091	79.85756	73.24837	71.70702	-307.40463	606.69673	1
109	N	76.10570	78.02111	73.23071	479.90863	-504.50129	222.86849	1
110	C	74.91031	78.68370	72.80304	75.51268	-600.91904	506.73700	1
111	H	75.23793	79.58138	72.22988	-2033.61562	1795.30103	254.89480	1
112	C	74.22600	77.55137	71.92250	523.79067	517.99274	284.45581	1
113	H	73.12871	77.69572	71.81008	1599.61665	-1127.00911	1895.98173	1
114	H	74.66231	77.53839	70.89317	-1881.83093	1275.82488	-1501.55016	1
115	C	74.60147	76.25039	72.69611	-600.05639	-404.05026	316.64485	1

116	H	73.94898	76.11317	73.58587	-2597.05260	496.36221	657.73249	1
117	H	74.50813	75.32234	72.09113	-1666.24518	1294.38985	-1723.90591	1
118	C	76.09598	76.56752	73.12596	493.57570	-129.95376	-602.56394	1
119	H	76.39787	76.13522	74.11043	-1469.08415	-637.84797	2204.22581	1
120	H	76.87057	76.31791	72.35759	-1038.97840	1068.88701	-2280.71789	1
121	C	74.07922	79.10696	74.13692	188.88100	241.05089	-727.87821	1
122	O	74.50695	78.98862	75.26170	531.88613	-49.19943	427.07960	1
123	N	72.88650	79.70013	73.79572	708.14833	26.93417	-179.73509	1
124	H	72.86259	79.54127	72.78326	-2232.69501	-1179.09831	1023.94816	1
125	C	71.72030	79.34161	74.63840	-738.32412	259.92548	104.42456	1
126	H	72.15103	79.40868	75.66531	2028.89123	1260.02983	1311.33324	1
127	C	70.61558	80.32855	74.34652	-258.65678	-345.52513	661.28459	1
128	H	70.37071	80.25174	73.26255	-1826.06090	-1801.46097	-918.64554	1
129	C	69.35624	80.00971	75.13270	-541.23400	531.92970	-218.41428	1
130	H	68.53600	80.75080	74.92599	1311.73218	-2219.18200	882.19023	1
131	H	68.96129	78.98756	74.86799	-1048.71298	1223.58118	-2196.97971	1
132	H	69.54452	80.01864	76.24126	419.06414	1903.92898	1903.44670	1
133	C	71.05258	81.75827	74.61524	-423.86431	152.66566	-648.55262	1
134	H	70.26102	82.50091	74.32163	105.68386	-2342.50080	1387.51238	1
135	H	71.28012	81.92342	75.70383	-1695.63603	-1484.73621	-1531.02793	1
136	H	71.98582	82.01306	74.04113	-1853.57121	-487.39031	1936.59343	1
137	C	71.29366	77.80174	74.22615	539.71428	-510.58232	267.58633	1
138	O	70.27839	77.60813	73.60771	-15.93758	-278.34085	-624.49402	1
139	N	72.21782	76.93716	74.60300	-676.81886	12.05292	276.17960	1
140	H	73.05349	77.23183	75.13400	-1694.44250	-373.84189	-2100.66098	1
141	C	71.87944	75.53306	74.68505	412.33078	-664.70360	108.35451	1
142	H	71.01753	75.53686	75.38831	1765.77476	1294.44366	1621.76594	1
143	C	71.46995	74.97686	73.26127	-179.66635	-721.95667	-264.73915	1
144	H	71.11497	75.80379	72.60330	-607.34922	2587.87032	-598.10018	1
145	H	72.35094	74.53034	72.74760	-359.69332	-1479.13954	-2259.74260	1
146	C	70.33917	73.91003	73.43845	-240.01076	616.02425	431.85322	1
147	H	70.57170	73.20002	74.26271	-1359.17131	782.54425	2227.99181	1
148	H	69.37812	74.39750	73.71775	-820.36667	85.81767	-2596.78715	1
149	C	70.21374	73.14480	72.05947	-513.07015	236.18570	-551.87280	1
150	H	70.01789	73.85589	71.22399	1816.11944	-1183.11722	-1650.94321	1
151	H	71.16884	72.63205	71.80138	-1800.04429	-1361.53473	1526.34643	1
152	C	69.05962	72.12537	72.19876	726.08972	-253.19732	-179.64713	1
153	H	69.20763	71.36620	72.99258	1224.27271	-456.51798	-2390.90304	1
154	H	68.05309	72.57947	72.29333	1206.40339	-1150.93514	-2154.90344	1
155	N	68.99999	71.29842	70.87026	329.70796	-633.68968	-155.67358	1
156	H	68.23645	70.56358	70.82111	1348.31305	1938.76845	1359.00643	1
157	H	68.82950	71.83847	69.97259	2096.92035	1446.54551	-966.48890	1
158	H	69.85704	70.72416	70.62065	-1197.07217	-2303.53719	827.28733	1
159	C	73.24086	74.91932	75.28805	-378.01186	-556.17301	-413.96481	1
160	O	74.06763	75.68475	75.81453	-409.44433	-307.55053	-453.30833	1
161	N	73.30608	73.62044	75.12954	-429.02477	524.70884	274.08502	1
162	H	72.51033	73.17835	74.67036	1706.34263	-1425.96036	1574.38926	1
163	C	74.41767	72.84147	75.54472	-45.25864	-626.22952	478.93267	1
164	H	74.10420	71.81201	75.26043	1988.63164	570.90773	1772.87287	1
165	C	75.67251	73.35141	74.71669	551.77128	-20.49526	-564.54996	1
166	H	75.34503	73.91800	73.81678	1434.61535	-1753.10253	1513.99471	1
167	H	76.26641	74.07534	75.32162	-714.67738	1819.09770	1898.36494	1
168	C	76.55726	72.13165	74.29979	446.99263	-555.77305	338.97221	1
169	H	76.70577	71.42726	75.14790	1953.68466	1892.25957	-161.67766	1
170	H	76.06964	71.53918	73.49351	-403.03785	2688.07032	-188.43591	1
171	C	77.94468	72.72017	73.81825	567.86262	335.74681	434.04421	1
172	H	77.81050	73.38271	72.92967	-1080.02275	1568.26081	-1948.78900	1
173	H	78.39587	73.37047	74.60376	-919.54108	2111.34692	1456.13463	1
174	C	78.88781	71.54054	73.48772	195.81897	173.33862	-745.11536	1
175	H	79.14582	70.89862	74.35361	1405.67949	-2301.21089	-390.08113	1
176	H	78.56790	70.91293	72.63168	-940.37328	-1118.32446	2299.72133	1
177	N	80.25092	72.17045	73.04271	319.26422	656.36007	-42.02424	1

178	H	81.04076	71.49778	72.81672	1961.03633	619.91968	1787.09422	1
179	H	80.23460	72.78618	72.17841	854.14343	-2156.80752	1429.08711	1
180	H	80.71467	72.81240	73.74777	1237.02905	-1378.50857	-1998.28500	1
181	C	74.57718	73.02955	77.16401	532.53319	-268.57236	517.55729	1
182	O	73.62525	73.27506	77.86552	266.16714	-290.73804	-558.88002	1
183	N	75.83264	72.71747	77.53912	-226.25352	640.49678	-270.32839	1
184	H	76.40772	72.51161	76.72121	2007.69063	-1035.27229	1523.50231	1
185	C	76.48626	73.48808	78.56160	-540.76542	-573.33303	49.50000	1
186	H	77.56672	73.34693	78.33928	-2374.20950	-1036.76023	843.75774	1
187	C	76.07099	75.00062	78.29999	-77.09082	666.87422	-415.84136	1
188	H	74.94666	75.07531	78.33500	-985.81834	617.19825	2463.91927	1
189	O	76.44318	75.50127	77.00427	293.29899	-391.65602	-477.80926	1
190	H	75.50714	75.62912	76.58043	2528.72714	-681.76262	-751.27122	1
191	C	76.68050	75.78503	79.51255	252.47363	-605.14473	440.05134	1
192	H	76.43378	76.87979	79.45548	-2052.65063	1456.49051	-1043.51830	1
193	H	76.29792	75.40674	80.49003	-2152.98800	-1661.97574	-161.70652	1
194	H	77.79332	75.70739	79.53385	-473.12726	-1584.27339	2165.61725	1
195	C	76.11329	72.88138	80.01884	360.36307	488.46713	505.10056	1
196	O	75.10317	72.26179	80.29069	-200.08817	-528.03552	-385.82850	1
197	N	77.08101	73.25059	80.93094	-597.54095	-226.44775	355.20479	1
198	H	77.74294	73.72647	80.30065	2179.23655	-1300.70981	-991.33835	1
199	C	77.63430	72.10739	81.64178	-687.68921	297.39807	-249.45179	1
200	H	77.77907	71.31918	80.87254	-349.16256	-2467.37713	-1101.72831	1
201	C	78.99745	72.61145	82.28216	672.47345	361.54328	-201.62880	1
202	H	78.81695	73.50139	82.92826	1541.41502	582.18425	2169.97026	1
203	H	79.43143	71.81485	82.93012	-2534.67717	60.25153	997.72295	1
204	C	79.94884	72.95851	81.12443	574.26774	-389.43119	-377.02542	1
205	C	80.61179	71.89724	80.44042	688.82679	-287.33580	-257.96133	1
206	H	80.47002	70.84724	80.75516	331.14182	1470.38163	2269.80013	1
207	C	80.12654	74.31279	80.71146	-383.52382	-675.04808	144.24917	1
208	H	79.60747	75.13490	81.23714	4.09847	1517.59662	2262.86397	1
209	C	81.44004	72.21484	79.36382	-134.76730	428.45285	-649.50303	1
210	H	81.95866	71.39508	78.83724	-903.23433	1600.49020	2011.53387	1
211	C	80.96582	74.57928	79.62602	-335.53281	-615.00040	-364.39058	1
212	H	81.09977	75.63008	79.31489	1596.45398	-1369.33862	1732.02659	1
213	C	81.64968	73.55062	78.91468	585.48547	-340.24194	-406.23938	1
214	O	82.49949	73.80871	77.80682	-419.15649	-173.04408	-511.94141	1
215	H	82.45883	74.79372	77.79225	-1071.84350	1559.71507	-1960.13012	1
216	C	76.64095	71.64342	82.82044	291.41878	-183.13091	710.72246	1
217	O	76.67685	70.49688	83.22284	379.87695	523.47396	-222.23622	1
218	N	75.94449	72.68107	83.31960	564.30591	373.09380	277.24371	1
219	H	76.05794	73.53579	82.77077	-120.59931	-2436.07824	-1214.35098	1
220	C	74.67868	72.39088	83.93601	404.07514	-299.37480	608.84009	1
221	H	74.18323	73.38709	83.93997	-1071.07882	-841.69025	2359.66467	1
222	C	73.97865	71.35141	82.96780	-683.12807	68.71770	-390.13096	1
223	H	74.24380	71.58960	81.88812	2068.88918	1596.58590	770.89603	1
224	H	74.39734	70.33144	83.15369	1379.86429	2342.49779	-179.85638	1
225	C	72.44034	71.39009	83.19415	-176.39967	537.49466	550.97268	1
226	H	72.18098	71.59187	84.25646	-396.28051	1942.22168	1869.33314	1
227	H	71.96379	72.21165	82.61620	-94.44700	586.00678	-2659.20016	1
228	C	71.88624	69.94685	82.73771	-291.69381	-718.18079	-150.72929	1
229	H	72.04073	69.74666	81.64552	-2303.38776	1089.76242	964.62032	1
230	H	72.25125	69.09883	83.39445	884.16729	2568.80533	-207.74283	1
231	N	70.54290	70.18676	82.99411	-594.49522	-252.81478	342.29276	1
232	H	70.19013	69.82444	83.87118	-1735.17426	2084.05705	-263.71605	1
233	C	69.72579	70.80782	82.22306	595.23177	-271.52487	442.22352	1
234	N	70.21799	71.31701	81.02338	585.53813	-424.79750	-105.81303	1
235	H	71.17092	71.28900	80.66028	959.88797	1327.56823	-2177.11905	1
236	H	69.68236	71.84520	80.33391	1578.48647	16.27378	-2220.76233	1
237	N	68.45518	70.84027	82.80005	-452.17763	-390.33541	-421.51853	1
238	H	68.11955	70.44771	83.67916	470.26107	1974.25629	-1817.92087	1
239	H	67.64014	71.26762	82.35825	1856.67307	-1573.97321	-1224.35416	1

240	C	74.99098	71.83928	85.42649	-531.47271	-581.45780	-55.06206	1
241	O	75.75240	72.40762	86.17011	-243.00837	192.73507	609.52485	1
242	N	74.21574	70.75303	85.74544	343.49288	-644.25607	38.09164	1
243	H	73.61717	70.52525	84.94345	-1691.16043	-1535.97525	-1484.73099	1
244	C	74.95227	69.57408	86.27598	542.66492	350.14337	454.42563	1
245	H	76.02250	69.87899	86.32677	1209.57979	-2396.95920	463.86744	1
246	C	74.35084	69.20410	87.61277	-737.14309	145.93010	242.71942	1
247	H	73.27387	68.97553	87.44611	-1050.18303	159.36419	-2509.06125	1
248	C	75.01689	67.97148	88.19754	-706.77696	-252.88343	-245.16230	1
249	H	74.51822	67.63821	89.14897	-1624.64039	-1665.49085	1417.86935	1
250	H	74.98902	67.10221	87.48150	2566.10521	598.51109	693.22305	1
251	H	76.09946	68.16059	88.43757	-1972.69758	107.10018	-1876.34312	1
252	C	74.42969	70.35731	88.59746	412.85148	672.58832	-27.69222	1
253	H	73.89722	70.12685	89.56111	1447.02277	1762.76533	-1490.78944	1
254	H	75.49619	70.60783	88.85299	1320.77379	-145.20455	2378.68491	1
255	H	73.96936	71.29026	88.16772	-1512.10848	1470.52031	1724.75147	1
256	C	74.62022	68.38397	85.19173	-607.11113	499.56689	73.73769	1
257	O	73.50657	68.25080	84.70896	357.97126	460.81534	356.68785	1
258	N	75.69117	67.63835	85.00568	536.55407	-368.62270	332.76306	1
259	H	76.54073	67.88858	85.50873	524.38866	2297.69985	1367.20941	1
260	C	75.56383	66.39577	84.33549	46.50277	-774.29190	-147.97904	1
261	H	74.46572	66.26158	84.19927	1676.51875	1883.29066	1032.55549	1
262	C	76.35904	66.45451	82.92851	-559.41456	-34.19198	-556.30433	1
263	H	77.45703	66.45326	83.12625	-64.66664	395.18769	2695.05373	1
264	H	76.15894	65.53266	82.33280	-2703.44278	-60.40056	333.79418	1
265	C	75.97457	67.68475	82.15554	-519.76435	377.31045	459.42366	1
266	H	76.23033	68.59138	82.77537	-1746.74323	1667.50644	-1261.73691	1
267	C	76.75574	67.75941	80.84907	570.95554	16.46261	-545.27700	1
268	H	76.52505	68.70110	80.28691	2391.58273	28.05277	-1305.07271	1
269	H	77.86169	67.73997	81.02689	175.75588	917.63458	2559.43867	1
270	H	76.51229	66.89993	80.17273	-1063.97851	-2155.34650	1283.00462	1
271	C	74.48426	67.71854	81.85321	193.76014	2.62946	-765.53141	1
272	H	74.21670	68.58565	81.19502	507.39394	-846.55087	2539.60089	1
273	H	74.14055	66.78718	81.33340	1337.57841	1818.19054	1526.01994	1
274	H	73.88215	67.82248	82.81013	1100.88635	-1172.91350	-2199.08909	1
275	C	76.27440	65.29709	85.27417	-549.21115	475.64486	-309.38218	1
276	O	76.71072	65.54493	86.36814	556.06106	-390.37755	-78.24250	1
277	O	76.35066	63.98263	84.75229	-572.27940	-310.19032	-209.75862	1
278	H	75.87977	64.13282	83.88813	-1380.08193	2212.14486	790.85944	1

Listing 20: C00020.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.8085	3234
		0.2500	300.00	0.00	0.00	0.00	-1294.0363	0.0000	300.0000
3	H	75.02491	70.21798	67.06212	-2043.14101	-1757.64893	399.89339		1
4	N	75.27755	70.77793	66.24906	426.75047	490.45733	-334.42467		1
5	H	74.56010	71.50013	66.25008	442.25559	-1110.30854	-2448.52907		1
6	C	76.60637	71.25210	66.20595	415.32972	-666.39213	83.73172		1
7	H	77.23499	70.36096	66.41421	879.32219	2491.00447	667.35213		1
8	C	76.88367	71.92619	64.77038	31.35357	477.41777	628.23362		1
9	H	76.03540	72.60534	64.51266	1168.38489	2240.25337	-1019.71136		1
10	H	77.79382	72.57276	64.82154	-360.43770	2534.90498	931.67112		1
11	C	77.05327	70.84892	63.72893	463.18208	512.70242	-382.34388		1
12	H	76.24898	70.09278	63.87340	1725.29117	1863.52247	-987.07854		1
13	C	76.92389	71.43090	62.32729	710.42801	-144.27427	-313.15367		1
14	H	77.05070	70.64378	61.53950	364.20195	-1033.13725	2494.72524		1
15	H	75.92147	71.90521	62.16537	2567.61904	335.80679	847.48802		1
16	H	77.69795	72.21852	62.13554	-2587.99029	680.92867	-512.16411		1
17	C	78.40714	70.16588	63.86809	268.17616	741.64379	-40.42634		1
18	H	78.54454	69.35906	63.10252	1283.54314	-1945.37420	-1411.27812		1
19	H	79.24957	70.89354	63.73656	-1258.57796	1317.15249	-2026.02085		1

20	H	78.53479	69.69269	64.87543	-2502.84526	909.80597	575.92391	1
21	C	76.83978	72.44725	67.33216	619.36578	-458.64843	-172.09273	1
22	O	78.09245	73.02542	67.31352	-81.40433	433.87611	522.34594	1
23	N	75.73038	73.38413	67.10132	175.23996	-622.20190	341.55523	1
24	H	74.82330	73.00393	67.37902	-876.57256	-303.22879	-2561.90213	1
25	C	76.01478	74.64510	67.73108	-571.88214	-534.10783	-106.15033	1
26	H	76.97320	74.96651	67.26537	-2713.20841	-16.25800	-248.80809	1
27	C	74.78597	75.61009	67.41777	166.60354	288.16399	-716.09568	1
28	H	73.88533	75.18551	67.93693	-2097.85574	1636.78449	-586.18044	1
29	O	74.44297	75.74856	66.02381	-317.80580	-363.38227	484.43082	1
30	H	73.60424	75.24869	65.98372	1863.74748	-1451.84923	1357.29467	1
31	C	75.23751	76.93214	68.14074	503.80731	517.99032	318.51606	1
32	H	74.45044	77.71866	68.08490	640.61020	-2157.10410	-1536.29104	1
33	H	75.45984	76.76142	69.22197	1687.88455	465.60692	2087.56452	1
34	H	76.15798	77.35494	67.67542	-1293.07895	-1899.88581	-1463.57452	1
35	C	76.11471	74.39852	69.33356	-153.07550	-733.68902	248.70981	1
36	O	75.14619	74.63755	70.00698	186.15459	-480.78787	-449.34387	1
37	N	77.30520	73.84849	69.71889	-487.53139	543.18517	42.03850	1
38	C	77.57172	73.60477	71.12251	-699.35871	69.34393	360.10701	1
39	H	76.62037	73.32712	71.62932	2.81126	-221.99807	-2715.58072	1
40	C	78.67062	72.47656	71.00902	-507.46439	-592.59194	122.07761	1
41	H	79.24981	72.33393	71.94935	-1975.08116	525.87560	-1801.71556	1
42	H	78.23008	71.49003	70.74478	1588.27743	-1913.22100	1113.83566	1
43	C	79.51995	73.07197	69.82781	-613.62442	-457.55993	-194.14490	1
44	H	80.20557	73.87225	70.19855	1707.54637	-721.27992	1996.92523	1
45	H	80.16391	72.32038	69.31452	758.23357	2100.81767	1560.55011	1
46	C	78.42557	73.67518	68.88949	-352.41524	704.96076	49.21465	1
47	H	78.66550	74.64245	68.37207	1714.76886	-2070.42778	443.35792	1
48	H	76.53427	72.09330	68.35626	1224.15040	1801.50881	1636.97633	1
49	C	78.30312	74.93279	71.72832	566.85117	537.05831	117.62814	1
50	O	79.03634	75.63258	71.07095	-550.26779	-406.08867	4.21666	1
51	N	77.99555	75.04304	73.02975	566.34832	-425.77725	180.18749	1
52	H	77.45236	74.26968	73.41818	644.44502	2646.80550	-52.73430	1
53	C	79.00363	75.65090	73.85438	612.34801	-281.48662	411.56221	1
54	H	79.63155	76.28012	73.18174	1667.23498	-1490.75142	1556.16753	1
55	C	78.12072	76.52257	74.87230	-714.45746	-175.43074	286.98927	1
56	H	77.20449	75.92419	75.12549	-787.09484	1763.03619	-1922.46060	1
57	O	77.62354	77.75238	74.30522	-429.46514	516.51932	-128.40526	1
58	H	76.68520	77.52670	74.15598	1981.82785	436.16847	-1818.18182	1
59	C	78.99964	76.67781	76.16187	630.79189	-468.94448	76.03230	1
60	H	78.45655	77.25421	76.94734	-1775.71861	2062.30353	131.89849	1
61	H	79.26941	75.68661	76.60086	-1855.14608	88.94118	1993.53760	1
62	H	79.94925	77.22147	75.94963	-1504.82350	-780.94249	-2132.90992	1
63	C	79.81875	74.42435	74.51279	288.57638	618.62814	-397.00270	1
64	O	79.28947	73.30659	74.63102	321.70495	-185.26452	574.37218	1
65	N	80.97999	74.83280	74.97406	-447.05792	-446.53431	367.76425	1
66	H	81.20411	75.80276	74.75428	350.31316	1975.63644	-1843.31522	1
67	C	82.02640	73.86452	75.15057	-511.23061	374.03917	-471.51480	1
68	H	82.08883	73.31915	74.18327	2234.79579	-898.70890	-1273.45190	1
69	C	83.32954	74.71880	75.49260	529.53781	-159.34528	563.72604	1
70	H	84.19574	74.00667	75.56824	654.59388	2347.94251	1217.51488	1
71	H	83.52971	75.38210	74.61095	-1526.55661	2103.42026	817.87394	1
72	O	83.29781	75.48941	76.72989	-554.84278	14.12789	399.58769	1
73	H	82.72921	76.22483	76.44258	1297.06236	2061.84854	1220.68812	1
74	C	81.66627	72.85056	76.36552	-662.15484	-412.13544	123.62687	1
75	O	82.02901	71.69898	76.29858	-540.01537	-317.05804	274.91456	1
76	N	81.13325	73.48792	77.42863	-202.76299	-690.00100	-131.49145	1
77	H	80.90036	74.44598	77.16476	-702.62132	-2617.37191	281.70413	1
78	C	80.38615	72.73736	78.45771	-491.73914	576.34187	222.73509	1
79	H	79.93522	71.91869	77.85108	1977.17978	-1823.58850	-434.68928	1
80	C	81.34659	72.22087	79.50392	-649.50797	-328.66843	306.11224	1
81	H	81.72765	73.09399	80.08044	2075.07803	1452.16490	-1004.45904	1

82	C	80.65922	71.26290	80.46254	-615.18735	-489.99689	-70.96352	1
83	H	81.33727	70.96324	81.30730	-1226.32661	-1724.38906	-1716.47170	1
84	H	79.73468	71.71261	80.91698	2381.64273	-969.84735	900.46860	1
85	H	80.34189	70.31885	79.94200	2122.74991	1702.23946	-141.36228	1
86	C	82.56524	71.53867	78.90159	-501.86074	-479.61276	-376.42482	1
87	H	83.27980	71.17805	79.69129	993.79261	-2246.95401	-1177.81305	1
88	H	82.27309	70.64766	78.27712	42.71279	-626.15391	-2651.37258	1
89	H	83.13238	72.23931	78.22557	-2026.39012	-1590.33709	-887.82922	1
90	C	79.27556	73.83261	78.99369	-672.89153	382.57394	-156.34072	1
91	O	78.46337	74.27600	78.20852	410.04627	221.86223	500.35950	1
92	N	79.41220	74.13479	80.27098	-378.11782	-443.79414	-441.10984	1
93	H	80.15649	73.70306	80.81341	2404.15973	-568.14894	1149.30085	1
94	C	78.48160	75.02443	80.87452	-544.54484	466.16019	331.29119	1
95	H	77.78943	75.34842	80.05962	-1409.80988	-170.17955	2325.32679	1
96	C	77.81476	74.19828	82.05719	-184.48284	116.78282	-758.89137	1
97	H	77.32145	73.28050	81.63665	1893.78641	1861.14652	611.04528	1
98	H	78.59200	73.83865	82.77018	-2170.79665	-974.19311	1327.50117	1
99	C	76.77924	75.10870	82.78431	389.51668	672.81878	-138.49152	1
100	H	77.31426	75.94854	83.28897	510.64577	1933.03327	1851.02484	1
101	H	76.11210	75.60784	82.04722	-2302.30869	-1105.72939	-948.89774	1
102	C	75.90561	74.31153	83.82562	-559.93427	-126.34590	542.30857	1
103	O	75.00536	74.86983	84.39613	-670.36003	-111.83166	76.36448	1
104	N	76.26669	73.01647	83.97431	-216.06729	-537.07037	446.51379	1
105	H	77.07890	72.52402	83.58589	-1251.96487	1074.12894	-2168.52500	1
106	H	75.87285	72.39462	84.68870	-2451.83023	-720.73851	944.84612	1
107	C	79.33141	76.22195	81.60223	546.24052	-563.88337	-85.11809	1
108	O	79.53588	76.13459	82.78373	71.70702	-307.40463	606.69673	1
109	N	79.73054	77.15677	80.72300	479.90863	-504.50129	222.86849	1
110	C	80.53495	78.25317	81.15023	75.51268	-600.91904	506.73700	1
111	H	81.05439	77.90193	82.07145	-2033.61562	1795.30103	254.89480	1
112	C	81.45256	78.48263	79.87941	523.79067	517.99274	284.45581	1
113	H	81.80775	79.53432	79.79791	1599.61665	-1127.00911	1895.98173	1
114	H	82.36824	77.85316	79.94248	-1881.83093	1275.82488	-1501.55016	1
115	C	80.57590	78.04553	78.66004	-600.05639	-404.05026	316.64485	1
116	H	80.05619	78.91154	78.19125	-2597.05260	496.36221	657.73249	1
117	H	81.18347	77.58998	77.84617	-1666.24518	1294.38985	-1723.90591	1
118	C	79.54428	77.01751	79.28412	493.57570	-129.95376	-602.56394	1
119	H	78.45306	77.24155	79.06427	-1469.08415	-637.84797	2204.22581	1
120	H	79.75581	75.94588	79.05002	-1038.97840	1068.88701	-2280.71789	1
121	C	79.57238	79.55008	81.47134	188.88100	241.05089	-727.87821	1
122	O	79.60486	80.04561	82.57376	531.88613	-49.19943	427.07960	1
123	N	78.92027	79.96096	80.39430	708.14833	26.93417	-179.73509	1
124	H	79.02587	79.40736	79.54700	-2232.69501	-1179.09831	1023.94816	1
125	C	77.79627	80.83079	80.54480	-738.32412	259.92548	104.42456	1
126	H	77.32538	80.56221	81.51610	2028.89123	1260.02983	1311.33324	1
127	C	78.33640	82.32026	80.52147	-258.65678	-345.52513	661.28459	1
128	H	78.81261	82.54105	79.54139	-1826.06090	-1801.46097	-918.64554	1
129	C	77.10736	83.25939	80.77440	-541.23400	531.92970	-218.41428	1
130	H	77.40367	84.33448	80.76861	1311.73218	-2219.18200	882.19023	1
131	H	76.32547	83.12565	79.98982	-1048.71298	1223.58118	-2196.97971	1
132	H	76.62853	83.05155	81.75989	419.06414	1903.92898	1903.44670	1
133	C	79.36428	82.53539	81.68748	-423.86431	152.66566	-648.55262	1
134	H	79.65858	83.60684	81.78707	105.68386	-2342.50080	1387.51238	1
135	H	78.94376	82.20827	82.67010	-1695.63603	-1484.73621	-1531.02793	1
136	H	80.29961	81.94901	81.51714	-1853.57121	-487.39031	1936.59343	1
137	C	76.88659	80.58109	79.20222	539.71428	-510.58232	267.58633	1
138	O	77.29763	80.88673	78.10585	-15.93758	-278.34085	-624.49402	1
139	N	75.69097	80.13189	79.56463	-676.81886	12.05292	276.17960	1
140	H	75.53892	79.97335	80.56094	-1694.44250	-373.84189	-2100.66098	1
141	C	74.85550	79.44430	78.63314	412.33078	-664.70360	108.35451	1
142	H	73.84711	79.46958	79.10351	1765.77476	1294.44366	1621.76594	1
143	C	74.94862	80.22609	77.26065	-179.66635	-721.95667	-264.73915	1

144	H	75.14168	81.30432	77.46950	-607.34922	2587.87032	-598.10018	1
145	H	75.83775	79.88600	76.67821	-359.69332	-1479.13954	-2259.74260	1
146	C	73.64107	80.04803	76.41927	-240.01076	616.02425	431.85322	1
147	H	73.58256	79.03210	75.96798	-1359.17131	782.54425	2227.99181	1
148	H	72.73339	80.15726	77.05423	-820.36667	85.81767	-2596.78715	1
149	C	73.68026	81.17139	75.30591	-513.07015	236.18570	-551.87280	1
150	H	73.69403	82.18287	75.77366	1816.11944	-1183.11722	-1650.94321	1
151	H	74.62112	81.10228	74.71269	-1800.04429	-1361.53473	1526.34643	1
152	C	72.44847	81.02050	74.38372	726.08972	-253.19732	-179.64713	1
153	H	72.47569	80.13960	73.70910	1224.27271	-456.51798	-2390.90304	1
154	H	71.47087	81.06996	74.90382	1206.40339	-1150.93514	-2154.90344	1
155	N	72.44206	82.26234	73.42845	329.70796	-633.68968	-155.67358	1
156	H	71.65610	82.28940	72.71700	1348.31305	1938.76845	1359.00643	1
157	H	72.34739	83.21954	73.87813	2096.92035	1446.54551	-966.48890	1
158	H	73.29137	82.39595	72.80619	-1197.07217	-2303.53719	827.28733	1
159	C	75.41071	77.91733	78.44032	-378.01186	-556.17301	-413.96481	1
160	O	76.55409	77.55020	78.62632	-409.44433	-307.55053	-453.30833	1
161	N	74.35103	77.13655	78.07021	-429.02477	524.70884	274.08502	1
162	H	73.60368	77.83533	77.97096	1706.34263	-1425.96036	1574.38926	1
163	C	74.59402	76.30651	76.89638	-45.25864	-626.22952	478.93267	1
164	H	74.88623	77.00557	76.08252	1988.63164	570.90773	1772.87287	1
165	C	75.72504	75.27108	77.24069	551.77128	-20.49526	-564.54996	1
166	H	76.73354	75.74877	77.24981	1434.61535	-1753.10253	1513.99471	1
167	H	75.58994	74.85820	78.26604	-714.67738	1819.09770	1898.36494	1
168	C	75.62954	74.13937	76.15720	446.99263	-555.77305	338.97221	1
169	H	74.65102	73.60779	76.22747	1953.68466	1892.25957	-161.67766	1
170	H	75.66776	74.55781	75.12606	-403.03785	2688.07032	-188.43591	1
171	C	76.84100	73.16691	76.42738	567.86262	335.74681	434.04421	1
172	H	77.81395	73.70291	76.27021	-1080.02275	1568.26081	-1948.78900	1
173	H	76.84554	72.83141	77.49212	-919.54108	2111.34692	1456.13463	1
174	C	76.73172	71.95183	75.46549	195.81897	173.33862	-745.11536	1
175	H	75.96005	71.20637	75.74130	1405.67949	-2301.21089	-390.08113	1
176	H	76.63391	72.21978	74.39319	-940.37328	-1118.32446	2299.72133	1
177	N	78.09219	71.22369	75.55541	319.26422	656.36007	-42.02424	1
178	H	78.18176	70.32256	75.00573	1961.03633	619.91968	1787.09422	1
179	H	78.95167	71.86057	75.19724	854.14343	-2156.80752	1429.08711	1
180	H	78.38398	70.89060	76.51741	1237.02905	-1378.50857	-1998.28500	1
181	C	73.23747	75.49394	76.56087	532.53319	-268.57236	517.55729	1
182	O	73.09038	75.06346	75.41128	266.16714	-290.73804	-558.88002	1
183	N	72.50926	75.26568	77.63637	-226.25352	640.49678	-270.32839	1
184	H	72.91864	75.69688	78.46578	2007.69063	-1035.27229	1523.50231	1
185	C	71.13128	74.92720	77.62800	-540.76542	-573.33303	49.50000	1
186	H	70.79970	75.16568	78.66249	-2374.20950	-1036.76023	843.75774	1
187	C	70.40989	75.81994	76.51430	-77.09082	666.87422	-415.84136	1
188	H	70.87060	75.57881	75.51367	-985.81834	617.19825	2463.91927	1
189	O	70.53133	77.24551	76.66707	293.29899	-391.65602	-477.80926	1
190	H	71.01676	77.47967	75.84912	2528.72714	-681.76262	-751.27122	1
191	C	68.95323	75.23109	76.59417	252.47363	-605.14473	440.05134	1
192	H	68.29601	75.64609	75.79583	-2052.65063	1456.49051	-1043.51830	1
193	H	68.95029	74.11824	76.49011	-2152.98800	-1661.97574	-161.70652	1
194	H	68.47521	75.46813	77.57312	-473.12726	-1584.27339	2165.61725	1
195	C	70.88143	73.34519	77.26028	360.36307	488.46713	505.10056	1
196	O	70.07737	72.73498	77.91949	-200.08817	-528.03552	-385.82850	1
197	N	71.54026	72.99030	76.17201	-597.54095	-226.44775	355.20479	1
198	H	72.15655	73.70162	75.68898	2179.23655	-1300.70981	-991.33835	1
199	C	71.66717	71.63018	75.79717	-687.68921	297.39807	-249.45179	1
200	H	72.57532	71.62778	75.15381	-349.16256	-2467.37713	-1101.72831	1
201	C	71.79093	70.66048	77.06496	672.47345	361.54328	-201.62880	1
202	H	70.82934	70.67801	77.63337	1541.41502	582.18425	2169.97026	1
203	H	71.93040	69.61490	76.70483	-2534.67717	60.25153	997.72295	1
204	C	72.94878	71.06371	77.99119	574.26774	-389.43119	-377.02542	1
205	C	74.29971	70.73761	77.66738	688.82679	-287.33580	-257.96133	1

206	H	74.53988	70.22764	76.71778	331.14182	1470.38163	2269.80013	1
207	C	72.65145	71.73377	79.21615	-383.52382	-675.04808	144.24917	1
208	H	71.60794	72.01592	79.45655	4.09847	1517.59662	2262.86397	1
209	C	75.30506	71.04536	78.58940	-134.76730	428.45285	-649.50303	1
210	H	76.34701	70.77942	78.33869	-903.23433	1600.49020	2011.53387	1
211	C	73.69038	72.01026	80.11175	-335.53281	-615.00040	-364.39058	1
212	H	73.44012	72.50874	81.06505	1596.45398	-1369.33862	1732.02659	1
213	C	75.04690	71.66738	79.84512	585.48547	-340.24194	-406.23938	1
214	O	76.10788	71.92731	80.77040	-419.15649	-173.04408	-511.94141	1
215	H	75.57624	72.27088	81.52831	-1071.84350	1559.71507	-1960.13012	1
216	C	70.33454	71.17974	74.97911	291.41878	-183.13091	710.72246	1
217	O	70.08535	70.00001	74.85188	379.87695	523.47396	-222.23622	1
218	N	69.69223	72.21507	74.43113	564.30591	373.09380	277.24371	1
219	H	70.03402	73.14698	74.66211	-120.59931	-2436.07824	-1214.35098	1
220	C	68.43685	71.94131	73.82024	404.07514	-299.37480	608.84009	1
221	H	68.35688	70.82672	73.86355	-1071.07882	-841.69025	2359.66467	1
222	C	67.31553	72.68324	74.66869	-683.12807	68.71770	-390.13096	1
223	H	67.45902	72.50855	75.75866	2068.88918	1596.58590	770.89603	1
224	H	67.38477	73.78505	74.52838	1379.86429	2342.49779	-179.85638	1
225	C	65.93329	72.14562	74.18831	-176.39967	537.49466	550.97268	1
226	H	65.87485	72.16462	73.07290	-396.28051	1942.22168	1869.33314	1
227	H	65.80458	71.07673	74.47090	-94.44700	586.00678	-2659.20016	1
228	C	64.77777	73.04556	74.82620	-291.69381	-718.18079	-150.72929	1
229	H	64.58356	72.89826	75.91899	-2303.38776	1089.76242	964.62032	1
230	H	64.86186	74.14565	74.63427	884.16729	2568.80533	-207.74283	1
231	N	63.66734	72.57395	74.10667	-594.49522	-252.81478	342.29276	1
232	H	63.85047	71.90486	73.37479	-1735.17426	2084.05705	-263.71605	1
233	C	62.46363	72.93441	74.30097	595.23177	-271.52487	442.22352	1
234	N	62.21322	73.86575	75.31447	585.53813	-424.79750	-105.81303	1
235	H	62.86677	74.31894	75.95150	959.88797	1327.56823	-2177.11905	1
236	H	61.29096	74.22577	75.56183	1578.48647	16.27378	-2220.76233	1
237	N	61.59535	72.28921	73.40800	-452.17763	-390.33541	-421.51853	1
238	H	61.78013	71.61660	72.66557	470.26107	1974.25629	-1817.92087	1
239	H	60.58722	72.44697	73.39645	1856.67307	-1573.97321	-1224.35416	1
240	C	68.33345	72.53498	72.29822	-531.47271	-581.45780	-55.06206	1
241	O	67.42827	72.12612	71.59614	-243.00837	192.73507	609.52485	1
242	N	69.21255	73.47868	72.00213	343.49288	-644.25607	38.09164	1
243	H	69.90959	73.73610	72.69757	-1691.16043	-1535.97525	-1484.73099	1
244	C	69.05858	74.10640	70.72539	542.66492	350.14337	454.42563	1
245	H	68.69727	73.26571	70.09088	1209.57979	-2396.95920	463.86744	1
246	C	67.93128	75.21510	70.86711	-737.14309	145.93010	242.71942	1
247	H	68.17548	75.93809	71.67396	-1050.18303	159.36419	-2509.06125	1
248	C	67.79566	75.92907	69.47939	-706.77696	-252.88343	-245.16230	1
249	H	66.91664	76.61500	69.45104	-1624.64039	-1665.49085	1417.86935	1
250	H	68.70733	76.54285	69.25025	2566.10521	598.51109	693.22305	1
251	H	67.67025	75.19286	68.65037	-1972.69758	107.10018	-1876.34312	1
252	C	66.53217	74.55694	71.13841	412.85148	672.58832	-27.69222	1
253	H	65.70342	75.29842	71.04503	1447.02277	1762.76533	-1490.78944	1
254	H	66.32331	73.73000	70.41672	1320.77379	-145.20455	2378.68491	1
255	H	66.47445	74.12288	72.16519	-1512.10848	1470.52031	1724.75147	1
256	C	70.50259	74.71249	70.23754	-607.11113	499.56689	73.73769	1
257	O	71.17213	74.04601	69.48183	357.97126	460.81534	356.68785	1
258	N	70.77508	75.91122	70.73562	536.55407	-368.62270	332.76306	1
259	H	70.11556	76.35905	71.36961	524.38866	2297.69985	1367.20941	1
260	C	72.01246	76.52034	70.40020	46.50277	-774.29190	-147.97904	1
261	H	72.62114	75.73026	69.89807	1676.51875	1883.29066	1032.55549	1
262	C	71.74273	77.81185	69.50470	-559.41456	-34.19198	-556.30433	1
263	H	71.19022	78.56551	70.10806	-64.66664	395.18769	2695.05373	1
264	H	72.70758	78.29306	69.23467	-2703.44278	-60.40056	333.79418	1
265	C	70.92114	77.49308	68.21210	-519.76435	377.31045	459.42366	1
266	H	69.91359	77.09055	68.48426	-1746.74323	1667.50644	-1261.73691	1
267	C	70.78828	78.82567	67.38676	570.95554	16.46261	-545.27700	1

268	H	70.20114	78.67242	66.45158	2391.58273	28.05277	-1305.07271	1
269	H	70.27496	79.62311	67.97256	175.75588	917.63458	2559.43867	1
270	H	71.78584	79.22334	67.08807	-1063.97851	-2155.34650	1283.00462	1
271	C	71.67746	76.45690	67.30558	193.76014	2.62946	-765.53141	1
272	H	71.12399	76.26026	66.35777	507.39394	-846.55087	2539.60089	1
273	H	72.69370	76.82399	67.02461	1337.57841	1818.19054	1526.01994	1
274	H	71.79554	75.47601	67.82891	1100.88635	-1172.91350	-2199.08909	1
275	C	72.63380	77.14195	71.77271	-549.21115	475.64486	-309.38218	1
276	O	71.99941	77.88263	72.47735	556.06106	-390.37755	-78.24250	1
277	O	73.99623	76.89395	72.02314	-572.27940	-310.19032	-209.75862	1
278	H	74.17442	76.21257	71.31089	-1380.08193	2212.14486	790.85944	1

Listing 21: C00021.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1294.0188	0.0000	300.0000
3	H	74.92939	76.99095	81.98003	-2043.14101	-1757.64893	399.89339		1
4	N	74.85370	77.74287	81.29333	426.75047	490.45733	-334.42467		1
5	H	73.97356	78.22362	81.56500	442.25559	-1110.30854	-2448.52907		1
6	C	76.01257	78.56109	81.27914	415.32972	-666.39213	83.73172		1
7	H	76.41291	78.56091	82.31597	879.32219	2491.00447	667.35213		1
8	C	77.05677	77.98184	80.19701	31.35357	477.41777	628.23362		1
9	H	76.54281	77.91706	79.20810	1168.38489	2240.25337	-1019.71136		1
10	H	77.89233	78.70989	80.06030	-360.43770	2534.90498	931.67112		1
11	C	77.59894	76.63039	80.58742	463.18208	512.70242	-382.34388		1
12	H	76.74894	75.97924	80.89015	1725.29117	1863.52247	-987.07854		1
13	C	78.29898	75.98735	79.39628	710.42801	-144.27427	-313.15367		1
14	H	78.71362	74.97882	79.65388	364.20195	-1033.13725	2494.72524		1
15	H	77.60167	75.84901	78.52988	2567.61904	335.80679	847.48802		1
16	H	79.15501	76.61436	79.03567	-2587.99029	680.92867	-512.16411		1
17	C	78.57578	76.74455	81.74938	268.17616	741.64379	-40.42634		1
18	H	79.00304	75.74722	82.03060	1283.54314	-1945.37420	-1411.27812		1
19	H	79.43877	77.41353	81.49559	-1258.57796	1317.15249	-2026.02085		1
20	H	78.08772	77.16801	82.66469	-2502.84526	909.80597	575.92391		1
21	C	75.57971	80.04526	80.74324	619.36578	-458.64843	-172.09273		1
22	O	76.07535	81.06334	81.17175	-81.40433	433.87611	522.34594		1
23	N	74.76467	79.88835	79.69703	175.23996	-622.20190	341.55523		1
24	H	74.47910	78.92652	79.51144	-876.57256	-303.22879	-2561.90213		1
25	C	74.12604	81.03393	79.14868	-571.88214	-534.10783	-106.15033		1
26	H	74.76101	81.87762	79.50979	-2713.20841	-16.25800	-248.80809		1
27	C	74.11982	80.86754	77.55381	166.60354	288.16399	-716.09568		1
28	H	73.55483	79.93528	77.27767	-2097.85574	1636.78449	-586.18044		1
29	O	75.40623	80.70675	76.92842	-317.80580	-363.38227	484.43082		1
30	H	75.30492	79.82106	76.52374	1863.74748	-1451.84923	1357.29467		1
31	C	73.29213	82.12805	77.11126	503.80731	517.99032	318.51606		1
32	H	73.11138	82.13332	76.01143	640.61020	-2157.10410	-1536.29104		1
33	H	72.29500	82.16905	77.61292	1687.88455	465.60692	2087.56452		1
34	H	73.82659	83.07305	77.36550	-1293.07895	-1899.88581	-1463.57452		1
35	C	72.60407	81.12541	79.73832	-153.07550	-733.68902	248.70981		1
36	O	72.18464	82.24324	79.89478	186.15459	-480.78787	-449.34387		1
37	N	71.93216	79.97200	79.83336	-487.53139	543.18517	42.03850		1
38	C	70.80580	79.87977	80.71760	-699.35871	69.34393	360.10701		1
39	H	70.42635	80.91727	80.87714	2.81126	-221.99807	-2715.58072		1
40	C	69.84464	78.88827	79.91673	-507.46439	-592.59194	122.07761		1
41	H	69.08445	78.39937	80.56526	-1975.08116	525.87560	-1801.71556		1
42	H	69.28808	79.41630	79.11149	1588.27743	-1913.22100	1113.83566		1
43	C	70.88528	77.88971	79.32926	-613.62442	-457.55993	-194.14490		1
44	H	71.28111	77.20856	80.11692	1707.54637	-721.27992	1996.92523		1
45	H	70.48417	77.24501	78.51534	758.23357	2100.81767	1560.55011		1
46	C	71.98834	78.91802	78.82650	-352.41524	704.96076	49.21465		1
47	H	73.02142	78.50199	78.78344	1714.76886	-2070.42778	443.35792		1

48	H	71.74858	79.41325	77.85614	1224.15040	1801.50881	1636.97633	1
49	C	71.22344	79.11157	82.09059	566.85117	537.05831	117.62814	1
50	O	72.33354	78.60291	82.28164	-550.26779	-406.08867	4.21666	1
51	N	70.16775	79.11643	82.86215	566.34832	-425.77725	180.18749	1
52	H	69.34543	79.58258	82.48706	644.44502	2646.80550	-52.73430	1
53	C	70.11807	78.33773	84.05777	612.34801	-281.48662	411.56221	1
54	H	71.09455	78.55170	84.54777	1667.23498	-1490.75142	1556.16753	1
55	C	68.81211	78.73392	84.88272	-714.45746	-175.43074	286.98927	1
56	H	67.91481	78.36507	84.31213	-787.09484	1763.03619	-1922.46060	1
57	O	68.59773	80.13837	85.10669	-429.46514	516.51932	-128.40526	1
58	H	67.73873	80.27742	84.65847	1981.82785	436.16847	-1818.18182	1
59	C	68.99845	77.85016	86.17257	630.79189	-468.94448	76.03230	1
60	H	68.09007	77.87686	86.81839	-1775.71861	2062.30353	131.89849	1
61	H	69.19979	76.77797	85.91957	-1855.14608	88.94118	1993.53760	1
62	H	69.85250	78.21039	86.79157	-1504.82350	-780.94249	-2132.90992	1
63	C	69.95547	76.76985	83.61804	288.57638	618.62814	-397.00270	1
64	O	68.88274	76.23813	83.72098	321.70495	-185.26452	574.37218	1
65	N	71.10514	76.32136	83.10333	-447.05792	-446.53431	367.76425	1
66	H	71.86005	77.03393	82.95237	350.31316	1975.63644	-1843.31522	1
67	C	71.56498	75.01800	83.48147	-511.23061	374.03917	-471.51480	1
68	H	72.50226	74.96047	82.88452	2234.79579	-898.70890	-1273.45190	1
69	C	71.90712	75.01283	85.04731	529.53781	-159.34528	563.72604	1
70	H	72.55977	74.11547	85.22100	654.59388	2347.94251	1217.51488	1
71	H	72.53045	75.92344	85.25969	-1526.55661	2103.42026	817.87394	1
72	O	70.79224	75.01040	85.97596	-554.84278	14.12789	399.58769	1
73	H	70.54493	74.06446	85.91818	1297.06236	2061.84854	1220.68812	1
74	C	70.51519	73.85837	83.09285	-662.15484	-412.13544	123.62687	1
75	O	70.48145	72.81682	83.71467	-540.01537	-317.05804	274.91456	1
76	N	69.84815	74.14306	81.95613	-202.76299	-690.00100	-131.49145	1
77	H	69.91163	75.12059	81.66896	-702.62132	-2617.37191	281.70413	1
78	C	68.68147	73.33536	81.72790	-491.73914	576.34187	222.73509	1
79	H	69.06239	72.32051	81.98654	1977.17978	-1823.58850	-434.68928	1
80	C	67.53430	73.81719	82.70944	-649.50797	-328.66843	306.11224	1
81	H	67.37643	74.91601	82.62091	2075.07803	1452.16490	-1004.45904	1
82	C	66.23268	73.02754	82.33991	-615.18735	-489.99689	-70.96352	1
83	H	65.38066	73.29929	83.00667	-1226.32661	-1724.38906	-1716.47170	1
84	H	65.91926	73.24625	81.28888	2381.64273	-969.84735	900.46860	1
85	H	66.38251	71.92521	82.42187	2122.74991	1702.23946	-141.36228	1
86	C	67.94642	73.44778	84.17791	-501.86074	-479.61276	-376.42482	1
87	H	67.09796	73.57276	84.89147	993.79261	-2246.95401	-1177.81305	1
88	H	68.30184	72.39092	84.25413	42.71279	-626.15391	-2651.37258	1
89	H	68.78078	74.10458	84.53412	-2026.39012	-1590.33709	-887.82922	1
90	C	68.27642	73.54365	80.15864	-672.89153	382.57394	-156.34072	1
91	O	67.36017	74.25182	79.82557	410.04627	221.86223	500.35950	1
92	N	69.08713	72.80270	79.41853	-378.11782	-443.79414	-441.10984	1
93	H	69.86385	72.23387	79.81346	2404.15973	-568.14894	1149.30085	1
94	C	69.18610	73.01951	77.99525	-544.54484	466.16019	331.29119	1
95	H	68.18437	72.78229	77.57196	-1409.80988	-170.17955	2325.32679	1
96	C	69.55526	74.54872	77.78503	-184.48284	116.78282	-758.89137	1
97	H	68.85752	75.18125	78.37992	1893.78641	1861.14652	611.04528	1
98	H	70.56999	74.76236	78.19092	-2170.79665	-974.19311	1327.50117	1
99	C	69.48120	74.92471	76.27264	389.51668	672.81878	-138.49152	1
100	H	70.29518	74.41408	75.70996	510.64577	1933.03327	1851.02484	1
101	H	68.53077	74.54322	75.83936	-2302.30869	-1105.72939	-948.89774	1
102	C	69.56059	76.49143	76.04101	-559.93427	-126.34590	542.30857	1
103	O	70.12236	76.94536	75.07830	-670.36003	-111.83166	76.36448	1
104	N	68.87848	77.19008	76.97507	-216.06729	-537.07037	446.51379	1
105	H	68.29854	76.83433	77.74329	-1251.96487	1074.12894	-2168.52500	1
106	H	68.70937	78.20044	76.92874	-2451.83023	-720.73851	944.84612	1
107	C	70.35817	71.97382	77.64481	546.24052	-563.88337	-85.11809	1
108	O	70.88158	71.36687	78.56381	71.70702	-307.40463	606.69673	1
109	N	70.57528	71.84981	76.33582	479.90863	-504.50129	222.86849	1

110	C	71.85916	71.43240	75.83467	75.51268	-600.91904	506.73700	1
111	H	72.14262	70.60452	76.52444	-2033.61562	1795.30103	254.89480	1
112	C	71.53402	70.97470	74.35167	523.79067	517.99274	284.45581	1
113	H	72.39239	71.11065	73.64875	1599.61665	-1127.00911	1895.98173	1
114	H	71.27085	69.89346	74.31531	-1881.83093	1275.82488	-1501.55016	1
115	C	70.30322	71.86171	73.98666	-600.05639	-404.05026	316.64485	1
116	H	70.61750	72.89959	73.73352	-2597.05260	496.36221	657.73249	1
117	H	69.72084	71.48087	73.11736	-1666.24518	1294.38985	-1723.90591	1
118	C	69.49717	71.80668	75.35606	493.57570	-129.95376	-602.56394	1
119	H	68.79502	72.65138	75.53511	-1469.08415	-637.84797	2204.22581	1
120	H	68.96189	70.84504	75.54091	-1038.97840	1068.88701	-2280.71789	1
121	C	72.91492	72.66296	75.95757	188.88100	241.05089	-727.87821	1
122	O	72.76129	73.56969	76.74140	531.88613	-49.19943	427.07960	1
123	N	73.98355	72.41854	75.19830	708.14833	26.93417	-179.73509	1
124	H	74.01643	71.62907	74.55162	-2232.69501	-1179.09831	1023.94816	1
125	C	74.95086	73.47270	75.11250	-738.32412	259.92548	104.42456	1
126	H	75.00942	73.85828	76.15661	2028.89123	1260.02983	1311.33324	1
127	C	76.29665	72.83857	74.55790	-258.65678	-345.52513	661.28459	1
128	H	76.18926	72.56475	73.48384	-1826.06090	-1801.46097	-918.64554	1
129	C	77.51322	73.81288	74.73219	-541.23400	531.92970	-218.41428	1
130	H	78.48829	73.28430	74.57244	1311.73218	-2219.18200	882.19023	1
131	H	77.47322	74.65097	73.99607	-1048.71298	1223.58118	-2196.97971	1
132	H	77.54290	74.25781	75.75542	419.06414	1903.92898	1903.44670	1
133	C	76.63540	71.55595	75.39166	-423.86431	152.66566	-648.55262	1
134	H	77.63301	71.13965	75.11673	105.68386	-2342.50080	1387.51238	1
135	H	76.64626	71.76603	76.48709	-1695.63603	-1484.73621	-1531.02793	1
136	H	75.88117	70.75151	75.20902	-1853.57121	-487.39031	1936.59343	1
137	C	74.34227	74.59435	74.09895	539.71428	-510.58232	267.58633	1
138	O	73.35592	74.43876	73.37854	-15.93758	-278.34085	-624.49402	1
139	N	75.16468	75.61962	74.12100	-676.81886	12.05292	276.17960	1
140	H	75.93283	75.55558	74.78376	-1694.44250	-373.84189	-2100.66098	1
141	C	74.87714	76.82543	73.40039	412.33078	-664.70360	108.35451	1
142	H	73.78688	76.97762	73.57243	1765.77476	1294.44366	1621.76594	1
143	C	75.79790	77.94167	74.04206	-179.66635	-721.95667	-264.73915	1
144	H	75.75505	77.91098	75.15356	-607.34922	2587.87032	-598.10018	1
145	H	76.86163	77.74696	73.78477	-359.69332	-1479.13954	-2259.74260	1
146	C	75.35044	79.33977	73.50103	-240.01076	616.02425	431.85322	1
147	H	75.08522	79.27309	72.41481	-1359.17131	782.54425	2227.99181	1
148	H	74.44059	79.71022	74.02546	-820.36667	85.81767	-2596.78715	1
149	C	76.57978	80.31277	73.70329	-513.07015	236.18570	-551.87280	1
150	H	76.83566	80.41775	74.78311	1816.11944	-1183.11722	-1650.94321	1
151	H	77.48834	79.89236	73.21464	-1800.04429	-1361.53473	1526.34643	1
152	C	76.23497	81.68633	73.08101	726.08972	-253.19732	-179.64713	1
153	H	75.94568	81.64906	72.01147	1224.27271	-456.51798	-2390.90304	1
154	H	75.50099	82.28820	73.65430	1206.40339	-1150.93514	-2154.90344	1
155	N	77.56168	82.51301	73.09641	329.70796	-633.68968	-155.67358	1
156	H	77.52394	83.47725	72.65622	1348.31305	1938.76845	1359.00643	1
157	H	77.97222	82.72923	74.04979	2096.92035	1446.54551	-966.48890	1
158	H	78.38878	82.07549	72.59322	-1197.07217	-2303.53719	827.28733	1
159	C	75.19176	76.65988	71.81970	-378.01186	-556.17301	-413.96481	1
160	O	75.24770	77.64474	71.11317	-409.44433	-307.55053	-453.30833	1
161	N	75.40079	75.38190	71.44399	-429.02477	524.70884	274.08502	1
162	H	75.25656	74.72933	72.21917	1706.34263	-1425.96036	1574.38926	1
163	C	74.73556	75.03558	70.18549	-45.25864	-626.22952	478.93267	1
164	H	73.75009	75.54564	70.27629	1988.63164	570.90773	1772.87287	1
165	C	75.63780	75.64159	69.04867	551.77128	-20.49526	-564.54996	1
166	H	75.80800	76.73130	69.23349	1434.61535	-1753.10253	1513.99471	1
167	H	76.64671	75.17012	69.06550	-714.67738	1819.09770	1898.36494	1
168	C	74.94571	75.40999	67.66212	446.99263	-555.77305	338.97221	1
169	H	74.81255	74.32021	67.46865	1953.68466	1892.25957	-161.67766	1
170	H	73.92696	75.85788	67.63518	-403.03785	2688.07032	-188.43591	1
171	C	75.89046	76.07069	66.58050	567.86262	335.74681	434.04421	1

172	H	75.93178	77.17609	66.71573	-1080.02275	1568.26081	-1948.78900	1
173	H	76.93846	75.71214	66.70237	-919.54108	2111.34692	1456.13463	1
174	C	75.35599	75.70752	65.17562	195.81897	173.33862	-745.11536	1
175	H	75.37632	74.62473	64.94005	1405.67949	-2301.21089	-390.08113	1
176	H	74.35983	76.12911	64.93431	-940.37328	-1118.32446	2299.72133	1
177	N	76.32958	76.35662	64.13474	319.26422	656.36007	-42.02424	1
178	H	76.10759	76.16463	63.11554	1961.03633	619.91968	1787.09422	1
179	H	76.39930	77.41576	64.13661	854.14343	-2156.80752	1429.08711	1
180	H	77.35039	76.06934	64.18365	1237.02905	-1378.50857	-1998.28500	1
181	C	74.61704	73.43172	70.11176	532.53319	-268.57236	517.55729	1
182	O	75.11924	72.82482	69.16830	266.16714	-290.73804	-558.88002	1
183	N	73.87644	72.99471	71.10275	-226.25352	640.49678	-270.32839	1
184	H	73.47683	73.67250	71.79093	2007.69063	-1035.27229	1523.50231	1
185	C	73.73677	71.62164	71.42733	-540.76542	-573.33303	49.50000	1
186	H	73.00574	71.63617	72.27232	-2374.20950	-1036.76023	843.75774	1
187	C	73.17761	70.82605	70.15502	-77.09082	666.87422	-415.84136	1
188	H	73.83345	71.05261	69.26697	-985.81834	617.19825	2463.91927	1
189	O	71.83599	71.17519	69.76963	293.29899	-391.65602	-477.80926	1
190	H	71.99230	71.57066	68.88907	2528.72714	-681.76262	-751.27122	1
191	C	73.39736	69.33076	70.58796	252.47363	-605.14473	440.05134	1
192	H	73.10343	68.62375	69.77785	-2052.65063	1456.49051	-1043.51830	1
193	H	74.46534	69.12102	70.83585	-2152.98800	-1661.97574	-161.70652	1
194	H	72.79213	69.07288	71.48788	-473.12726	-1584.27339	2165.61725	1
195	C	75.18469	71.02699	71.92366	360.36307	488.46713	505.10056	1
196	O	75.24996	70.53216	73.02246	-200.08817	-528.03552	-385.82850	1
197	N	76.09608	71.10829	70.96764	-597.54095	-226.44775	355.20479	1
198	H	75.86387	71.56033	70.04642	2179.23655	-1300.70981	-991.33835	1
199	C	77.44654	70.86514	71.31370	-687.68921	297.39807	-249.45179	1
200	H	77.39339	70.35052	72.29982	-349.16256	-2467.37713	-1101.72831	1
201	C	78.07436	69.98932	70.12855	672.47345	361.54328	-201.62880	1
202	H	77.97833	70.50586	69.14705	1541.41502	582.18425	2169.97026	1
203	H	79.16081	69.82189	70.30675	-2534.67717	60.25153	997.72295	1
204	C	77.30877	68.65972	70.10501	574.26774	-389.43119	-377.02542	1
205	C	77.59513	67.67871	71.10107	688.82679	-287.33580	-257.96133	1
206	H	78.38062	67.85572	71.85808	331.14182	1470.38163	2269.80013	1
207	C	76.28643	68.43294	69.13412	-383.52382	-675.04808	144.24917	1
208	H	76.05555	69.19688	68.36982	4.09847	1517.59662	2262.86397	1
209	C	76.85212	66.49914	71.10454	-134.76730	428.45285	-649.50303	1
210	H	77.06884	65.74118	71.87731	-903.23433	1600.49020	2011.53387	1
211	C	75.57335	67.23273	69.17774	-335.53281	-615.00040	-364.39058	1
212	H	74.78464	67.06567	68.42345	1596.45398	-1369.33862	1732.02659	1
213	C	75.82304	66.22740	70.15715	585.48547	-340.24194	-406.23938	1
214	O	75.09974	65.00785	70.21516	-419.15649	-173.04408	-511.94141	1
215	H	74.50270	65.13135	69.44003	-1071.84350	1559.71507	-1960.13012	1
216	C	78.20061	72.32316	71.39626	291.41878	-183.13091	710.72246	1
217	O	78.43977	72.78145	72.49427	379.87695	523.47396	-222.23622	1
218	N	78.43796	72.84451	70.20555	564.30591	373.09380	277.24371	1
219	H	78.07459	72.34586	69.39558	-120.59931	-2436.07824	-1214.35098	1
220	C	79.20375	74.03554	70.05356	404.07514	-299.37480	608.84009	1
221	H	78.98862	74.35842	69.00894	-1071.07882	-841.69025	2359.66467	1
222	C	78.70162	75.07476	71.14767	-683.12807	68.71770	-390.13096	1
223	H	77.58767	75.08522	71.17355	2068.88918	1596.58590	770.89603	1
224	H	79.02235	74.75288	72.17207	1379.86429	2342.49779	-179.85638	1
225	C	79.26445	76.48967	70.82207	-176.39967	537.49466	550.97268	1
226	H	80.37075	76.52252	70.95823	-396.28051	1942.22168	1869.33314	1
227	H	79.08390	76.76362	69.75929	-94.44700	586.00678	-2659.20016	1
228	C	78.51370	77.50260	71.81711	-291.69381	-718.18079	-150.72929	1
229	H	77.42879	77.61910	71.54717	-2303.38776	1089.76242	964.62032	1
230	H	78.63053	77.28161	72.90762	884.16729	2568.80533	-207.74283	1
231	N	79.16129	78.70026	71.51602	-594.49522	-252.81478	342.29276	1
232	H	79.20825	78.93940	70.53567	-1735.17426	2084.05705	-263.71605	1
233	C	79.65420	79.52281	72.35672	595.23177	-271.52487	442.22352	1

234	N	79.56892	79.22238	73.71716	585.53813	-424.79750	-105.81303	1
235	H	79.17015	78.40496	74.17768	959.88797	1327.56823	-2177.11905	1
236	H	79.91897	79.81715	74.46951	1578.48647	16.27378	-2220.76233	1
237	N	80.19458	80.63838	71.70350	-452.17763	-390.33541	-421.51853	1
238	H	80.29781	80.83545	70.70926	470.26107	1974.25629	-1817.92087	1
239	H	80.68494	81.39056	72.18868	1856.67307	-1573.97321	-1224.35416	1
240	C	80.78467	73.72488	70.26729	-531.47271	-581.45780	-55.06206	1
241	O	81.57282	74.64789	70.44542	-243.00837	192.73507	609.52485	1
242	N	81.06425	72.44088	70.15438	343.49288	-644.25607	38.09164	1
243	H	80.25455	71.85775	69.95979	-1691.16043	-1535.97525	-1484.73099	1
244	C	82.43397	71.93363	70.21696	542.66492	350.14337	454.42563	1
245	H	82.85790	72.49923	71.08106	1209.57979	-2396.95920	463.86744	1
246	C	82.42682	70.42446	70.37662	-737.14309	145.93010	242.71942	1
247	H	81.86908	69.99608	69.51352	-1050.18303	159.36419	-2509.06125	1
248	C	83.83669	69.86142	70.34810	-706.77696	-252.88343	-245.16230	1
249	H	83.84144	68.73933	70.42272	-1624.64039	-1665.49085	1417.86935	1
250	H	84.36758	70.13548	69.39225	2566.10521	598.51109	693.22305	1
251	H	84.45894	70.25480	71.19843	-1972.69758	107.10018	-1876.34312	1
252	C	81.72238	69.98360	71.64698	412.85148	672.58832	-27.69222	1
253	H	81.63159	68.86390	71.70541	1447.02277	1762.76533	-1490.78944	1
254	H	82.27949	70.32067	72.56384	1320.77379	-145.20455	2378.68491	1
255	H	80.68486	70.41133	71.71726	-1512.10848	1470.52031	1724.75147	1
256	C	83.15443	72.37751	68.78564	-607.11113	499.56689	73.73769	1
257	O	83.37007	71.57054	67.91835	357.97126	460.81534	356.68785	1
258	N	83.41986	73.67325	68.81319	536.55407	-368.62270	332.76306	1
259	H	83.10614	74.27152	69.61085	524.38866	2297.69985	1367.20941	1
260	C	84.00861	74.23103	67.65524	46.50277	-774.29190	-147.97904	1
261	H	84.17388	73.37527	66.95886	1676.51875	1883.29066	1032.55549	1
262	C	83.01160	75.37243	67.08615	-559.41456	-34.19198	-556.30433	1
263	H	82.83772	76.13409	67.88318	-64.66664	395.18769	2695.05373	1
264	H	83.48306	75.91722	66.23393	-2703.44278	-60.40056	333.79418	1
265	C	81.71196	74.73888	66.67222	-519.76435	377.31045	459.42366	1
266	H	81.38270	74.05419	67.48725	-1746.74323	1667.50644	-1261.73691	1
267	C	80.63775	75.80107	66.47332	570.95554	16.46261	-545.27700	1
268	H	79.65987	75.34980	66.16398	2391.58273	28.05277	-1305.07271	1
269	H	80.45324	76.38286	67.41310	175.75588	917.63458	2559.43867	1
270	H	80.92910	76.53616	65.67938	-1063.97851	-2155.34650	1283.00462	1
271	C	81.87950	73.93130	65.39186	193.76014	2.62946	-765.53141	1
272	H	80.90739	73.49222	65.04895	507.39394	-846.55087	2539.60089	1
273	H	82.27168	74.56315	64.55342	1337.57841	1818.19054	1526.01994	1
274	H	82.59544	73.08020	65.53048	1100.88635	-1172.91350	-2199.08909	1
275	C	85.36155	74.99622	68.10985	-549.21115	475.64486	-309.38218	1
276	O	85.54158	75.43436	69.21506	556.06106	-390.37755	-78.24250	1
277	O	86.28950	75.25206	67.07343	-572.27940	-310.19032	-209.75862	1
278	H	85.82836	74.76884	66.33214	-1380.08193	2212.14486	790.85944	1

Listing 22: C00022.xmolout

		276							
1		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	1.0227	4091
2		0.2500	300.00	0.00	0.00	0.00	-1293.9901	0.0000	300.0000
3	H	69.64461	64.28404	66.57395	-2043.14101	-1757.64893		399.89339	1
4	N	69.66103	65.29891	66.51328	426.75047	490.45733		-334.42467	1
5	H	68.82788	65.49263	65.96341	442.25559	-1110.30854		-2448.52907	1
6	C	70.86071	65.86502	66.03854	415.32972	-666.39213		83.73172	1
7	H	71.65041	65.28495	66.56193	879.32219	2491.00447		667.35213	1
8	C	70.97374	65.77580	64.43145	31.35357	477.41777		628.23362	1
9	H	70.01617	66.10902	63.96394	1168.38489	2240.25337		-1019.71136	1
10	H	71.74824	66.51068	64.09656	-360.43770	2534.90498		931.67112	1
11	C	71.33212	64.38703	63.97385	463.18208	512.70242		-382.34388	1
12	H	70.55640	63.67788	64.33984	1725.29117	1863.52247		-987.07854	1
13	C	71.36237	64.33381	62.45058	710.42801	-144.27427		-313.15367	1

14	H	71.60904	63.30698	62.07605	364.20195	-1033.13725	2494.72524	1
15	H	70.37629	64.62349	62.00443	2567.61904	335.80679	847.48802	1
16	H	72.13229	65.03201	62.03122	-2587.99029	680.92867	-512.16411	1
17	C	72.68756	63.94920	64.51245	268.17616	741.64379	-40.42634	1
18	H	72.99435	62.95393	64.09856	1283.54314	-1945.37420	-1411.27812	1
19	H	73.49258	64.68184	64.24507	-1258.57796	1317.15249	-2026.02085	1
20	H	72.68450	63.85397	65.62847	-2502.84526	909.80597	575.92391	1
21	C	70.88749	67.44245	66.37150	619.36578	-458.64843	-172.09273	1
22	O	71.44419	68.21155	65.59214	-81.40433	433.87611	522.34594	1
23	N	70.39948	67.75795	67.60796	175.23996	-622.20190	341.55523	1
24	H	70.02784	66.84382	67.91063	-876.57256	-303.22879	-2561.90213	1
25	C	69.42582	68.84536	67.60185	-571.88214	-534.10783	-106.15033	1
26	H	68.71352	68.55183	66.80067	-2713.20841	-16.25800	-248.80809	1
27	C	68.75238	68.76021	69.03629	166.60354	288.16399	-716.09568	1
28	H	69.54555	68.86868	69.82786	-2097.85574	1636.78449	-586.18044	1
29	O	68.09563	67.50593	69.33190	-317.80580	-363.38227	484.43082	1
30	H	68.59616	67.20782	70.11398	1863.74748	-1451.84923	1357.29467	1
31	C	67.83832	70.04036	69.03518	503.80731	517.99032	318.51606	1
32	H	67.37014	70.21082	70.03247	640.61020	-2157.10410	-1536.29104	1
33	H	68.41441	70.96060	68.77097	1687.88455	465.60692	2087.56452	1
34	H	67.01237	69.94663	68.29234	-1293.07895	-1899.88581	-1463.57452	1
35	C	70.08454	70.28543	67.27665	-153.07550	-733.68902	248.70981	1
36	O	69.34579	71.02990	66.68360	186.15459	-480.78787	-449.34387	1
37	N	71.27286	70.57163	67.82528	-487.53139	543.18517	42.03850	1
38	C	72.01228	71.73959	67.43611	-699.35871	69.34393	360.10701	1
39	H	71.30175	72.42082	66.90924	2.81126	-221.99807	-2715.58072	1
40	C	72.56222	72.24316	68.84811	-507.46439	-592.59194	122.07761	1
41	H	73.41652	72.94975	68.75110	-1975.08116	525.87560	-1801.71556	1
42	H	71.77431	72.76650	69.43372	1588.27743	-1913.22100	1113.83566	1
43	C	72.95294	70.88182	69.49784	-613.62442	-457.55993	-194.14490	1
44	H	73.91375	70.50560	69.07945	1707.54637	-721.27992	1996.92523	1
45	H	73.08906	70.94136	70.60085	758.23357	2100.81767	1560.55011	1
46	C	71.73024	69.96075	69.06673	-352.41524	704.96076	49.21465	1
47	H	71.99129	68.90100	68.83590	1714.76886	-2070.42778	443.35792	1
48	H	70.85828	69.98558	69.76192	1224.15040	1801.50881	1636.97633	1
49	C	73.31366	71.31970	66.56514	566.85117	537.05831	117.62814	1
50	O	74.30992	72.04648	66.54715	-550.26779	-406.08867	4.21666	1
51	N	73.06417	70.23313	65.89256	566.34832	-425.77725	180.18749	1
52	H	72.13380	69.75369	65.98679	644.44502	2646.80550	-52.73430	1
53	C	74.09442	69.50694	65.23678	612.34801	-281.48662	411.56221	1
54	H	73.53731	68.65180	64.78917	1667.23498	-1490.75142	1556.16753	1
55	C	74.76755	70.45005	64.13081	-714.45746	-175.43074	286.98927	1
56	H	75.11579	71.40590	64.61778	-787.09484	1763.03619	-1922.46060	1
57	O	73.89892	70.85536	63.05816	-429.46514	516.51932	-128.40526	1
58	H	73.84088	71.81883	63.21739	1981.82785	436.16847	-1818.18182	1
59	C	76.01807	69.59433	63.71339	630.79189	-468.94448	76.03230	1
60	H	76.64283	70.12738	62.95985	-1775.71861	2062.30353	131.89849	1
61	H	76.67458	69.36937	64.58658	-1855.14608	88.94118	1993.53760	1
62	H	75.71456	68.62021	63.26438	-1504.82350	-780.94249	-2132.90992	1
63	C	75.15288	68.99136	66.38094	288.57638	618.62814	-397.00270	1
64	O	75.12950	67.82717	66.69232	321.70495	-185.26452	574.37218	1
65	N	75.97817	69.96103	66.74956	-447.05792	-446.53431	367.76425	1
66	H	75.76873	70.94504	66.48520	350.31316	1975.63644	-1843.31522	1
67	C	76.84283	69.73908	67.88032	-511.23061	374.03917	-471.51480	1
68	H	76.15614	69.59192	68.74378	2234.79579	-898.70890	-1273.45190	1
69	C	77.74908	68.44366	67.63286	529.53781	-159.34528	563.72604	1
70	H	78.26490	68.21493	68.60747	654.59388	2347.94251	1217.51488	1
71	H	77.05204	67.58108	67.42032	-1526.55661	2103.42026	817.87394	1
72	O	78.80787	68.55878	66.64429	-554.84278	14.12789	399.58769	1
73	H	78.30354	68.32314	65.84397	1297.06236	2061.84854	1220.68812	1
74	C	77.76397	71.05291	68.00009	-662.15484	-412.13544	123.62687	1
75	O	77.88188	71.88211	67.13026	-540.01537	-317.05804	274.91456	1

76	N	78.41428	70.98247	69.17788	-202.76299	-690.00100	-131.49145	1
77	H	78.14380	70.21475	69.79402	-702.62132	-2617.37191	281.70413	1
78	C	79.19745	72.11352	69.67622	-491.73914	576.34187	222.73509	1
79	H	79.53104	71.76048	70.67991	1977.17978	-1823.58850	-434.68928	1
80	C	80.34992	72.33606	68.71965	-649.50797	-328.66843	306.11224	1
81	H	79.92630	72.69287	67.75116	2075.07803	1452.16490	-1004.45904	1
82	C	81.34712	73.35816	69.23563	-615.18735	-489.99689	-70.96352	1
83	H	82.23806	73.44376	68.55570	-1226.32661	-1724.38906	-1716.47170	1
84	H	80.90383	74.38596	69.32253	2381.64273	-969.84735	900.46860	1
85	H	81.73338	73.07984	70.25378	2122.74991	1702.23946	-141.36228	1
86	C	81.07945	71.03680	68.41722	-501.86074	-479.61276	-376.42482	1
87	H	81.91461	71.18786	67.68037	993.79261	-2246.95401	-1177.81305	1
88	H	81.52898	70.58903	69.34486	42.71279	-626.15391	-2651.37258	1
89	H	80.38082	70.26959	67.98003	-2026.39012	-1590.33709	-887.82922	1
90	C	78.05808	73.32426	69.81403	-672.89153	382.57394	-156.34072	1
91	O	77.10993	73.14637	70.53755	410.04627	221.86223	500.35950	1
92	N	78.40658	74.41047	69.14559	-378.11782	-443.79414	-441.10984	1
93	H	79.22716	74.32193	68.55107	2404.15973	-568.14894	1149.30085	1
94	C	77.53081	75.52861	68.99131	-544.54484	466.16019	331.29119	1
95	H	78.15377	76.24999	68.41267	-1409.80988	-170.17955	2325.32679	1
96	C	76.28332	75.00638	68.13734	-184.48284	116.78282	-758.89137	1
97	H	76.62314	74.32831	67.32155	1893.78641	1861.14652	611.04528	1
98	H	75.59816	74.39763	68.76976	-2170.79665	-974.19311	1327.50117	1
99	C	75.56716	76.26727	67.57383	389.51668	672.81878	-138.49152	1
100	H	75.22081	76.90930	68.42096	510.64577	1933.03327	1851.02484	1
101	H	76.29859	76.90625	67.03097	-2302.30869	-1105.72939	-948.89774	1
102	C	74.34695	75.96811	66.62048	-559.93427	-126.34590	542.30857	1
103	O	73.71990	76.89516	66.17266	-670.36003	-111.83166	76.36448	1
104	N	74.11501	74.66403	66.37739	-216.06729	-537.07037	446.51379	1
105	H	74.60668	73.78407	66.67345	-1251.96487	1074.12894	-2168.52500	1
106	H	73.34779	74.38483	65.74806	-2451.83023	-720.73851	944.84612	1
107	C	77.04363	76.10967	70.41280	546.24052	-563.88337	-85.11809	1
108	O	75.98343	76.72160	70.41840	71.70702	-307.40463	606.69673	1
109	N	77.92768	75.99318	71.39542	479.90863	-504.50129	222.86849	1
110	C	77.54069	75.83367	72.77409	75.51268	-600.91904	506.73700	1
111	H	76.60132	75.23333	72.76059	-2033.61562	1795.30103	254.89480	1
112	C	78.82000	75.12227	73.39678	523.79067	517.99274	284.45581	1
113	H	78.88098	75.23576	74.50276	1599.61665	-1127.00911	1895.98173	1
114	H	78.82899	74.03020	73.18254	-1881.83093	1275.82488	-1501.55016	1
115	C	79.96612	75.86027	72.63810	-600.05639	-404.05026	316.64485	1
116	H	80.12716	76.88005	73.05491	-2597.05260	496.36221	657.73249	1
117	H	80.94766	75.33724	72.69126	-1666.24518	1294.38985	-1723.90591	1
118	C	79.36649	75.91861	71.16790	493.57570	-129.95376	-602.56394	1
119	H	79.67442	76.79530	70.55128	-1469.08415	-637.84797	2204.22581	1
120	H	79.50783	74.98383	70.57628	-1038.97840	1068.88701	-2280.71789	1
121	C	77.36275	77.29013	73.46109	188.88100	241.05089	-727.87821	1
122	O	77.87763	77.52071	74.52325	531.88613	-49.19943	427.07960	1
123	N	76.54108	78.07120	72.74427	708.14833	26.93417	-179.73509	1
124	H	76.16254	77.66541	71.84714	-2232.69501	-1179.09831	1023.94816	1
125	C	76.74938	79.53508	72.82502	-738.32412	259.92548	104.42456	1
126	H	77.84849	79.65236	72.96887	2028.89123	1260.02983	1311.33324	1
127	C	76.24185	80.14490	71.53963	-258.65678	-345.52513	661.28459	1
128	H	75.21172	79.75957	71.36442	-1826.06090	-1801.46097	-918.64554	1
129	C	76.17523	81.66000	71.61961	-541.23400	531.92970	-218.41428	1
130	H	75.74391	82.10894	70.68305	1311.73218	-2219.18200	882.19023	1
131	H	75.53571	82.00078	72.48281	-1048.71298	1223.58118	-2196.97971	1
132	H	77.19507	82.11023	71.76866	419.06414	1903.92898	1903.44670	1
133	C	77.09415	79.74276	70.34774	-423.86431	152.66566	-648.55262	1
134	H	76.66949	80.13352	69.38277	105.68386	-2342.50080	1387.51238	1
135	H	78.14254	80.13916	70.43703	-1695.63603	-1484.73621	-1531.02793	1
136	H	77.17088	78.62398	70.25034	-1853.57121	-487.39031	1936.59343	1
137	C	75.91951	80.10109	74.12908	539.71428	-510.58232	267.58633	1

138	O	76.09432	81.21943	74.55661	-15.93758	-278.34085	-624.49402	1
139	N	74.96182	79.22092	74.56661	-676.81886	12.05292	276.17960	1
140	H	75.20647	78.38104	74.02709	-1694.44250	-373.84189	-2100.66098	1
141	C	74.97249	79.13325	76.02762	412.33078	-664.70360	108.35451	1
142	H	76.04173	79.27557	76.29341	1765.77476	1294.44366	1621.76594	1
143	C	74.03812	80.29275	76.52357	-179.66635	-721.95667	-264.73915	1
144	H	74.42688	81.27153	76.15270	-607.34922	2587.87032	-598.10018	1
145	H	73.02350	80.18090	76.07727	-359.69332	-1479.13954	-2259.74260	1
146	C	73.95597	80.26393	78.08942	-240.01076	616.02425	431.85322	1
147	H	73.55954	79.28605	78.44494	-1359.17131	782.54425	2227.99181	1
148	H	74.96275	80.37468	78.54768	-820.36667	85.81767	-2596.78715	1
149	C	73.00318	81.44849	78.52191	-513.07015	236.18570	-551.87280	1
150	H	73.40042	82.42563	78.16239	1816.11944	-1183.11722	-1650.94321	1
151	H	72.00043	81.33942	78.04766	-1800.04429	-1361.53473	1526.34643	1
152	C	72.87902	81.44229	80.06371	726.08972	-253.19732	-179.64713	1
153	H	72.40148	80.53530	80.48251	1224.27271	-456.51798	-2390.90304	1
154	H	73.82037	81.65622	80.61002	1206.40339	-1150.93514	-2154.90344	1
155	N	71.91862	82.61787	80.44980	329.70796	-633.68968	-155.67358	1
156	H	71.72839	82.73693	81.48648	1348.31305	1938.76845	1359.00643	1
157	H	72.23174	83.59676	80.18347	2096.92035	1446.54551	-966.48890	1
158	H	70.93238	82.59243	80.05736	-1197.07217	-2303.53719	827.28733	1
159	C	74.40323	77.66730	76.40212	-378.01186	-556.17301	-413.96481	1
160	O	73.21330	77.47640	76.65002	-409.44433	-307.55053	-453.30833	1
161	N	75.38829	76.79386	76.36033	-429.02477	524.70884	274.08502	1
162	H	76.33148	77.10728	76.12548	1706.34263	-1425.96036	1574.38926	1
163	C	75.09817	75.44633	76.73983	-45.25864	-626.22952	478.93267	1
164	H	74.08697	75.29441	76.29579	1988.63164	570.90773	1772.87287	1
165	C	76.24217	74.50701	76.18912	551.77128	-20.49526	-564.54996	1
166	H	76.39426	74.64303	75.09467	1434.61535	-1753.10253	1513.99471	1
167	H	77.21751	74.75818	76.66517	-714.67738	1819.09770	1898.36494	1
168	C	75.80597	73.04338	76.53513	446.99263	-555.77305	338.97221	1
169	H	75.52934	72.97728	77.61351	1953.68466	1892.25957	-161.67766	1
170	H	74.89541	72.75451	75.96386	-403.03785	2688.07032	-188.43591	1
171	C	77.00462	72.06132	76.22372	567.86262	335.74681	434.04421	1
172	H	77.28628	72.09799	75.14611	-1080.02275	1568.26081	-1948.78900	1
173	H	77.91779	72.35979	76.78857	-919.54108	2111.34692	1456.13463	1
174	C	76.54237	70.64334	76.63511	195.81897	173.33862	-745.11536	1
175	H	76.27251	70.53971	77.70516	1405.67949	-2301.21089	-390.08113	1
176	H	75.73975	70.21710	76.00080	-940.37328	-1118.32446	2299.72133	1
177	N	77.75658	69.67270	76.45002	319.26422	656.36007	-42.02424	1
178	H	77.56866	68.65573	76.68676	1961.03633	619.91968	1787.09422	1
179	H	78.16838	69.58769	75.47551	854.14343	-2156.80752	1429.08711	1
180	H	78.61932	69.86537	77.03778	1237.02905	-1378.50857	-1998.28500	1
181	C	75.04392	75.36630	78.38202	532.53319	-268.57236	517.55729	1
182	O	75.87053	74.75639	79.00868	266.16714	-290.73804	-558.88002	1
183	N	73.98301	76.04811	78.79440	-226.25352	640.49678	-270.32839	1
184	H	73.35695	76.49759	78.08061	2007.69063	-1035.27229	1523.50231	1
185	C	73.51100	75.87942	80.12614	-540.76542	-573.33303	49.50000	1
186	H	72.55171	76.44415	80.12160	-2374.20950	-1036.76023	843.75774	1
187	C	73.26548	74.31220	80.33915	-77.09082	666.87422	-415.84136	1
188	H	74.27096	73.80557	80.33086	-985.81834	617.19825	2463.91927	1
189	O	72.47167	73.67093	79.32174	293.29899	-391.65602	-477.80926	1
190	H	73.12955	73.06412	78.92981	2528.72714	-681.76262	-751.27122	1
191	C	72.64660	74.24166	81.78185	252.47363	-605.14473	440.05134	1
192	H	72.50202	73.18618	82.11136	-2052.65063	1456.49051	-1043.51830	1
193	H	73.30445	74.74883	82.54284	-2152.98800	-1661.97574	-161.70652	1
194	H	71.64744	74.73555	81.81927	-473.12726	-1584.27339	2165.61725	1
195	C	74.60571	76.54095	81.13604	360.36307	488.46713	505.10056	1
196	O	74.70630	76.15366	82.28896	-200.08817	-528.03552	-385.82850	1
197	N	75.20250	77.58881	80.57943	-597.54095	-226.44775	355.20479	1
198	H	74.97165	77.79222	79.60911	2179.23655	-1300.70981	-991.33835	1
199	C	76.03437	78.40826	81.39139	-687.68921	297.39807	-249.45179	1

200	H	76.51299	77.68657	82.09220	-349.16256	-2467.37713	-1101.72831	1
201	C	77.01037	79.35195	80.55476	672.47345	361.54328	-201.62880	1
202	H	76.41727	80.15550	80.06163	1541.41502	582.18425	2169.97026	1
203	H	77.69192	79.87451	81.26564	-2534.67717	60.25153	997.72295	1
204	C	77.82393	78.58755	79.49593	574.26774	-389.43119	-377.02542	1
205	C	78.67176	77.49488	79.84413	688.82679	-287.33580	-257.96133	1
206	H	78.74697	77.14912	80.89120	331.14182	1470.38163	2269.80013	1
207	C	77.74196	79.04747	78.14840	-383.52382	-675.04808	144.24917	1
208	H	77.11015	79.91481	77.88441	4.09847	1517.59662	2262.86397	1
209	C	79.40002	76.86982	78.83062	-134.76730	428.45285	-649.50303	1
210	H	80.05506	76.02152	79.09534	-903.23433	1600.49020	2011.53387	1
211	C	78.48768	78.38545	77.17126	-335.53281	-615.00040	-364.39058	1
212	H	78.41591	78.74705	76.12323	1596.45398	-1369.33862	1732.02659	1
213	C	79.32894	77.27388	77.46669	585.48547	-340.24194	-406.23938	1
214	O	80.08134	76.60462	76.46698	-419.15649	-173.04408	-511.94141	1
215	H	79.65692	76.99318	75.65822	-1071.84350	1559.71507	-1960.13012	1
216	C	75.13168	79.53726	82.14567	291.41878	-183.13091	710.72246	1
217	O	75.54098	80.66989	82.27432	379.87695	523.47396	-222.23622	1
218	N	73.96419	79.02272	82.54154	564.30591	373.09380	277.24371	1
219	H	73.82560	78.01479	82.39882	-120.59931	-2436.07824	-1214.35098	1
220	C	73.22728	79.73061	83.53701	404.07514	-299.37480	608.84009	1
221	H	73.59455	80.78010	83.44656	-1071.07882	-841.69025	2359.66467	1
222	C	71.70137	79.51386	83.17856	-683.12807	68.71770	-390.13096	1
223	H	71.51075	79.77516	82.11409	2068.88918	1596.58590	770.89603	1
224	H	71.42743	78.43925	83.27579	1379.86429	2342.49779	-179.85638	1
225	C	70.82850	80.39375	84.12531	-176.39967	537.49466	550.97268	1
226	H	70.94677	80.07859	85.18927	-396.28051	1942.22168	1869.33314	1
227	H	71.12338	81.46614	84.08375	-94.44700	586.00678	-2659.20016	1
228	C	69.34098	80.16596	83.58802	-291.69381	-718.18079	-150.72929	1
229	H	69.16056	80.48474	82.53122	-2303.38776	1089.76242	964.62032	1
230	H	68.95405	79.12062	83.69492	884.16729	2568.80533	-207.74283	1
231	N	68.54725	80.99144	84.39159	-594.49522	-252.81478	342.29276	1
232	H	69.01201	81.48846	85.13523	-1735.17426	2084.05705	-263.71605	1
233	C	67.29297	81.13738	84.24085	595.23177	-271.52487	442.22352	1
234	N	66.68127	80.42751	83.20079	585.53813	-424.79750	-105.81303	1
235	H	67.09160	79.78054	82.52859	959.88797	1327.56823	-2177.11905	1
236	H	65.68479	80.45295	82.98367	1578.48647	16.27378	-2220.76233	1
237	N	66.76592	82.02096	85.19260	-452.17763	-390.33541	-421.51853	1
238	H	67.21348	82.52883	85.95417	470.26107	1974.25629	-1817.92087	1
239	H	65.77488	82.26108	85.24092	1856.67307	-1573.97321	-1224.35416	1
240	C	73.57462	79.04202	84.98220	-531.47271	-581.45780	-55.06206	1
241	O	72.70759	78.74039	85.76808	-243.00837	192.73507	609.52485	1
242	N	74.89761	78.95663	85.14015	343.49288	-644.25607	38.09164	1
243	H	75.43407	79.23760	84.31785	-1691.16043	-1535.97525	-1484.73099	1
244	C	75.49301	78.13315	86.19206	542.66492	350.14337	454.42563	1
245	H	74.95201	78.42002	87.12424	1209.57979	-2396.95920	463.86744	1
246	C	75.31635	76.66493	85.84676	-737.14309	145.93010	242.71942	1
247	H	75.88326	76.45991	84.91051	-1050.18303	159.36419	-2509.06125	1
248	C	75.87081	75.78003	86.94804	-706.77696	-252.88343	-245.16230	1
249	H	75.79698	74.68886	86.68579	-1624.64039	-1665.49085	1417.86935	1
250	H	76.95692	76.00143	87.15653	2566.10521	598.51109	693.22305	1
251	H	75.31602	75.92686	87.91558	-1972.69758	107.10018	-1876.34312	1
252	C	73.86214	76.31950	85.57883	412.85148	672.58832	-27.69222	1
253	H	73.71501	75.22057	85.38791	1447.02277	1762.76533	-1490.78944	1
254	H	73.20289	76.61308	86.44494	1320.77379	-145.20455	2378.68491	1
255	H	73.47183	76.87843	84.68052	-1512.10848	1470.52031	1724.75147	1
256	C	77.11042	78.51463	86.17056	-607.11113	499.56689	73.73769	1
257	O	77.72717	78.61090	85.13830	357.97126	460.81534	356.68785	1
258	N	77.54411	78.63236	87.41893	536.55407	-368.62270	332.76306	1
259	H	76.88310	78.45466	88.17363	524.38866	2297.69985	1367.20941	1
260	C	78.94108	78.67817	87.64550	46.50277	-774.29190	-147.97904	1
261	H	79.38965	78.84742	86.63937	1676.51875	1883.29066	1032.55549	1

262	C	79.26801	79.83626	88.72399	-559.41456	-34.19198	-556.30433	1
263	H	78.88806	79.52345	89.72553	-64.66664	395.18769	2695.05373	1
264	H	80.37055	79.96054	88.84393	-2703.44278	-60.40056	333.79418	1
265	C	78.61989	81.12703	88.30175	-519.76435	377.31045	459.42366	1
266	H	77.54130	80.92707	88.10880	-1746.74323	1667.50644	-1261.73691	1
267	C	78.72981	82.16426	89.41260	570.95554	16.46261	-545.27700	1
268	H	78.22387	83.12439	89.13411	2391.58273	28.05277	-1305.07271	1
269	H	78.25918	81.80417	90.36360	175.75588	917.63458	2559.43867	1
270	H	79.79851	82.40817	89.64414	-1063.97851	-2155.34650	1283.00462	1
271	C	79.24076	81.67396	87.02356	193.76014	2.62946	-765.53141	1
272	H	78.77515	82.64796	86.72262	507.39394	-846.55087	2539.60089	1
273	H	80.34043	81.85410	87.14152	1337.57841	1818.19054	1526.01994	1
274	H	79.10703	80.96528	86.16515	1100.88635	-1172.91350	-2199.08909	1
275	C	79.36109	77.27264	88.32042	-549.21115	475.64486	-309.38218	1
276	O	78.56928	76.45586	88.71288	556.06106	-390.37755	-78.24250	1
277	O	80.75049	77.06789	88.49343	-572.27940	-310.19032	-209.75862	1
278	H	81.08234	77.90702	88.06790	-1380.08193	2212.14486	790.85944	1

Listing 23: C00023.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.9865	0.0000	300.0000
3	H	70.24329	64.92098	78.43268	-2043.14101	-1757.64893	399.89339		1
4	N	70.07379	65.33491	77.51672	426.75047	490.45733	-334.42467		1
5	H	69.12054	65.69838	77.61394	442.25559	-1110.30854	-2448.52907		1
6	C	70.99129	66.35360	77.16564	415.32972	-666.39213	83.73172		1
7	H	71.78995	66.29215	77.93732	879.32219	2491.00447	667.35213		1
8	C	71.56401	66.08885	75.67739	31.35357	477.41777	628.23362		1
9	H	70.73310	66.19372	74.94031	1168.38489	2240.25337	-1019.71136		1
10	H	72.32057	66.86010	75.40117	-360.43770	2534.90498	931.67112		1
11	C	72.15519	64.70810	75.61729	463.18208	512.70242	-382.34388		1
12	H	71.42469	64.00720	76.08191	1725.29117	1863.52247	-987.07854		1
13	C	72.39302	64.27567	74.17538	710.42801	-144.27427	-313.15367		1
14	H	72.68189	63.19530	74.11206	364.20195	-1033.13725	2494.72524		1
15	H	71.47779	64.41290	73.54397	2567.61904	335.80679	847.48802		1
16	H	73.21928	64.86245	73.69859	-2587.99029	680.92867	-512.16411		1
17	C	73.47079	64.63936	76.38257	268.17616	741.64379	-40.42634		1
18	H	73.89520	63.60262	76.38268	1283.54314	-1945.37420	-1411.27812		1
19	H	74.24225	65.31298	75.92839	-1258.57796	1317.15249	-2026.02085		1
20	H	73.34675	64.94834	77.45217	-2502.84526	909.80597	575.92391		1
21	C	70.12237	67.71303	77.22188	619.36578	-458.64843	-172.09273		1
22	O	68.98516	67.74802	77.71898	-81.40433	433.87611	522.34594		1
23	N	70.86590	68.69376	76.78698	175.23996	-622.20190	341.55523		1
24	H	71.77524	68.42529	76.41395	-876.57256	-303.22879	-2561.90213		1
25	C	70.38060	70.00387	76.44592	-571.88214	-534.10783	-106.15033		1
26	H	70.18069	69.95912	75.35282	-2713.20841	-16.25800	-248.80809		1
27	C	69.05478	70.37017	77.25306	166.60354	288.16399	-716.09568		1
28	H	69.15084	69.94716	78.29627	-2097.85574	1636.78449	-586.18044		1
29	O	67.85404	69.76936	76.76141	-317.80580	-363.38227	484.43082		1
30	H	67.90371	68.86881	77.26648	1863.74748	-1451.84923	1357.29467		1
31	C	69.07887	71.94127	77.28066	503.80731	517.99032	318.51606		1
32	H	68.24453	72.34898	77.89747	640.61020	-2157.10410	-1536.29104		1
33	H	70.03004	72.34042	77.70346	1687.88455	465.60692	2087.56452		1
34	H	68.96849	72.36639	76.25602	-1293.07895	-1899.88581	-1463.57452		1
35	C	71.70914	70.90449	76.68358	-153.07550	-733.68902	248.70981		1
36	O	72.28285	71.21223	75.65124	186.15459	-480.78787	-449.34387		1
37	N	72.07962	71.10282	77.94757	-487.53139	543.18517	42.03850		1
38	C	73.19827	71.91992	78.32865	-699.35871	69.34393	360.10701		1
39	H	73.13912	72.85827	77.73327	2.81126	-221.99807	-2715.58072		1
40	C	73.00268	72.07988	79.89402	-507.46439	-592.59194	122.07761		1
41	H	73.94872	72.34854	80.41699	-1975.08116	525.87560	-1801.71556		1

42	H	72.25514	72.86529	80.14547	1588.27743	-1913.22100	1113.83566	1
43	C	72.48280	70.65365	80.25346	-613.62442	-457.55993	-194.14490	1
44	H	73.30471	69.90222	80.21072	1707.54637	-721.27992	1996.92523	1
45	H	72.02806	70.58032	81.26689	758.23357	2100.81767	1560.55011	1
46	C	71.43763	70.43719	79.07549	-352.41524	704.96076	49.21465	1
47	H	71.24368	69.37599	78.79390	1714.76886	-2070.42778	443.35792	1
48	H	70.46776	70.96297	79.23757	1224.15040	1801.50881	1636.97633	1
49	C	74.61496	71.12903	78.12453	566.85117	537.05831	117.62814	1
50	O	75.56252	71.37041	78.83570	-550.26779	-406.08867	4.21666	1
51	N	74.55054	70.34321	77.05887	566.34832	-425.77725	180.18749	1
52	H	73.67340	70.30898	76.51410	644.44502	2646.80550	-52.73430	1
53	C	75.48815	69.27576	76.94015	612.34801	-281.48662	411.56221	1
54	H	76.26285	69.53574	77.69926	1667.23498	-1490.75142	1556.16753	1
55	C	74.70168	67.92356	77.29390	-714.45746	-175.43074	286.98927	1
56	H	74.02434	67.67615	76.43180	-787.09484	1763.03619	-1922.46060	1
57	O	73.84816	67.97101	78.45171	-429.46514	516.51932	-128.40526	1
58	H	72.96704	68.05112	78.02953	1981.82785	436.16847	-1818.18182	1
59	C	75.87904	66.88472	77.36153	630.79189	-468.94448	76.03230	1
60	H	75.51229	65.85927	77.59837	-1775.71861	2062.30353	131.89849	1
61	H	76.43601	66.82517	76.38662	-1855.14608	88.94118	1993.53760	1
62	H	76.61836	67.15534	78.15146	-1504.82350	-780.94249	-2132.90992	1
63	C	76.03079	69.26925	75.40503	288.57638	618.62814	-397.00270	1
64	O	76.36221	68.19854	74.87810	321.70495	-185.26452	574.37218	1
65	N	76.10414	70.48315	74.92130	-447.05792	-446.53431	367.76425	1
66	H	75.78880	71.18727	75.59024	350.31316	1975.63644	-1843.31522	1
67	C	76.64236	70.87178	73.66966	-511.23061	374.03917	-471.51480	1
68	H	76.53773	71.98261	73.71600	2234.79579	-898.70890	-1273.45190	1
69	C	78.17421	70.41593	73.64141	529.53781	-159.34528	563.72604	1
70	H	78.71571	70.95519	72.81591	654.59388	2347.94251	1217.51488	1
71	H	78.62636	70.79795	74.59670	-1526.55661	2103.42026	817.87394	1
72	O	78.46986	69.01845	73.49019	-554.84278	14.12789	399.58769	1
73	H	77.67048	68.62234	74.00074	1297.06236	2061.84854	1220.68812	1
74	C	75.77229	70.25700	72.44379	-662.15484	-412.13544	123.62687	1
75	O	76.26956	70.07908	71.35753	-540.01537	-317.05804	274.91456	1
76	N	74.48822	70.10631	72.78950	-202.76299	-690.00100	-131.49145	1
77	H	74.26199	70.34202	73.75562	-702.62132	-2617.37191	281.70413	1
78	C	73.50364	69.71302	71.78247	-491.73914	576.34187	222.73509	1
79	H	74.15847	69.28373	70.98440	1977.17978	-1823.58850	-434.68928	1
80	C	72.55775	68.71376	72.42217	-649.50797	-328.66843	306.11224	1
81	H	72.08254	69.18869	73.30861	2075.07803	1452.16490	-1004.45904	1
82	C	71.46546	68.29121	71.45671	-615.18735	-489.99689	-70.96352	1
83	H	70.74164	67.57436	71.93323	-1226.32661	-1724.38906	-1716.47170	1
84	H	70.87285	69.17344	71.08828	2381.64273	-969.84735	900.46860	1
85	H	71.89283	67.77935	70.55065	2122.74991	1702.23946	-141.36228	1
86	C	73.30903	67.49176	72.92180	-501.86074	-479.61276	-376.42482	1
87	H	72.62045	66.76293	73.42718	993.79261	-2246.95401	-1177.81305	1
88	H	73.81339	66.94438	72.07860	42.71279	-626.15391	-2651.37258	1
89	H	74.11386	67.77257	73.65789	-2026.39012	-1590.33709	-887.82922	1
90	C	72.78502	71.11979	71.25332	-672.89153	382.57394	-156.34072	1
91	O	73.26980	71.69321	70.30739	410.04627	221.86223	500.35950	1
92	N	71.74779	71.49083	71.98458	-378.11782	-443.79414	-441.10984	1
93	H	71.46298	70.89139	72.75571	2404.15973	-568.14894	1149.30085	1
94	C	70.93106	72.55363	71.47926	-544.54484	466.16019	331.29119	1
95	H	71.26938	72.65329	70.41958	-1409.80988	-170.17955	2325.32679	1
96	C	69.43523	72.02773	71.62749	-184.48284	116.78282	-758.89137	1
97	H	69.36572	70.96830	71.29373	1893.78641	1861.14652	611.04528	1
98	H	69.11663	72.03019	72.69415	-2170.79665	-974.19311	1327.50117	1
99	C	68.51187	72.94127	70.76706	389.51668	672.81878	-138.49152	1
100	H	68.55237	73.98984	71.14445	510.64577	1933.03327	1851.02484	1
101	H	68.90772	73.01671	69.72993	-2302.30869	-1105.72939	-948.89774	1
102	C	67.01730	72.44374	70.71533	-559.93427	-126.34590	542.30857	1
103	O	66.20754	73.07399	70.08623	-670.36003	-111.83166	76.36448	1

104	N	66.78536	71.30231	71.39855	-216.06729	-537.07037	446.51379	1
105	H	67.42162	70.73704	71.97268	-1251.96487	1074.12894	-2168.52500	1
106	H	65.86289	70.85983	71.47615	-2451.83023	-720.73851	944.84612	1
107	C	71.06794	73.96610	72.26131	546.24052	-563.88337	-85.11809	1
108	O	70.56050	74.92741	71.69798	71.70702	-307.40463	606.69673	1
109	N	71.72774	73.95673	73.41975	479.90863	-504.50129	222.86849	1
110	C	71.38315	74.81378	74.51774	75.51268	-600.91904	506.73700	1
111	H	70.27060	74.85466	74.55186	-2033.61562	1795.30103	254.89480	1
112	C	72.10344	74.12527	75.74812	523.79067	517.99274	284.45581	1
113	H	72.28442	74.83820	76.58747	1599.61665	-1127.00911	1895.98173	1
114	H	71.49869	73.28464	76.15866	-1881.83093	1275.82488	-1501.55016	1
115	C	73.42036	73.61366	75.07810	-600.05639	-404.05026	316.64485	1
116	H	74.16821	74.43878	74.97997	-2597.05260	496.36221	657.73249	1
117	H	73.92832	72.79684	75.64648	-1666.24518	1294.38985	-1723.90591	1
118	C	72.91290	73.13897	73.65147	493.57570	-129.95376	-602.56394	1
119	H	73.61755	73.30952	72.80033	-1469.08415	-637.84797	2204.22581	1
120	H	72.55728	72.08040	73.62247	-1038.97840	1068.88701	-2280.71789	1
121	C	72.07572	76.29720	74.41280	188.88100	241.05089	-727.87821	1
122	O	72.47179	76.80381	75.43611	531.88613	-49.19943	427.07960	1
123	N	71.97693	76.78549	73.19174	708.14833	26.93417	-179.73509	1
124	H	71.47117	76.21775	72.47123	-2232.69501	-1179.09831	1023.94816	1
125	C	72.71233	77.92562	72.77670	-738.32412	259.92548	104.42456	1
126	H	72.21889	78.22640	71.82637	2028.89123	1260.02983	1311.33324	1
127	C	72.64399	79.03427	73.91233	-258.65678	-345.52513	661.28459	1
128	H	73.09883	78.65837	74.86574	-1826.06090	-1801.46097	-918.64554	1
129	C	73.36658	80.33506	73.42265	-541.23400	531.92970	-218.41428	1
130	H	73.15111	81.19422	74.10080	1311.73218	-2219.18200	882.19023	1
131	H	74.48967	80.21214	73.38891	-1048.71298	1223.58118	-2196.97971	1
132	H	73.03017	80.63121	72.40119	419.06414	1903.92898	1903.44670	1
133	C	71.13753	79.41181	74.13081	-423.86431	152.66566	-648.55262	1
134	H	71.01877	80.20759	74.90308	105.68386	-2342.50080	1387.51238	1
135	H	70.66602	79.78431	73.19148	-1695.63603	-1484.73621	-1531.02793	1
136	H	70.54865	78.52729	74.47022	-1853.57121	-487.39031	1936.59343	1
137	C	74.28472	77.50825	72.54699	539.71428	-510.58232	267.58633	1
138	O	74.97464	76.97899	73.38273	-15.93758	-278.34085	-624.49402	1
139	N	74.66755	78.01976	71.36198	-676.81886	12.05292	276.17960	1
140	H	73.88272	78.36577	70.80923	-1694.44250	-373.84189	-2100.66098	1
141	C	75.72380	77.28734	70.68821	412.33078	-664.70360	108.35451	1
142	H	75.43331	76.21452	70.72528	1765.77476	1294.44366	1621.76594	1
143	C	75.78682	77.88433	69.23445	-179.66635	-721.95667	-264.73915	1
144	H	74.86451	77.64475	68.65851	-607.34922	2587.87032	-598.10018	1
145	H	75.82694	78.99592	69.28533	-359.69332	-1479.13954	-2259.74260	1
146	C	77.06128	77.32654	68.51232	-240.01076	616.02425	431.85322	1
147	H	77.95630	77.43488	69.16693	-1359.17131	782.54425	2227.99181	1
148	H	76.96441	76.23765	68.30397	-820.36667	85.81767	-2596.78715	1
149	C	77.26033	78.15485	67.18105	-513.07015	236.18570	-551.87280	1
150	H	76.44531	77.94343	66.45111	1816.11944	-1183.11722	-1650.94321	1
151	H	77.20933	79.24933	67.38448	-1800.04429	-1361.53473	1526.34643	1
152	C	78.64453	77.77900	66.60197	726.08972	-253.19732	-179.64713	1
153	H	79.50073	78.02060	67.26318	1224.27271	-456.51798	-2390.90304	1
154	H	78.72764	76.73417	66.24223	1206.40339	-1150.93514	-2154.90344	1
155	N	78.87532	78.66266	65.33023	329.70796	-633.68968	-155.67358	1
156	H	79.79993	78.51725	64.83105	1348.31305	1938.76845	1359.00643	1
157	H	78.18673	78.54659	64.53100	2096.92035	1446.54551	-966.48890	1
158	H	78.87615	79.71533	65.46778	-1197.07217	-2303.53719	827.28733	1
159	C	77.13393	77.57193	71.44559	-378.01186	-556.17301	-413.96481	1
160	O	78.03859	76.77193	71.35218	-409.44433	-307.55053	-453.30833	1
161	N	77.15561	78.81412	71.92035	-429.02477	524.70884	274.08502	1
162	H	76.25746	79.30193	71.95656	1706.34263	-1425.96036	1574.38926	1
163	C	78.19051	79.23954	72.83018	-45.25864	-626.22952	478.93267	1
164	H	78.18061	78.43082	73.59410	1988.63164	570.90773	1772.87287	1
165	C	79.55651	79.28661	72.04278	551.77128	-20.49526	-564.54996	1

166	H	79.62210	78.41621	71.34963	1434.61535	-1753.10253	1513.99471	1
167	H	79.58769	80.18507	71.38590	-714.67738	1819.09770	1898.36494	1
168	C	80.77273	79.28353	73.03131	446.99263	-555.77305	338.97221	1
169	H	80.71613	80.11698	73.76786	1953.68466	1892.25957	-161.67766	1
170	H	80.79818	78.35377	73.64326	-403.03785	2688.07032	-188.43591	1
171	C	82.06848	79.41792	72.13516	567.86262	335.74681	434.04421	1
172	H	82.17530	78.53980	71.45747	-1080.02275	1568.26081	-1948.78900	1
173	H	81.99520	80.30720	71.46762	-919.54108	2111.34692	1456.13463	1
174	C	83.29083	79.54571	73.07346	195.81897	173.33862	-745.11536	1
175	H	83.27335	80.43537	73.73419	1405.67949	-2301.21089	-390.08113	1
176	H	83.51498	78.63772	73.66792	-940.37328	-1118.32446	2299.72133	1
177	N	84.55281	79.75708	72.16980	319.26422	656.36007	-42.02424	1
178	H	85.47130	79.87461	72.68711	1961.03633	619.91968	1787.09422	1
179	H	84.79618	78.98074	71.48820	854.14343	-2156.80752	1429.08711	1
180	H	84.55930	80.61180	71.54014	1237.02905	-1378.50857	-1998.28500	1
181	C	77.61845	80.65651	73.36714	532.53319	-268.57236	517.55729	1
182	O	76.41439	80.77165	73.57416	266.16714	-290.73804	-558.88002	1
183	N	78.58798	81.52244	73.58916	-226.25352	640.49678	-270.32839	1
184	H	79.52739	81.23059	73.32045	2007.69063	-1035.27229	1523.50231	1
185	C	78.39345	82.89438	73.89280	-540.76542	-573.33303	49.50000	1
186	H	79.40614	83.33486	73.75290	-2374.20950	-1036.76023	843.75774	1
187	C	77.35724	83.51504	72.83360	-77.09082	666.87422	-415.84136	1
188	H	76.45765	82.84317	72.74411	-985.81834	617.19825	2463.91927	1
189	O	77.88901	83.62891	71.50300	293.29899	-391.65602	-477.80926	1
190	H	77.29648	83.02316	71.01238	2528.72714	-681.76262	-751.27122	1
191	C	76.92104	84.85581	73.52607	252.47363	-605.14473	440.05134	1
192	H	76.37484	85.52264	72.81845	-2052.65063	1456.49051	-1043.51830	1
193	H	76.24048	84.67440	74.39401	-2152.98800	-1661.97574	-161.70652	1
194	H	77.80171	85.42198	73.91718	-473.12726	-1584.27339	2165.61725	1
195	C	77.90458	83.08947	75.43530	360.36307	488.46713	505.10056	1
196	O	77.90329	84.21902	75.88101	-200.08817	-528.03552	-385.82850	1
197	N	77.58096	81.95977	76.06293	-597.54095	-226.44775	355.20479	1
198	H	77.59795	81.10647	75.50133	2179.23655	-1300.70981	-991.33835	1
199	C	76.89469	82.09466	77.29703	-687.68921	297.39807	-249.45179	1
200	H	76.91422	83.19187	77.50539	-349.16256	-2467.37713	-1101.72831	1
201	C	75.41989	81.49900	77.08691	672.47345	361.54328	-201.62880	1
202	H	75.45546	80.58142	76.45469	1541.41502	582.18425	2169.97026	1
203	H	74.97012	81.21504	78.06559	-2534.67717	60.25153	997.72295	1
204	C	74.59761	82.60532	76.41341	574.26774	-389.43119	-377.02542	1
205	C	73.82174	83.51416	77.19430	688.82679	-287.33580	-257.96133	1
206	H	73.77936	83.42090	78.29458	331.14182	1470.38163	2269.80013	1
207	C	74.66568	82.74998	74.99636	-383.52382	-675.04808	144.24917	1
208	H	75.30431	82.04244	74.39319	4.09847	1517.59662	2262.86397	1
209	C	73.12642	84.52738	76.53629	-134.76730	428.45285	-649.50303	1
210	H	72.52771	85.23222	77.13908	-903.23433	1600.49020	2011.53387	1
211	C	73.94797	83.77715	74.38104	-335.53281	-615.00040	-364.39058	1
212	H	74.00946	83.87391	73.28288	1596.45398	-1369.33862	1732.02659	1
213	C	73.15489	84.70110	75.12185	585.48547	-340.24194	-406.23938	1
214	O	72.42231	85.75167	74.51129	-419.15649	-173.04408	-511.94141	1
215	H	72.66807	85.59940	73.56811	-1071.84350	1559.71507	-1960.13012	1
216	C	77.58164	81.21488	78.49064	291.41878	-183.13091	710.72246	1
217	O	77.66521	81.70999	79.59450	379.87695	523.47396	-222.23622	1
218	N	77.91781	79.97656	78.14764	564.30591	373.09380	277.24371	1
219	H	77.74842	79.63016	77.20434	-120.59931	-2436.07824	-1214.35098	1
220	C	78.41449	79.17086	79.23238	404.07514	-299.37480	608.84009	1
221	H	79.10176	79.90313	79.71574	-1071.07882	-841.69025	2359.66467	1
222	C	77.18774	78.87732	80.19081	-683.12807	68.71770	-390.13096	1
223	H	76.69550	79.83718	80.47625	2068.88918	1596.58590	770.89603	1
224	H	76.40056	78.28795	79.66861	1379.86429	2342.49779	-179.85638	1
225	C	77.71967	78.13020	81.45399	-176.39967	537.49466	550.97268	1
226	H	78.28927	77.22020	81.16375	-396.28051	1942.22168	1869.33314	1
227	H	78.44459	78.76438	82.01053	-94.44700	586.00678	-2659.20016	1

228	C	76.47717	77.74375	82.38008	-291.69381	-718.18079	-150.72929	1
229	H	75.96316	78.59544	82.89411	-2303.38776	1089.76242	964.62032	1
230	H	75.69249	77.11138	81.89152	884.16729	2568.80533	-207.74283	1
231	N	77.10819	76.95599	83.35656	-594.49522	-252.81478	342.29276	1
232	H	78.08526	76.75187	83.21389	-1735.17426	2084.05705	-263.71605	1
233	C	76.54106	76.48026	84.38982	595.23177	-271.52487	442.22352	1
234	N	75.18382	76.76062	84.58187	585.53813	-424.79750	-105.81303	1
235	H	74.55032	77.31815	84.01069	959.88797	1327.56823	-2177.11905	1
236	H	74.62972	76.44125	85.37717	1578.48647	16.27378	-2220.76233	1
237	N	77.44329	75.73018	85.15858	-452.17763	-390.33541	-421.51853	1
238	H	78.43226	75.52678	85.02292	470.26107	1974.25629	-1817.92087	1
239	H	77.18176	75.26763	86.02991	1856.67307	-1573.97321	-1224.35416	1
240	C	79.17418	77.87409	78.60344	-531.47271	-581.45780	-55.06206	1
241	O	80.23589	77.99209	78.04494	-243.00837	192.73507	609.52485	1
242	N	78.53116	76.72306	78.91699	343.49288	-644.25607	38.09164	1
243	H	77.60065	76.92423	79.28879	-1691.16043	-1535.97525	-1484.73099	1
244	C	78.69310	75.54654	78.05065	542.66492	350.14337	454.42563	1
245	H	79.79585	75.42114	77.94535	1209.57979	-2396.95920	463.86744	1
246	C	78.01208	74.40773	78.78036	-737.14309	145.93010	242.71942	1
247	H	76.97128	74.72821	79.01393	-1050.18303	159.36419	-2509.06125	1
248	C	77.92536	73.13586	77.96195	-706.77696	-252.88343	-245.16230	1
249	H	77.40738	72.30923	78.53869	-1624.64039	-1665.49085	1417.86935	1
250	H	77.31827	73.29684	77.00635	2566.10521	598.51109	693.22305	1
251	H	78.94187	72.75620	77.66408	-1972.69758	107.10018	-1876.34312	1
252	C	78.70314	74.10601	80.10054	412.85148	672.58832	-27.69222	1
253	H	78.17242	73.29672	80.67294	1447.02277	1762.76533	-1490.78944	1
254	H	79.76222	73.76310	79.94281	1320.77379	-145.20455	2378.68491	1
255	H	78.74467	75.01438	80.76129	-1512.10848	1470.52031	1724.75147	1
256	C	77.98903	75.93980	76.60338	-607.11113	499.56689	73.73769	1
257	O	77.24855	76.88332	76.46621	357.97126	460.81534	356.68785	1
258	N	78.39246	75.07254	75.68239	536.55407	-368.62270	332.76306	1
259	H	78.97396	74.30205	76.00399	524.38866	2297.69985	1367.20941	1
260	C	77.73407	75.09207	74.42040	46.50277	-774.29190	-147.97904	1
261	H	77.48078	76.16766	74.26611	1676.51875	1883.29066	1032.55549	1
262	C	78.67972	74.42096	73.29533	-559.41456	-34.19198	-556.30433	1
263	H	78.56887	73.31246	73.36208	-64.66664	395.18769	2695.05373	1
264	H	78.30799	74.69945	72.27725	-2703.44278	-60.40056	333.79418	1
265	C	80.13082	74.78961	73.44907	-519.76435	377.31045	459.42366	1
266	H	80.40451	74.75263	74.52712	-1746.74323	1667.50644	-1261.73691	1
267	C	81.01048	73.79810	72.69666	570.95554	16.46261	-545.27700	1
268	H	82.09698	74.05594	72.78857	2391.58273	28.05277	-1305.07271	1
269	H	80.88309	72.75374	73.08221	175.75588	917.63458	2559.43867	1
270	H	80.76575	73.77909	71.60347	-1063.97851	-2155.34650	1283.00462	1
271	C	80.38721	76.19680	72.92909	193.76014	2.62946	-765.53141	1
272	H	81.47675	76.46099	72.95303	507.39394	-846.55087	2539.60089	1
273	H	80.03253	76.30888	71.86526	1337.57841	1818.19054	1526.01994	1
274	H	79.83759	76.96147	73.53991	1100.88635	-1172.91350	-2199.08909	1
275	C	76.43975	74.15178	74.50348	-549.21115	475.64486	-309.38218	1
276	O	76.16847	73.43530	75.44172	556.06106	-390.37755	-78.24250	1
277	O	75.68062	74.06053	73.31152	-572.27940	-310.19032	-209.75862	1
278	H	75.91943	74.95593	72.92598	-1380.08193	2212.14486	790.85944	1

Listing 24: C00024.xmolout

1		276						
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750 11100
		0.2500	300.00	0.00	0.00	0.00	-1293.9706	0.0000 300.0000
3	H	71.43720	78.94080	86.11812	-2043.14101	-1757.64893	399.89339	1
4	N	71.38973	79.41802	85.21883	426.75047	490.45733	-334.42467	1
5	H	70.43836	79.78301	85.25721	442.25559	-1110.30854	-2448.52907	1
6	C	72.36730	80.43794	85.09025	415.32972	-666.39213	83.73172	1
7	H	72.45879	80.90359	86.09531	879.32219	2491.00447	667.35213	1

8	C	73.74606	79.76737	84.60098	31.35357	477.41777	628.23362	1
9	H	73.56990	79.25612	83.62384	1168.38489	2240.25337	-1019.71136	1
10	H	74.50401	80.56287	84.40071	-360.43770	2534.90498	931.67112	1
11	C	74.26231	78.78423	85.62231	463.18208	512.70242	-382.34388	1
12	H	73.43357	78.09638	85.90197	1725.29117	1863.52247	-987.07854	1
13	C	75.39268	77.95360	85.02796	710.42801	-144.27427	-313.15367	1
14	H	75.78599	77.20381	85.76220	364.20195	-1033.13725	2494.72524	1
15	H	75.05788	77.38733	84.12057	2567.61904	335.80679	847.48802	1
16	H	76.25609	78.59704	84.71726	-2587.99029	680.92867	-512.16411	1
17	C	74.75576	79.49445	86.87492	268.17616	741.64379	-40.42634	1
18	H	75.16067	78.77027	87.62849	1283.54314	-1945.37420	-1411.27812	1
19	H	75.57678	80.22028	86.63932	-1258.57796	1317.15249	-2026.02085	1
20	H	73.93759	80.07222	87.37696	-2502.84526	909.80597	575.92391	1
21	C	71.89961	81.49962	83.95023	619.36578	-458.64843	-172.09273	1
22	O	72.32623	82.63380	83.95762	-81.40433	433.87611	522.34594	1
23	N	71.14598	80.91290	83.01710	175.23996	-622.20190	341.55523	1
24	H	70.85897	79.95138	83.19463	-876.57256	-303.22879	-2561.90213	1
25	C	70.51891	81.74050	82.04268	-571.88214	-534.10783	-106.15033	1
26	H	71.09741	82.69329	82.03688	-2713.20841	-16.25800	-248.80809	1
27	C	70.55026	80.90531	80.66796	166.60354	288.16399	-716.09568	1
28	H	70.04401	79.91601	80.85869	-2097.85574	1636.78449	-586.18044	1
29	O	71.85733	80.59563	80.16051	-317.80580	-363.38227	484.43082	1
30	H	71.82569	79.61728	80.14820	1863.74748	-1451.84923	1357.29467	1
31	C	69.63464	81.75577	79.71460	503.80731	517.99032	318.51606	1
32	H	69.42327	81.20718	78.76733	640.61020	-2157.10410	-1536.29104	1
33	H	68.64992	81.99493	80.18245	1687.88455	465.60692	2087.56452	1
34	H	70.11728	82.72092	79.43645	-1293.07895	-1899.88581	-1463.57452	1
35	C	68.96339	81.88184	82.48361	-153.07550	-733.68902	248.70981	1
36	O	68.33318	80.87188	82.75722	186.15459	-480.78787	-449.34387	1
37	N	68.53583	83.13434	82.37997	-487.53139	543.18517	42.03850	1
38	C	67.20436	83.51347	82.78723	-699.35871	69.34393	360.10701	1
39	H	67.03694	82.99484	83.75995	2.81126	-221.99807	-2715.58072	1
40	C	67.26527	85.10038	82.83889	-507.46439	-592.59194	122.07761	1
41	H	66.27203	85.56085	82.62374	-1975.08116	525.87560	-1801.71556	1
42	H	67.58624	85.47100	83.83823	1588.27743	-1913.22100	1113.83566	1
43	C	68.33018	85.41756	81.74312	-613.62442	-457.55993	-194.14490	1
44	H	67.88087	85.35530	80.72654	1707.54637	-721.27992	1996.92523	1
45	H	68.77590	86.43381	81.83327	758.23357	2100.81767	1560.55011	1
46	C	69.38198	84.24934	81.97959	-352.41524	704.96076	49.21465	1
47	H	69.97158	83.95726	81.08032	1714.76886	-2070.42778	443.35792	1
48	H	70.07711	84.42170	82.83618	1224.15040	1801.50881	1636.97633	1
49	C	66.10695	83.11244	81.66851	566.85117	537.05831	117.62814	1
50	O	65.35545	83.98619	81.24515	-550.26779	-406.08867	4.21666	1
51	N	66.15866	81.83424	81.35295	566.34832	-425.77725	180.18749	1
52	H	66.84195	81.22643	81.86364	644.44502	2646.80550	-52.73430	1
53	C	64.91836	81.25123	80.90094	612.34801	-281.48662	411.56221	1
54	H	64.12461	81.74373	81.50706	1667.23498	-1490.75142	1556.16753	1
55	C	64.74403	81.52352	79.34532	-714.45746	-175.43074	286.98927	1
56	H	65.58821	81.04636	78.76417	-787.09484	1763.03619	-1922.46060	1
57	O	64.81882	82.88029	78.87649	-429.46514	516.51932	-128.40526	1
58	H	64.97366	83.37030	79.76229	1981.82785	436.16847	-1818.18182	1
59	C	63.41534	80.74357	79.04404	630.79189	-468.94448	76.03230	1
60	H	63.19364	80.72103	77.95158	-1775.71861	2062.30353	131.89849	1
61	H	63.46615	79.68467	79.39881	-1855.14608	88.94118	1993.53760	1
62	H	62.54180	81.21657	79.55049	-1504.82350	-780.94249	-2132.90992	1
63	C	65.02243	79.63728	81.10658	288.57638	618.62814	-397.00270	1
64	O	64.06110	79.02573	81.50513	321.70495	-185.26452	574.37218	1
65	N	66.17574	79.16829	80.65185	-447.05792	-446.53431	367.76425	1
66	H	66.97102	79.72320	80.28047	350.31316	1975.63644	-1843.31522	1
67	C	66.39657	77.75256	80.71344	-511.23061	374.03917	-471.51480	1
68	H	66.15490	77.42096	81.74804	2234.79579	-898.70890	-1273.45190	1
69	C	65.41210	77.08392	79.63905	529.53781	-159.34528	563.72604	1

70	H	65.46865	75.96893	79.77200	654.59388	2347.94251	1217.51488	1
71	H	64.37407	77.39668	79.93606	-1526.55661	2103.42026	817.87394	1
72	O	65.67648	77.36702	78.24217	-554.84278	14.12789	399.58769	1
73	H	65.33013	78.27874	78.19810	1297.06236	2061.84854	1220.68812	1
74	C	67.96064	77.71440	80.30685	-662.15484	-412.13544	123.62687	1
75	O	68.47970	78.73336	79.86386	-540.01537	-317.05804	274.91456	1
76	N	68.49754	76.52970	80.55313	-202.76299	-690.00100	-131.49145	1
77	H	67.91744	75.77947	80.93052	-702.62132	-2617.37191	281.70413	1
78	C	69.83321	76.27241	80.16410	-491.73914	576.34187	222.73509	1
79	H	70.14546	77.16212	79.56967	1977.17978	-1823.58850	-434.68928	1
80	C	70.66106	76.06101	81.50894	-649.50797	-328.66843	306.11224	1
81	H	70.17110	75.28566	82.13627	2075.07803	1452.16490	-1004.45904	1
82	C	72.12329	75.64232	81.13883	-615.18735	-489.99689	-70.96352	1
83	H	72.75393	75.50691	82.04906	-1226.32661	-1724.38906	-1716.47170	1
84	H	72.14074	74.67931	80.57460	2381.64273	-969.84735	900.46860	1
85	H	72.62092	76.40953	80.50016	2122.74991	1702.23946	-141.36228	1
86	C	70.73499	77.42258	82.28096	-501.86074	-479.61276	-376.42482	1
87	H	71.21049	77.30861	83.28392	993.79261	-2246.95401	-1177.81305	1
88	H	71.32950	78.18021	81.71984	42.71279	-626.15391	-2651.37258	1
89	H	69.71797	77.85357	82.44139	-2026.39012	-1590.33709	-887.82922	1
90	C	69.77745	74.84196	79.34896	-672.89153	382.57394	-156.34072	1
91	O	69.49314	73.80296	79.89981	410.04627	221.86223	500.35950	1
92	N	70.05367	75.05090	78.06702	-378.11782	-443.79414	-441.10984	1
93	H	70.32955	75.98321	77.76172	2404.15973	-568.14894	1149.30085	1
94	C	70.24411	73.88976	77.25802	-544.54484	466.16019	331.29119	1
95	H	69.59130	73.11498	77.72101	-1409.80988	-170.17955	2325.32679	1
96	C	69.89108	74.27659	75.76264	-184.48284	116.78282	-758.89137	1
97	H	68.83266	74.61444	75.68944	1893.78641	1861.14652	611.04528	1
98	H	70.50890	75.14155	75.43143	-2170.79665	-974.19311	1327.50117	1
99	C	70.15018	73.03709	74.84868	389.51668	672.81878	-138.49152	1
100	H	71.17287	72.62498	75.01868	510.64577	1933.03327	1851.02484	1
101	H	69.47571	72.20082	75.13768	-2302.30869	-1105.72939	-948.89774	1
102	C	69.96628	73.37450	73.31826	-559.93427	-126.34590	542.30857	1
103	O	70.35835	72.60650	72.47761	-670.36003	-111.83166	76.36448	1
104	N	69.32122	74.54029	73.08967	-216.06729	-537.07037	446.51379	1
105	H	68.90363	75.19199	73.76331	-1251.96487	1074.12894	-2168.52500	1
106	H	69.02720	74.86005	72.16076	-2451.83023	-720.73851	944.84612	1
107	C	71.84259	73.52552	77.31639	546.24052	-563.88337	-85.11809	1
108	O	72.66995	74.34851	77.03259	71.70702	-307.40463	606.69673	1
109	N	71.99479	72.23959	77.66821	479.90863	-504.50129	222.86849	1
110	C	73.26201	71.58629	77.59493	75.51268	-600.91904	506.73700	1
111	H	74.04657	72.36539	77.73783	-2033.61562	1795.30103	254.89480	1
112	C	73.12125	70.50285	78.75276	523.79067	517.99274	284.45581	1
113	H	73.84575	69.66423	78.65252	1599.61665	-1127.00911	1895.98173	1
114	H	73.28742	70.95248	79.75668	-1881.83093	1275.82488	-1501.55016	1
115	C	71.63770	70.05844	78.57007	-600.05639	-404.05026	316.64485	1
116	H	71.53340	69.36279	77.70713	-2597.05260	496.36221	657.73249	1
117	H	71.21532	69.53172	79.45556	-1666.24518	1294.38985	-1723.90591	1
118	C	70.92926	71.44847	78.27260	493.57570	-129.95376	-602.56394	1
119	H	70.08347	71.39263	77.54719	-1469.08415	-637.84797	2204.22581	1
120	H	70.60434	72.02047	79.17893	-1038.97840	1068.88701	-2280.71789	1
121	C	73.38808	70.79777	76.16730	188.88100	241.05089	-727.87821	1
122	O	72.46526	70.64635	75.40551	531.88613	-49.19943	427.07960	1
123	N	74.60691	70.17254	76.11935	708.14833	26.93417	-179.73509	1
124	H	75.12249	70.64100	76.87058	-2232.69501	-1179.09831	1023.94816	1
125	C	75.26480	69.93429	74.81542	-738.32412	259.92548	104.42456	1
126	H	76.22648	69.49527	75.16739	2028.89123	1260.02983	1311.33324	1
127	C	74.44964	68.97195	73.99027	-258.65678	-345.52513	661.28459	1
128	H	73.66840	69.56288	73.45832	-1826.06090	-1801.46097	-918.64554	1
129	C	75.29835	68.23836	72.96371	-541.23400	531.92970	-218.41428	1
130	H	74.66529	67.61899	72.27258	1311.73218	-2219.18200	882.19023	1
131	H	75.90312	68.93868	72.32482	-1048.71298	1223.58118	-2196.97971	1

132	H	76.02625	67.54045	73.45854	419.06414	1903.92898	1903.44670	1
133	C	73.72254	67.93989	74.83875	-423.86431	152.66566	-648.55262	1
134	H	73.10275	67.24358	74.21179	105.68386	-2342.50080	1387.51238	1
135	H	74.44099	67.31110	75.43078	-1695.63603	-1484.73621	-1531.02793	1
136	H	73.03032	68.43789	75.57363	-1853.57121	-487.39031	1936.59343	1
137	C	75.49824	71.43563	74.16854	539.71428	-510.58232	267.58633	1
138	O	75.76272	72.36218	74.89384	-15.93758	-278.34085	-624.49402	1
139	N	75.49174	71.39741	72.84468	-676.81886	12.05292	276.17960	1
140	H	75.26164	70.50472	72.41196	-1694.44250	-373.84189	-2100.66098	1
141	C	75.50328	72.57074	72.04187	412.33078	-664.70360	108.35451	1
142	H	75.52423	72.14742	71.01136	1765.77476	1294.44366	1621.76594	1
143	C	74.18792	73.41291	72.31887	-179.66635	-721.95667	-264.73915	1
144	H	73.28318	72.76440	72.36880	-607.34922	2587.87032	-598.10018	1
145	H	74.24874	73.93106	73.30316	-359.69332	-1479.13954	-2259.74260	1
146	C	74.10930	74.42950	71.13270	-240.01076	616.02425	431.85322	1
147	H	75.05804	75.02102	71.08644	-1359.17131	782.54425	2227.99181	1
148	H	74.03457	73.89160	70.16048	-820.36667	85.81767	-2596.78715	1
149	C	72.88157	75.40807	71.31465	-513.07015	236.18570	-551.87280	1
150	H	71.91182	74.86040	71.25812	1816.11944	-1183.11722	-1650.94321	1
151	H	72.90003	75.89781	72.31552	-1800.04429	-1361.53473	1526.34643	1
152	C	73.02115	76.45067	70.17959	726.08972	-253.19732	-179.64713	1
153	H	73.92316	77.08863	70.25313	1224.27271	-456.51798	-2390.90304	1
154	H	72.93850	76.03314	69.15631	1206.40339	-1150.93514	-2154.90344	1
155	N	71.83367	77.46258	70.29389	329.70796	-633.68968	-155.67358	1
156	H	71.83210	78.24506	69.57714	1348.31305	1938.76845	1359.00643	1
157	H	70.85339	77.07221	70.17922	2096.92035	1446.54551	-966.48890	1
158	H	71.75047	78.01002	71.19952	-1197.07217	-2303.53719	827.28733	1
159	C	76.80589	73.50525	72.38173	-378.01186	-556.17301	-413.96481	1
160	O	76.71726	74.72013	72.32371	-409.44433	-307.55053	-453.30833	1
161	N	77.88202	72.76538	72.54919	-429.02477	524.70884	274.08502	1
162	H	77.71864	71.76185	72.59207	1706.34263	-1425.96036	1574.38926	1
163	C	79.15178	73.37429	72.85182	-45.25864	-626.22952	478.93267	1
164	H	79.37974	73.92405	71.90194	1988.63164	570.90773	1772.87287	1
165	C	78.97789	74.38783	74.05185	551.77128	-20.49526	-564.54996	1
166	H	78.14808	75.10993	73.84470	1434.61535	-1753.10253	1513.99471	1
167	H	78.69945	73.85581	74.99018	-714.67738	1819.09770	1898.36494	1
168	C	80.35265	75.12413	74.18990	446.99263	-555.77305	338.97221	1
169	H	81.15371	74.39025	74.44317	1953.68466	1892.25957	-161.67766	1
170	H	80.64840	75.58999	73.21940	-403.03785	2688.07032	-188.43591	1
171	C	80.21465	76.21888	75.32130	567.86262	335.74681	434.04421	1
172	H	79.54311	77.04562	74.99313	-1080.02275	1568.26081	-1948.78900	1
173	H	79.74066	75.78670	76.23235	-919.54108	2111.34692	1456.13463	1
174	C	81.63062	76.74836	75.64940	195.81897	173.33862	-745.11536	1
175	H	82.31805	75.98926	76.07343	1405.67949	-2301.21089	-390.08113	1
176	H	82.12979	77.28997	74.82087	-940.37328	-1118.32446	2299.72133	1
177	N	81.47605	77.81262	76.78752	319.26422	656.36007	-42.02424	1
178	H	82.37987	78.23453	77.14859	1961.03633	619.91968	1787.09422	1
179	H	80.91448	78.68442	76.56110	854.14343	-2156.80752	1429.08711	1
180	H	81.02289	77.48789	77.69083	1237.02905	-1378.50857	-1998.28500	1
181	C	80.20853	72.19859	73.19177	532.53319	-268.57236	517.55729	1
182	O	80.76017	72.14477	74.29469	266.16714	-290.73804	-558.88002	1
183	N	80.39338	71.39743	72.16322	-226.25352	640.49678	-270.32839	1
184	H	79.84682	71.52853	71.31369	2007.69063	-1035.27229	1523.50231	1
185	C	81.52095	70.52114	72.23240	-540.76542	-573.33303	49.50000	1
186	H	82.26814	71.09175	72.82927	-2374.20950	-1036.76023	843.75774	1
187	C	81.04483	69.22630	73.02300	-77.09082	666.87422	-415.84136	1
188	H	80.18828	68.72219	72.48986	-985.81834	617.19825	2463.91927	1
189	O	80.49375	69.44777	74.33763	293.29899	-391.65602	-477.80926	1
190	H	80.62687	70.44959	74.42119	2528.72714	-681.76262	-751.27122	1
191	C	82.31053	68.30660	72.93004	252.47363	-605.14473	440.05134	1
192	H	82.12731	67.30958	73.39517	-2052.65063	1456.49051	-1043.51830	1
193	H	82.60901	68.13132	71.86832	-2152.98800	-1661.97574	-161.70652	1

194	H	83.18806	68.75806	73.45006	-473.12726	-1584.27339	2165.61725	1
195	C	81.97847	70.17947	70.68562	360.36307	488.46713	505.10056	1
196	O	81.27135	69.55621	69.93336	-200.08817	-528.03552	-385.82850	1
197	N	83.18303	70.70333	70.50092	-597.54095	-226.44775	355.20479	1
198	H	83.60096	71.17625	71.30276	2179.23655	-1300.70981	-991.33835	1
199	C	83.97261	70.45811	69.35572	-687.68921	297.39807	-249.45179	1
200	H	84.96962	70.86442	69.63712	-349.16256	-2467.37713	-1101.72831	1
201	C	84.01872	68.88952	69.01791	672.47345	361.54328	-201.62880	1
202	H	82.99729	68.44091	69.06427	1541.41502	582.18425	2169.97026	1
203	H	84.39168	68.75324	67.97556	-2534.67717	60.25153	997.72295	1
204	C	84.96942	68.22314	70.02141	574.26774	-389.43119	-377.02542	1
205	C	86.34683	68.59922	70.02196	688.82679	-287.33580	-257.96133	1
206	H	86.73028	69.33575	69.29275	331.14182	1470.38163	2269.80013	1
207	C	84.48727	67.25664	70.95442	-383.52382	-675.04808	144.24917	1
208	H	83.42327	66.95231	70.94945	4.09847	1517.59662	2262.86397	1
209	C	87.19670	68.02565	70.96618	-134.76730	428.45285	-649.50303	1
210	H	88.26010	68.32235	70.96914	-903.23433	1600.49020	2011.53387	1
211	C	85.37743	66.71091	71.88257	-335.53281	-615.00040	-364.39058	1
212	H	84.98948	65.97196	72.60521	1596.45398	-1369.33862	1732.02659	1
213	C	86.75532	67.07245	71.92955	585.48547	-340.24194	-406.23938	1
214	O	87.66748	66.53008	72.87170	-419.15649	-173.04408	-511.94141	1
215	H	87.06456	65.91598	73.35316	-1071.84350	1559.71507	-1960.13012	1
216	C	83.37974	71.17352	68.01789	291.41878	-183.13091	710.72246	1
217	O	83.87019	70.91043	66.94196	379.87695	523.47396	-222.23622	1
218	N	82.46312	72.10905	68.28926	564.30591	373.09380	277.24371	1
219	H	82.11175	72.10636	69.24706	-120.59931	-2436.07824	-1214.35098	1
220	C	81.72692	72.63328	67.17622	404.07514	-299.37480	608.84009	1
221	H	82.42921	72.51395	66.31655	-1071.07882	-841.69025	2359.66467	1
222	C	80.43005	71.72603	67.00328	-683.12807	68.71770	-390.13096	1
223	H	80.69586	70.64693	67.07376	2068.88918	1596.58590	770.89603	1
224	H	79.69696	71.90937	67.82515	1379.86429	2342.49779	-179.85638	1
225	C	79.81414	72.07019	65.61515	-176.39967	537.49466	550.97268	1
226	H	79.54507	73.15584	65.57121	-396.28051	1942.22168	1869.33314	1
227	H	80.55607	71.91251	64.80028	-94.44700	586.00678	-2659.20016	1
228	C	78.51961	71.15581	65.38860	-291.69381	-718.18079	-150.72929	1
229	H	78.69165	70.05165	65.32820	-2303.38776	1089.76242	964.62032	1
230	H	77.69498	71.37346	66.11729	884.16729	2568.80533	-207.74283	1
231	N	78.12961	71.63773	64.13139	-594.49522	-252.81478	342.29276	1
232	H	78.31209	72.61436	63.95238	-1735.17426	2084.05705	-263.71605	1
233	C	77.53356	70.97218	63.22425	595.23177	-271.52487	442.22352	1
234	N	77.24120	69.62608	63.45967	585.53813	-424.79750	-105.81303	1
235	H	77.39972	69.06533	64.29560	959.88797	1327.56823	-2177.11905	1
236	H	76.73891	69.01600	62.81355	1578.48647	16.27378	-2220.76233	1
237	N	77.27320	71.77866	62.10798	-452.17763	-390.33541	-421.51853	1
238	H	77.47131	72.76330	61.93659	470.26107	1974.25629	-1817.92087	1
239	H	76.78447	71.44499	61.27642	1856.67307	-1573.97321	-1224.35416	1
240	C	81.26364	74.15799	67.45137	-531.47271	-581.45780	-55.06206	1
241	O	80.45878	74.69193	66.68342	-243.00837	192.73507	609.52485	1
242	N	81.87376	74.69656	68.48636	343.49288	-644.25607	38.09164	1
243	H	82.51842	74.05221	68.94482	-1691.16043	-1535.97525	-1484.73099	1
244	C	81.42696	75.90222	69.16912	542.66492	350.14337	454.42563	1
245	H	82.21632	76.09510	69.93416	1209.57979	-2396.95920	463.86744	1
246	C	81.26511	77.02949	68.15742	-737.14309	145.93010	242.71942	1
247	H	80.61188	76.65178	67.32894	-1050.18303	159.36419	-2509.06125	1
248	C	80.60007	78.24075	68.77978	-706.77696	-252.88343	-245.16230	1
249	H	80.43833	79.06021	68.02592	-1624.64039	-1665.49085	1417.86935	1
250	H	79.58909	77.98031	69.21799	2566.10521	598.51109	693.22305	1
251	H	81.22170	78.67188	69.61270	-1972.69758	107.10018	-1876.34312	1
252	C	82.59596	77.41601	67.54044	412.85148	672.58832	-27.69222	1
253	H	82.47522	78.20607	66.74871	1447.02277	1762.76533	-1490.78944	1
254	H	83.30876	77.82083	68.31091	1320.77379	-145.20455	2378.68491	1
255	H	83.09325	76.52881	67.05859	-1512.10848	1470.52031	1724.75147	1

256	C	79.96330	75.55399	69.88488	-607.11113	499.56689	73.73769	1
257	O	79.86237	75.71411	71.07675	357.97126	460.81534	356.68785	1
258	N	79.06549	75.17938	69.00135	536.55407	-368.62270	332.76306	1
259	H	79.32159	75.11776	67.99401	524.38866	2297.69985	1367.20941	1
260	C	77.77607	74.78120	69.44148	46.50277	-774.29190	-147.97904	1
261	H	77.82319	74.82833	70.55900	1676.51875	1883.29066	1032.55549	1
262	C	76.71133	75.77271	68.79036	-559.41456	-34.19198	-556.30433	1
263	H	76.75489	75.70288	67.68101	-64.66664	395.18769	2695.05373	1
264	H	75.67429	75.48852	69.07293	-2703.44278	-60.40056	333.79418	1
265	C	77.03882	77.22996	69.25635	-519.76435	377.31045	459.42366	1
266	H	78.10064	77.48057	69.00952	-1746.74323	1667.50644	-1261.73691	1
267	C	76.05693	78.21119	68.51824	570.95554	16.46261	-545.27700	1
268	H	76.21070	79.26615	68.84395	2391.58273	28.05277	-1305.07271	1
269	H	76.20373	78.18154	67.41354	175.75588	917.63458	2559.43867	1
270	H	74.99059	77.95589	68.71551	-1063.97851	-2155.34650	1283.00462	1
271	C	76.79976	77.35470	70.80520	193.76014	2.62946	-765.53141	1
272	H	77.00440	78.38820	71.16945	507.39394	-846.55087	2539.60089	1
273	H	75.75085	77.10669	71.08567	1337.57841	1818.19054	1526.01994	1
274	H	77.46397	76.66314	71.38024	1100.88635	-1172.91350	-2199.08909	1
275	C	77.52790	73.29673	68.81964	-549.21115	475.64486	-309.38218	1
276	O	76.97412	73.11532	67.76831	556.06106	-390.37755	-78.24250	1
277	O	78.08622	72.21807	69.53976	-572.27940	-310.19032	-209.75862	1
278	H	78.33224	72.69964	70.38011	-1380.08193	2212.14486	790.85944	1

Listing 25: C00025.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.7890	3156
		0.2500	300.00	0.00	0.00	0.00	-1293.9590	0.0000	300.0000
3	H	66.80058	61.07021	72.04983	-2043.14101	-1757.64893	399.89339		1
4	N	66.86297	62.06785	72.25056	426.75047	490.45733	-334.42467		1
5	H	66.83971	62.10426	73.27819	442.25559	-1110.30854	-2448.52907		1
6	C	68.03550	62.68018	71.75648	415.32972	-666.39213	83.73172		1
7	H	68.42401	62.05782	70.92112	879.32219	2491.00447	667.35213		1
8	C	67.66151	64.18160	71.29986	31.35357	477.41777	628.23362		1
9	H	67.23850	64.73423	72.17253	1168.38489	2240.25337	-1019.71136		1
10	H	68.57769	64.74048	70.99164	-360.43770	2534.90498	931.67112		1
11	C	66.65769	64.12182	70.17853	463.18208	512.70242	-382.34388		1
12	H	65.85822	63.40304	70.46960	1725.29117	1863.52247	-987.07854		1
13	C	66.02132	65.48885	69.95963	710.42801	-144.27427	-313.15367		1
14	H	65.25378	65.46219	69.14361	364.20195	-1033.13725	2494.72524		1
15	H	65.50996	65.86063	70.88487	2567.61904	335.80679	847.48802		1
16	H	66.78474	66.25672	69.67127	-2587.99029	680.92867	-512.16411		1
17	C	67.29541	63.64563	68.88053	268.17616	741.64379	-40.42634		1
18	H	66.55099	63.61187	68.04344	1283.54314	-1945.37420	-1411.27812		1
19	H	68.12645	64.32409	68.55683	-1258.57796	1317.15249	-2026.02085		1
20	H	67.72648	62.61664	68.98141	-2502.84526	909.80597	575.92391		1
21	C	68.99548	62.72613	73.06802	619.36578	-458.64843	-172.09273		1
22	O	68.54325	62.61061	74.19291	-81.40433	433.87611	522.34594		1
23	N	70.24903	62.95593	72.69613	175.23996	-622.20190	341.55523		1
24	H	70.45923	63.08166	71.70665	-876.57256	-303.22879	-2561.90213		1
25	C	71.26758	62.92166	73.68644	-571.88214	-534.10783	-106.15033		1
26	H	70.76401	62.55434	74.60995	-2713.20841	-16.25800	-248.80809		1
27	C	72.43260	61.96339	73.12266	166.60354	288.16399	-716.09568		1
28	H	72.76164	62.36547	72.12581	-2097.85574	1636.78449	-586.18044		1
29	O	72.04671	60.59944	72.89773	-317.80580	-363.38227	484.43082		1
30	H	72.19274	60.51940	71.93297	1863.74748	-1451.84923	1357.29467		1
31	C	73.58979	62.18219	74.16310	503.80731	517.99032	318.51606		1
32	H	74.51987	61.65036	73.85395	640.61020	-2157.10410	-1536.29104		1
33	H	73.85474	63.26150	74.27633	1687.88455	465.60692	2087.56452		1
34	H	73.31183	61.79747	75.17147	-1293.07895	-1899.88581	-1463.57452		1
35	C	71.88875	64.42062	73.78985	-153.07550	-733.68902	248.70981		1

36	O	72.32365	64.96483	72.78702	186.15459	-480.78787	-449.34387	1
37	N	71.91628	64.84169	75.05266	-487.53139	543.18517	42.03850	1
38	C	72.37182	66.16257	75.38731	-699.35871	69.34393	360.10701	1
39	H	71.94397	66.82172	74.59771	2.81126	-221.99807	-2715.58072	1
40	C	71.80775	66.37587	76.84977	-507.46439	-592.59194	122.07761	1
41	H	72.39451	67.12251	77.43182	-1975.08116	525.87560	-1801.71556	1
42	H	70.75452	66.73595	76.83447	1588.27743	-1913.22100	1113.83566	1
43	C	71.90517	64.92883	77.42973	-613.62442	-457.55993	-194.14490	1
44	H	72.95498	64.68620	77.70952	1707.54637	-721.27992	1996.92523	1
45	H	71.28530	64.76834	78.34038	758.23357	2100.81767	1560.55011	1
46	C	71.42565	64.06646	76.18548	-352.41524	704.96076	49.21465	1
47	H	71.85367	63.03857	76.13252	1714.76886	-2070.42778	443.35792	1
48	H	70.31777	64.01384	76.05684	1224.15040	1801.50881	1636.97633	1
49	C	74.01173	66.16825	75.35635	566.85117	537.05831	117.62814	1
50	O	74.67086	66.26097	76.36132	-550.26779	-406.08867	4.21666	1
51	N	74.40777	66.04431	74.09449	566.34832	-425.77725	180.18749	1
52	H	73.71358	65.92696	73.32094	644.44502	2646.80550	-52.73430	1
53	C	75.79632	66.21243	73.84018	612.34801	-281.48662	411.56221	1
54	H	76.31493	65.99294	74.80219	1667.23498	-1490.75142	1556.16753	1
55	C	76.13103	65.21853	72.63073	-714.45746	-175.43074	286.98927	1
56	H	75.50081	65.51787	71.74786	-787.09484	1763.03619	-1922.46060	1
57	O	75.83473	63.82818	72.86012	-429.46514	516.51932	-128.40526	1
58	H	75.09992	63.68851	72.22831	1981.82785	436.16847	-1818.18182	1
59	C	77.63798	65.56033	72.34050	630.79189	-468.94448	76.03230	1
60	H	78.01512	65.00999	71.44745	-1775.71861	2062.30353	131.89849	1
61	H	77.78657	66.64869	72.14825	-1855.14608	88.94118	1993.53760	1
62	H	78.29089	65.28107	73.19961	-1504.82350	-780.94249	-2132.90992	1
63	C	75.99052	67.75987	73.32395	288.57638	618.62814	-397.00270	1
64	O	75.39272	68.15461	72.32180	321.70495	-185.26452	574.37218	1
65	N	76.90567	68.34725	74.04536	-447.05792	-446.53431	367.76425	1
66	H	77.26008	67.76669	74.80430	350.31316	1975.63644	-1843.31522	1
67	C	77.28748	69.71442	73.96515	-511.23061	374.03917	-471.51480	1
68	H	78.27857	69.69558	74.47251	2234.79579	-898.70890	-1273.45190	1
69	C	77.39164	70.12198	72.42876	529.53781	-159.34528	563.72604	1
70	H	78.12617	70.96737	72.33102	654.59388	2347.94251	1217.51488	1
71	H	77.83382	69.23873	71.89657	-1526.55661	2103.42026	817.87394	1
72	O	76.18166	70.54983	71.76958	-554.84278	14.12789	399.58769	1
73	H	75.67231	69.64724	71.79659	1297.06236	2061.84854	1220.68812	1
74	C	76.24618	70.65219	74.79662	-662.15484	-412.13544	123.62687	1
75	O	75.30632	70.22452	75.42277	-540.01537	-317.05804	274.91456	1
76	N	76.71187	71.91387	74.78123	-202.76299	-690.00100	-131.49145	1
77	H	77.50785	72.02459	74.15396	-702.62132	-2617.37191	281.70413	1
78	C	75.89785	73.07004	75.16348	-491.73914	576.34187	222.73509	1
79	H	76.52553	73.92780	74.82070	1977.17978	-1823.58850	-434.68928	1
80	C	74.55842	72.99961	74.45740	-649.50797	-328.66843	306.11224	1
81	H	74.08349	72.02876	74.73584	2075.07803	1452.16490	-1004.45904	1
82	C	73.63086	74.12901	74.86752	-615.18735	-489.99689	-70.96352	1
83	H	72.64877	74.08191	74.32168	-1226.32661	-1724.38906	-1716.47170	1
84	H	73.40351	74.10189	75.97925	2381.64273	-969.84735	900.46860	1
85	H	74.08753	75.13244	74.64877	2122.74991	1702.23946	-141.36228	1
86	C	74.71182	73.02604	72.94720	-501.86074	-479.61276	-376.42482	1
87	H	73.71621	72.97715	72.42677	993.79261	-2246.95401	-1177.81305	1
88	H	75.22104	73.96740	72.60096	42.71279	-626.15391	-2651.37258	1
89	H	75.33071	72.14789	72.57021	-2026.39012	-1590.33709	-887.82922	1
90	C	75.74023	73.05441	76.81257	-672.89153	382.57394	-156.34072	1
91	O	74.74614	73.49817	77.35216	410.04627	221.86223	500.35950	1
92	N	76.85581	72.63695	77.38566	-378.11782	-443.79414	-441.10984	1
93	H	77.57271	72.33528	76.73011	2404.15973	-568.14894	1149.30085	1
94	C	76.81818	72.30826	78.77693	-544.54484	466.16019	331.29119	1
95	H	75.94500	72.88999	79.15333	-1409.80988	-170.17955	2325.32679	1
96	C	76.54561	70.74764	78.84633	-184.48284	116.78282	-758.89137	1
97	H	75.55221	70.49771	78.40826	1893.78641	1861.14652	611.04528	1

98	H	77.27995	70.18649	78.22522	-2170.79665	-974.19311	1327.50117	1
99	C	76.63314	70.31979	80.34440	389.51668	672.81878	-138.49152	1
100	H	77.51468	70.79444	80.83028	510.64577	1933.03327	1851.02484	1
101	H	75.76638	70.72261	80.91302	-2302.30869	-1105.72939	-948.89774	1
102	C	76.72649	68.75817	80.52867	-559.93427	-126.34590	542.30857	1
103	O	76.94750	68.30336	81.62084	-670.36003	-111.83166	76.36448	1
104	N	76.53802	68.05143	79.39153	-216.06729	-537.07037	446.51379	1
105	H	76.25606	68.37292	78.45810	-1251.96487	1074.12894	-2168.52500	1
106	H	76.48606	67.02747	79.35980	-2451.83023	-720.73851	944.84612	1
107	C	78.22859	72.80937	79.43857	546.24052	-563.88337	-85.11809	1
108	O	78.13165	73.79526	80.12472	71.70702	-307.40463	606.69673	1
109	N	79.32578	72.08219	79.18027	479.90863	-504.50129	222.86849	1
110	C	80.61279	72.57342	79.56890	75.51268	-600.91904	506.73700	1
111	H	80.47685	73.20265	80.47919	-2033.61562	1795.30103	254.89480	1
112	C	81.40652	71.20681	79.77018	523.79067	517.99274	284.45581	1
113	H	82.51066	71.34254	79.78105	1599.61665	-1127.00911	1895.98173	1
114	H	81.13295	70.71436	80.72994	-1881.83093	1275.82488	-1501.55016	1
115	C	80.89330	70.38944	78.54685	-600.05639	-404.05026	316.64485	1
116	H	81.39875	70.71632	77.61058	-2597.05260	496.36221	657.73249	1
117	H	81.06858	69.29422	78.63982	-1666.24518	1294.38985	-1723.90591	1
118	C	79.35128	70.77850	78.53284	493.57570	-129.95376	-602.56394	1
119	H	78.90978	70.89905	77.51582	-1469.08415	-637.84797	2204.22581	1
120	H	78.70345	70.10798	79.14649	-1038.97840	1068.88701	-2280.71789	1
121	C	81.24541	73.39261	78.30248	188.88100	241.05089	-727.87821	1
122	O	80.89583	73.18526	77.14557	531.88613	-49.19943	427.07960	1
123	N	82.19506	74.18575	78.74419	708.14833	26.93417	-179.73509	1
124	H	82.29918	74.16220	79.75709	-2232.69501	-1179.09831	1023.94816	1
125	C	83.01989	75.04743	77.91738	-738.32412	259.92548	104.42456	1
126	H	83.81875	75.39990	78.61395	2028.89123	1260.02983	1311.33324	1
127	C	83.56045	74.24258	76.74048	-258.65678	-345.52513	661.28459	1
128	H	82.68178	73.82600	76.18811	-1826.06090	-1801.46097	-918.64554	1
129	C	84.35652	75.11507	75.78948	-541.23400	531.92970	-218.41428	1
130	H	84.67661	74.54764	74.87208	1311.73218	-2219.18200	882.19023	1
131	H	83.75800	76.00355	75.44418	-1048.71298	1223.58118	-2196.97971	1
132	H	85.28936	75.51375	76.27622	419.06414	1903.92898	1903.44670	1
133	C	84.40519	73.07022	77.20260	-423.86431	152.66566	-648.55262	1
134	H	84.76646	72.44875	76.33744	105.68386	-2342.50080	1387.51238	1
135	H	85.31480	73.41246	77.76909	-1695.63603	-1484.73621	-1531.02793	1
136	H	83.82391	72.39062	77.88510	-1853.57121	-487.39031	1936.59343	1
137	C	82.08913	76.32518	77.38484	539.71428	-510.58232	267.58633	1
138	O	82.57198	77.42704	77.42776	-15.93758	-278.34085	-624.49402	1
139	N	80.92361	75.95876	76.88301	-676.81886	12.05292	276.17960	1
140	H	80.65785	74.95530	76.84040	-1694.44250	-373.84189	-2100.66098	1
141	C	79.96791	77.02284	76.73231	412.33078	-664.70360	108.35451	1
142	H	80.09778	77.66840	77.62969	1765.77476	1294.44366	1621.76594	1
143	C	80.42551	77.77868	75.42249	-179.66635	-721.95667	-264.73915	1
144	H	81.52725	77.95071	75.46251	-607.34922	2587.87032	-598.10018	1
145	H	80.25234	77.13697	74.52945	-359.69332	-1479.13954	-2259.74260	1
146	C	79.66505	79.13964	75.28210	-240.01076	616.02425	431.85322	1
147	H	78.56839	78.98029	75.19982	-1359.17131	782.54425	2227.99181	1
148	H	79.81137	79.78166	76.17951	-820.36667	85.81767	-2596.78715	1
149	C	80.23473	79.83977	73.98346	-513.07015	236.18570	-551.87280	1
150	H	81.23968	80.27648	74.18555	1816.11944	-1183.11722	-1650.94321	1
151	H	80.39056	79.09189	73.17268	-1800.04429	-1361.53473	1526.34643	1
152	C	79.24291	80.92970	73.51225	726.08972	-253.19732	-179.64713	1
153	H	78.30012	80.54086	73.06947	1224.27271	-456.51798	-2390.90304	1
154	H	79.01749	81.71432	74.26485	1206.40339	-1150.93514	-2154.90344	1
155	N	79.92154	81.70668	72.33233	329.70796	-633.68968	-155.67358	1
156	H	79.33964	82.48800	71.91324	1348.31305	1938.76845	1359.00643	1
157	H	80.82749	82.21495	72.54897	2096.92035	1446.54551	-966.48890	1
158	H	80.18187	81.15180	71.46599	-1197.07217	-2303.53719	827.28733	1
159	C	78.46917	76.39519	76.54107	-378.01186	-556.17301	-413.96481	1

160	O	78.23168	75.44412	75.83478	-409.44433	-307.55053	-453.30833	1
161	N	77.61335	77.19561	77.16909	-429.02477	524.70884	274.08502	1
162	H	77.97561	78.00052	77.67838	1706.34263	-1425.96036	1574.38926	1
163	C	76.22028	76.92240	77.10054	-45.25864	-626.22952	478.93267	1
164	H	76.16492	75.88854	76.68370	1988.63164	570.90773	1772.87287	1
165	C	75.64124	77.08733	78.56340	551.77128	-20.49526	-564.54996	1
166	H	76.29054	76.57449	79.30907	1434.61535	-1753.10253	1513.99471	1
167	H	75.63747	78.16346	78.85195	-714.67738	1819.09770	1898.36494	1
168	C	74.18823	76.50991	78.59256	446.99263	-555.77305	338.97221	1
169	H	73.58526	76.92613	77.75169	1953.68466	1892.25957	-161.67766	1
170	H	74.18861	75.40080	78.46155	-403.03785	2688.07032	-188.43591	1
171	C	73.57695	76.94187	79.98611	567.86262	335.74681	434.04421	1
172	H	74.12990	76.46516	80.82824	-1080.02275	1568.26081	-1948.78900	1
173	H	73.69230	78.04101	80.14227	-919.54108	2111.34692	1456.13463	1
174	C	72.08026	76.55630	80.01721	195.81897	173.33862	-745.11536	1
175	H	71.46540	77.02583	79.22339	1405.67949	-2301.21089	-390.08113	1
176	H	71.87859	75.46709	80.06065	-940.37328	-1118.32446	2299.72133	1
177	N	71.50620	77.13784	81.35348	319.26422	656.36007	-42.02424	1
178	H	70.47065	76.99237	81.53715	1961.03633	619.91968	1787.09422	1
179	H	71.93610	76.78034	82.25532	854.14343	-2156.80752	1429.08711	1
180	H	71.59897	78.18702	81.47766	1237.02905	-1378.50857	-1998.28500	1
181	C	75.52485	78.06244	76.13971	532.53319	-268.57236	517.55729	1
182	O	74.40729	78.51708	76.36209	266.16714	-290.73804	-558.88002	1
183	N	76.33642	78.31021	75.13704	-226.25352	640.49678	-270.32839	1
184	H	77.18155	77.74275	75.17212	2007.69063	-1035.27229	1523.50231	1
185	C	76.03806	79.16565	74.04622	-540.76542	-573.33303	49.50000	1
186	H	76.91430	79.03287	73.37482	-2374.20950	-1036.76023	843.75774	1
187	C	74.67932	78.63713	73.38654	-77.09082	666.87422	-415.84136	1
188	H	73.85706	78.67624	74.15508	-985.81834	617.19825	2463.91927	1
189	O	74.69810	77.27553	72.91634	293.29899	-391.65602	-477.80926	1
190	H	74.01947	76.87188	73.49334	2528.72714	-681.76262	-751.27122	1
191	C	74.43172	79.73932	72.29325	252.47363	-605.14473	440.05134	1
192	H	73.46408	79.57858	71.76439	-2052.65063	1456.49051	-1043.51830	1
193	H	74.40000	80.75910	72.73830	-2152.98800	-1661.97574	-161.70652	1
194	H	75.23613	79.73794	71.52177	-473.12726	-1584.27339	2165.61725	1
195	C	75.90970	80.70826	74.58709	360.36307	488.46713	505.10056	1
196	O	76.77826	81.48236	74.26334	-200.08817	-528.03552	-385.82850	1
197	N	74.79389	80.92695	75.27228	-597.54095	-226.44775	355.20479	1
198	H	74.22827	80.09946	75.57810	2179.23655	-1300.70981	-991.33835	1
199	C	74.64844	82.14928	75.97183	-687.68921	297.39807	-249.45179	1
200	H	73.66451	82.03819	76.47800	-349.16256	-2467.37713	-1101.72831	1
201	C	75.87273	82.30017	76.99008	672.47345	361.54328	-201.62880	1
202	H	76.83029	82.03323	76.48154	1541.41502	582.18425	2169.97026	1
203	H	75.96402	83.36850	77.30424	-2534.67717	60.25153	997.72295	1
204	C	75.63369	81.41727	78.22619	574.26774	-389.43119	-377.02542	1
205	C	74.38102	81.49834	78.90608	688.82679	-287.33580	-257.96133	1
206	H	73.57999	82.16513	78.53872	331.14182	1470.38163	2269.80013	1
207	C	76.66611	80.56788	78.72462	-383.52382	-675.04808	144.24917	1
208	H	77.64071	80.50421	78.20796	4.09847	1517.59662	2262.86397	1
209	C	74.18198	80.72299	80.04775	-134.76730	428.45285	-649.50303	1
210	H	73.20707	80.78345	80.56248	-903.23433	1600.49020	2011.53387	1
211	C	76.42786	79.82633	79.88728	-335.53281	-615.00040	-364.39058	1
212	H	77.23788	79.18130	80.27070	1596.45398	-1369.33862	1732.02659	1
213	C	75.18554	79.86716	80.58582	585.48547	-340.24194	-406.23938	1
214	O	74.91967	79.09898	81.75193	-419.15649	-173.04408	-511.94141	1
215	H	75.81046	78.70080	81.89282	-1071.84350	1559.71507	-1960.13012	1
216	C	74.75051	83.48990	75.04399	291.41878	-183.13091	710.72246	1
217	O	75.19655	84.51509	75.51504	379.87695	523.47396	-222.23622	1
218	N	74.13810	83.37206	73.81859	564.30591	373.09380	277.24371	1
219	H	73.99583	82.35582	73.77126	-120.59931	-2436.07824	-1214.35098	1
220	C	74.84291	84.09547	72.77975	404.07514	-299.37480	608.84009	1
221	H	75.66287	84.63637	73.30537	-1071.07882	-841.69025	2359.66467	1

222	C	75.37619	83.02937	71.74839	-683.12807	68.71770	-390.13096	1
223	H	75.97502	82.24125	72.26306	2068.88918	1596.58590	770.89603	1
224	H	74.52313	82.49856	71.26812	1379.86429	2342.49779	-179.85638	1
225	C	76.23855	83.77100	70.67716	-176.39967	537.49466	550.97268	1
226	H	75.72182	84.70858	70.34103	-396.28051	1942.22168	1869.33314	1
227	H	77.20974	84.10524	71.10641	-94.44700	586.00678	-2659.20016	1
228	C	76.46003	82.77981	69.44572	-291.69381	-718.18079	-150.72929	1
229	H	77.19400	81.95019	69.60967	-2303.38776	1089.76242	964.62032	1
230	H	75.52958	82.33632	69.00745	884.16729	2568.80533	-207.74283	1
231	N	76.98737	83.66985	68.49567	-594.49522	-252.81478	342.29276	1
232	H	77.08162	84.63445	68.77450	-1735.17426	2084.05705	-263.71605	1
233	C	77.33955	83.35349	67.31589	595.23177	-271.52487	442.22352	1
234	N	77.20783	82.01565	66.92828	585.53813	-424.79750	-105.81303	1
235	H	76.85802	81.21963	67.45992	959.88797	1327.56823	-2177.11905	1
236	H	77.45504	81.64763	66.00902	1578.48647	16.27378	-2220.76233	1
237	N	77.81077	84.47244	66.61325	-452.17763	-390.33541	-421.51853	1
238	H	77.88998	85.44959	66.89051	470.26107	1974.25629	-1817.92087	1
239	H	78.12780	84.43130	65.64409	1856.67307	-1573.97321	-1224.35416	1
240	C	73.83081	85.10718	72.02066	-531.47271	-581.45780	-55.06206	1
241	O	74.27202	85.86761	71.17611	-243.00837	192.73507	609.52485	1
242	N	72.55621	84.94604	72.36234	343.49288	-644.25607	38.09164	1
243	H	72.34852	84.27677	73.10261	-1691.16043	-1535.97525	-1484.73099	1
244	C	71.60357	85.78999	71.71747	542.66492	350.14337	454.42563	1
245	H	72.17583	86.71034	71.45828	1209.57979	-2396.95920	463.86744	1
246	C	71.07870	85.02945	70.42148	-737.14309	145.93010	242.71942	1
247	H	70.74046	84.00451	70.68471	-1050.18303	159.36419	-2509.06125	1
248	C	69.90882	85.86404	69.79780	-706.77696	-252.88343	-245.16230	1
249	H	69.49445	85.37558	68.88478	-1624.64039	-1665.49085	1417.86935	1
250	H	69.06711	85.99102	70.51941	2566.10521	598.51109	693.22305	1
251	H	70.24627	86.88607	69.50535	-1972.69758	107.10018	-1876.34312	1
252	C	72.22576	84.97506	69.35617	412.85148	672.58832	-27.69222	1
253	H	71.91556	84.42147	68.43882	1447.02277	1762.76533	-1490.78944	1
254	H	72.53640	85.99903	69.04101	1320.77379	-145.20455	2378.68491	1
255	H	73.13629	84.47238	69.76441	-1512.10848	1470.52031	1724.75147	1
256	C	70.30859	86.03309	72.68810	-607.11113	499.56689	73.73769	1
257	O	69.84318	87.14259	72.80378	357.97126	460.81534	356.68785	1
258	N	69.81476	84.87565	73.13237	536.55407	-368.62270	332.76306	1
259	H	70.33969	84.02261	72.93968	524.38866	2297.69985	1367.20941	1
260	C	68.91782	84.93148	74.22792	46.50277	-774.29190	-147.97904	1
261	H	68.73458	86.01644	74.40464	1676.51875	1883.29066	1032.55549	1
262	C	67.58368	84.09782	73.85988	-559.41456	-34.19198	-556.30433	1
263	H	67.84156	83.01622	73.76604	-64.66664	395.18769	2695.05373	1
264	H	66.84437	84.16353	74.69335	-2703.44278	-60.40056	333.79418	1
265	C	66.99116	84.60283	72.57212	-519.76435	377.31045	459.42366	1
266	H	67.78358	84.57290	71.79029	-1746.74323	1667.50644	-1261.73691	1
267	C	65.83948	83.70866	72.12906	570.95554	16.46261	-545.27700	1
268	H	65.39015	84.05889	71.16418	2391.58273	28.05277	-1305.07271	1
269	H	66.17219	82.64984	71.97543	175.75588	917.63458	2559.43867	1
270	H	65.01647	83.68969	72.88905	-1063.97851	-2155.34650	1283.00462	1
271	C	66.50115	86.03837	72.70466	193.76014	2.62946	-765.53141	1
272	H	66.00622	86.39505	71.76455	507.39394	-846.55087	2539.60089	1
273	H	65.75438	86.14559	73.53333	1337.57841	1818.19054	1526.01994	1
274	H	67.34637	86.74308	72.92068	1100.88635	-1172.91350	-2199.08909	1
275	C	69.65247	84.15444	75.44055	-549.21115	475.64486	-309.38218	1
276	O	70.45461	83.27434	75.26857	556.06106	-390.37755	-78.24250	1
277	O	69.18811	84.46573	76.73921	-572.27940	-310.19032	-209.75862	1
278	H	68.55724	85.20297	76.50532	-1380.08193	2212.14486	790.85944	1

Listing 26: C00026.xmolout

1	276							
2	150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100

		0.2500	300.00	0.00	0.00	0.00	-1293.9554	0.0000	300.0000	
3	H	72.57283	88.15144	73.34531	-2043.14101	-1757.64893		399.89339		1
4	N	73.38582	87.87093	72.80265	426.75047	490.45733		-334.42467		1
5	H	72.96830	87.50991	71.94767	442.25559	-1110.30854		-2448.52907		1
6	C	74.37926	88.85863	72.63170	415.32972	-666.39213		83.73172		1
7	H	74.41333	89.36381	73.62059	879.32219	2491.00447		667.35213		1
8	C	75.77006	88.12568	72.27449	31.35357	477.41777		628.23362		1
9	H	75.64421	87.52141	71.34449	1168.38489	2240.25337		-1019.71136		1
10	H	76.56247	88.88015	72.05069	-360.43770	2534.90498		931.67112		1
11	C	76.16563	87.24679	73.43245	463.18208	512.70242		-382.34388		1
12	H	75.26959	86.66799	73.74814	1725.29117	1863.52247		-987.07854		1
13	C	77.25055	86.26173	73.01591	710.42801	-144.27427		-313.15367		1
14	H	77.54190	85.58637	73.86139	364.20195	-1033.13725		2494.72524		1
15	H	76.91510	85.60878	72.16934	2567.61904	335.80679		847.48802		1
16	H	78.17936	86.79107	72.68013	-2587.99029	680.92867		-512.16411		1
17	C	76.65411	88.07007	74.61670	268.17616	741.64379		-40.42634		1
18	H	76.96996	87.41763	75.47129	1283.54314	-1945.37420		-1411.27812		1
19	H	77.53554	88.70500	74.34173	-1258.57796	1317.15249		-2026.02085		1
20	H	75.85866	88.75760	75.00305	-2502.84526	909.80597		575.92391		1
21	C	74.00458	89.88902	71.44395	619.36578	-458.64843		-172.09273		1
22	O	74.90037	90.59616	70.96381	-81.40433	433.87611		522.34594		1
23	N	72.72809	89.87916	71.17085	175.23996	-622.20190		341.55523		1
24	H	72.17179	89.25105	71.74788	-876.57256	-303.22879		-2561.90213		1
25	C	72.04889	90.61246	70.15074	-571.88214	-534.10783		-106.15033		1
26	H	71.27402	91.16872	70.72337	-2713.20841	-16.25800		-248.80809		1
27	C	73.02143	91.59010	69.35604	166.60354	288.16399		-716.09568		1
28	H	73.89595	90.99173	68.95796	-2097.85574	1636.78449		-586.18044		1
29	O	73.65479	92.61364	70.12761	-317.80580	-363.38227		484.43082		1
30	H	74.47592	92.07533	70.45711	1863.74748	-1451.84923		1357.29467		1
31	C	72.09646	92.06014	68.17489	503.80731	517.99032		318.51606		1
32	H	72.65886	92.67947	67.43825	640.61020	-2157.10410		-1536.29104		1
33	H	71.65633	91.19839	67.62002	1687.88455	465.60692		2087.56452		1
34	H	71.24829	92.68014	68.54765	-1293.07895	-1899.88581		-1463.57452		1
35	C	71.25908	89.45544	69.30514	-153.07550	-733.68902		248.70981		1
36	O	70.09228	89.34938	69.58247	186.15459	-480.78787		-449.34387		1
37	N	71.98112	88.74568	68.42638	-487.53139	543.18517		42.03850		1
38	C	71.38906	87.63986	67.73641	-699.35871	69.34393		360.10701		1
39	H	70.32607	87.92070	67.55601	2.81126	-221.99807		-2715.58072		1
40	C	72.32233	87.52868	66.45897	-507.46439	-592.59194		122.07761		1
41	H	72.25485	86.53718	65.95785	-1975.08116	525.87560		-1801.71556		1
42	H	72.06200	88.29438	65.69435	1588.27743	-1913.22100		1113.83566		1
43	C	73.72271	87.80715	67.09018	-613.62442	-457.55993		-194.14490		1
44	H	74.10133	86.90442	67.62453	1707.54637	-721.27992		1996.92523		1
45	H	74.50116	88.08688	66.34485	758.23357	2100.81767		1560.55011		1
46	C	73.38286	88.97783	68.10874	-352.41524	704.96076		49.21465		1
47	H	73.95356	88.95904	69.06788	1714.76886	-2070.42778		443.35792		1
48	H	73.43776	89.99864	67.66135	1224.15040	1801.50881		1636.97633		1
49	C	71.54589	86.31957	68.70516	566.85117	537.05831		117.62814		1
50	O	72.57824	85.65422	68.68068	-550.26779	-406.08867		4.21666		1
51	N	70.46855	86.18433	69.43717	566.34832	-425.77725		180.18749		1
52	H	69.79336	86.93876	69.30641	644.44502	2646.80550		-52.73430		1
53	C	70.10698	85.01923	70.16165	612.34801	-281.48662		411.56221		1
54	H	69.03745	85.19385	70.41636	1667.23498	-1490.75142		1556.16753		1
55	C	70.32893	83.73138	69.22468	-714.45746	-175.43074		286.98927		1
56	H	71.39468	83.72431	68.86030	-787.09484	1763.03619		-1922.46060		1
57	O	69.50484	83.65959	68.05312	-429.46514	516.51932		-128.40526		1
58	H	70.18198	83.67698	67.34473	1981.82785	436.16847		-1818.18182		1
59	C	70.14873	82.58961	70.28978	630.79189	-468.94448		76.03230		1
60	H	70.42303	81.59193	69.87413	-1775.71861	2062.30353		131.89849		1
61	H	70.79653	82.76957	71.18818	-1855.14608	88.94118		1993.53760		1
62	H	69.09428	82.52496	70.64638	-1504.82350	-780.94249		-2132.90992		1
63	C	71.01926	84.82771	71.49874	288.57638	618.62814		-397.00270		1

64	O	70.43462	84.66409	72.56818	321.70495	-185.26452	574.37218	1
65	N	72.29726	84.82772	71.24359	-447.05792	-446.53431	367.76425	1
66	H	72.63562	84.98469	70.25942	350.31316	1975.63644	-1843.31522	1
67	C	73.24373	84.45682	72.24065	-511.23061	374.03917	-471.51480	1
68	H	74.17535	84.89208	71.81129	2234.79579	-898.70890	-1273.45190	1
69	C	72.80314	85.13519	73.61579	529.53781	-159.34528	563.72604	1
70	H	73.72923	85.45810	74.16324	654.59388	2347.94251	1217.51488	1
71	H	72.23359	86.06453	73.34661	-1526.55661	2103.42026	817.87394	1
72	O	72.00504	84.36042	74.53331	-554.84278	14.12789	399.58769	1
73	H	71.11497	84.39442	74.00905	1297.06236	2061.84854	1220.68812	1
74	C	73.32718	82.83173	72.30189	-662.15484	-412.13544	123.62687	1
75	O	72.97584	82.11373	71.36860	-540.01537	-317.05804	274.91456	1
76	N	73.93940	82.49147	73.41806	-202.76299	-690.00100	-131.49145	1
77	H	74.13004	83.28229	74.03146	-702.62132	-2617.37191	281.70413	1
78	C	73.93745	81.17246	73.94474	-491.73914	576.34187	222.73509	1
79	H	74.29971	81.31044	74.98722	1977.17978	-1823.58850	-434.68928	1
80	C	72.45203	80.60377	73.87251	-649.50797	-328.66843	306.11224	1
81	H	71.98996	80.81929	72.88269	2075.07803	1452.16490	-1004.45904	1
82	C	72.45763	79.06681	74.17061	-615.18735	-489.99689	-70.96352	1
83	H	71.42350	78.65091	74.21440	-1226.32661	-1724.38906	-1716.47170	1
84	H	73.01601	78.48861	73.38153	2381.64273	-969.84735	900.46860	1
85	H	72.94489	78.84959	75.14825	2122.74991	1702.23946	-141.36228	1
86	C	71.64422	81.28909	75.02629	-501.86074	-479.61276	-376.42482	1
87	H	70.56794	80.99643	75.00923	993.79261	-2246.95401	-1177.81305	1
88	H	72.04841	81.01501	76.02934	42.71279	-626.15391	-2651.37258	1
89	H	71.69517	82.41134	74.93926	-2026.39012	-1590.33709	-887.82922	1
90	C	74.94955	80.21076	73.08491	-672.89153	382.57394	-156.34072	1
91	O	75.95300	79.82135	73.64103	410.04627	221.86223	500.35950	1
92	N	74.50209	79.98371	71.86903	-378.11782	-443.79414	-441.10984	1
93	H	73.66462	80.51061	71.52252	2404.15973	-568.14894	1149.30085	1
94	C	75.08020	78.96187	71.04759	-544.54484	466.16019	331.29119	1
95	H	74.37252	78.98805	70.18815	-1409.80988	-170.17955	2325.32679	1
96	C	76.50516	79.51072	70.61166	-184.48284	116.78282	-758.89137	1
97	H	76.41915	80.55743	70.24143	1893.78641	1861.14652	611.04528	1
98	H	77.18721	79.57456	71.48983	-2170.79665	-974.19311	1327.50117	1
99	C	77.06448	78.57623	69.49399	389.51668	672.81878	-138.49152	1
100	H	76.96442	77.50706	69.78612	510.64577	1933.03327	1851.02484	1
101	H	76.43835	78.65660	68.57813	-2302.30869	-1105.72939	-948.89774	1
102	C	78.56753	78.88998	69.14037	-559.93427	-126.34590	542.30857	1
103	O	79.14808	78.19501	68.34680	-670.36003	-111.83166	76.36448	1
104	N	79.07580	79.95914	69.79091	-216.06729	-537.07037	446.51379	1
105	H	78.61960	80.60683	70.44390	-1251.96487	1074.12894	-2168.52500	1
106	H	80.02476	80.31955	69.64438	-2451.83023	-720.73851	944.84612	1
107	C	74.97570	77.53139	71.79998	546.24052	-563.88337	-85.11809	1
108	O	73.82906	77.16535	72.04973	71.70702	-307.40463	606.69673	1
109	N	76.10881	76.89212	72.06025	479.90863	-504.50129	222.86849	1
110	C	76.19260	75.45433	72.13444	75.51268	-600.91904	506.73700	1
111	H	75.62850	75.07109	71.25320	-2033.61562	1795.30103	254.89480	1
112	C	77.75938	75.19288	72.13833	523.79067	517.99274	284.45581	1
113	H	78.02455	74.19927	72.56997	1599.61665	-1127.00911	1895.98173	1
114	H	78.19248	75.23230	71.11355	-1881.83093	1275.82488	-1501.55016	1
115	C	78.25100	76.38899	73.01196	-600.05639	-404.05026	316.64485	1
116	H	78.03276	76.21548	74.09004	-2597.05260	496.36221	657.73249	1
117	H	79.34396	76.58604	72.93176	-1666.24518	1294.38985	-1723.90591	1
118	C	77.35735	77.55673	72.41153	493.57570	-129.95376	-602.56394	1
119	H	77.08848	78.39904	73.12480	-1469.08415	-637.84797	2204.22581	1
120	H	77.76807	77.98317	71.46384	-1038.97840	1068.88701	-2280.71789	1
121	C	75.66689	74.83167	73.53839	188.88100	241.05089	-727.87821	1
122	O	76.34186	74.01105	74.10583	531.88613	-49.19943	427.07960	1
123	N	74.46442	75.28991	73.89198	708.14833	26.93417	-179.73509	1
124	H	73.95394	75.95597	73.25498	-2232.69501	-1179.09831	1023.94816	1
125	C	73.79679	74.68669	75.05118	-738.32412	259.92548	104.42456	1

126	H	74.66652	74.29727	75.63499	2028.89123	1260.02983	1311.33324	1
127	C	72.99891	75.76824	75.75444	-258.65678	-345.52513	661.28459	1
128	H	72.30657	76.22848	75.01413	-1826.06090	-1801.46097	-918.64554	1
129	C	72.16982	75.20428	76.89004	-541.23400	531.92970	-218.41428	1
130	H	71.70079	76.01524	77.51310	1311.73218	-2219.18200	882.19023	1
131	H	71.33436	74.55221	76.50174	-1048.71298	1223.58118	-2196.97971	1
132	H	72.80597	74.55132	77.58454	419.06414	1903.92898	1903.44670	1
133	C	73.91379	76.86375	76.27451	-423.86431	152.66566	-648.55262	1
134	H	73.33720	77.69261	76.76927	105.68386	-2342.50080	1387.51238	1
135	H	74.63961	76.46483	77.03522	-1695.63603	-1484.73621	-1531.02793	1
136	H	74.52230	77.31848	75.44352	-1853.57121	-487.39031	1936.59343	1
137	C	72.85047	73.44910	74.47549	539.71428	-510.58232	267.58633	1
138	O	71.65159	73.45213	74.62113	-15.93758	-278.34085	-624.49402	1
139	N	73.60493	72.53497	73.88208	-676.81886	12.05292	276.17960	1
140	H	74.61281	72.70783	73.87967	-1694.44250	-373.84189	-2100.66098	1
141	C	73.03239	71.26158	73.62399	412.33078	-664.70360	108.35451	1
142	H	71.92973	71.40219	73.71823	1765.77476	1294.44366	1621.76594	1
143	C	73.55136	70.75841	72.21690	-179.66635	-721.95667	-264.73915	1
144	H	73.18693	71.41435	71.39471	-607.34922	2587.87032	-598.10018	1
145	H	74.66298	70.80474	72.17446	-359.69332	-1479.13954	-2259.74260	1
146	C	73.04910	69.28668	72.04005	-240.01076	616.02425	431.85322	1
147	H	73.40225	68.66341	72.89517	-1359.17131	782.54425	2227.99181	1
148	H	71.93725	69.23883	72.05761	-820.36667	85.81767	-2596.78715	1
149	C	73.61755	68.72175	70.67708	-513.07015	236.18570	-551.87280	1
150	H	73.24562	69.31631	69.81121	1816.11944	-1183.11722	-1650.94321	1
151	H	74.72855	68.80305	70.64786	-1800.04429	-1361.53473	1526.34643	1
152	C	73.17456	67.24400	70.56717	726.08972	-253.19732	-179.64713	1
153	H	73.58556	66.58039	71.35401	1224.27271	-456.51798	-2390.90304	1
154	H	72.07975	67.09518	70.48090	1206.40339	-1150.93514	-2154.90344	1
155	N	73.75824	66.67408	69.23061	329.70796	-633.68968	-155.67358	1
156	H	73.53013	65.65837	69.02658	1348.31305	1938.76845	1359.00643	1
157	H	73.44863	67.14182	68.32955	2096.92035	1446.54551	-966.48890	1
158	H	74.81464	66.67488	69.12686	-1197.07217	-2303.53719	827.28733	1
159	C	73.68606	70.21778	74.72783	-378.01186	-556.17301	-413.96481	1
160	O	74.72653	69.64508	74.47987	-409.44433	-307.55053	-453.30833	1
161	N	72.92934	70.16163	75.80972	-429.02477	524.70884	274.08502	1
162	H	72.09339	70.74569	75.81508	1706.34263	-1425.96036	1574.38926	1
163	C	73.25264	69.33305	76.91909	-45.25864	-626.22952	478.93267	1
164	H	72.27852	69.18180	77.43563	1988.63164	570.90773	1772.87287	1
165	C	73.89054	68.00670	76.36381	551.77128	-20.49526	-564.54996	1
166	H	73.32031	67.64504	75.47951	1434.61535	-1753.10253	1513.99471	1
167	H	74.92651	68.20339	75.98609	-714.67738	1819.09770	1898.36494	1
168	C	73.92279	66.90161	77.50752	446.99263	-555.77305	338.97221	1
169	H	74.52061	67.28283	78.37740	1953.68466	1892.25957	-161.67766	1
170	H	72.89262	66.70640	77.89636	-403.03785	2688.07032	-188.43591	1
171	C	74.53588	65.64324	76.93243	567.86262	335.74681	434.04421	1
172	H	73.85530	65.21240	76.16342	-1080.02275	1568.26081	-1948.78900	1
173	H	75.46800	65.90391	76.38010	-919.54108	2111.34692	1456.13463	1
174	C	74.84815	64.63624	77.94652	195.81897	173.33862	-745.11536	1
175	H	75.68859	64.91533	78.61264	1405.67949	-2301.21089	-390.08113	1
176	H	73.97893	64.29864	78.54682	-940.37328	-1118.32446	2299.72133	1
177	N	75.35958	63.30937	77.29535	319.26422	656.36007	-42.02424	1
178	H	75.61331	62.56047	78.00634	1961.03633	619.91968	1787.09422	1
179	H	74.69347	62.77761	76.66174	854.14343	-2156.80752	1429.08711	1
180	H	76.24595	63.36101	76.71265	1237.02905	-1378.50857	-1998.28500	1
181	C	74.32919	70.10267	77.90993	532.53319	-268.57236	517.55729	1
182	O	74.37511	69.77167	79.07021	266.16714	-290.73804	-558.88002	1
183	N	75.05556	70.98877	77.25088	-226.25352	640.49678	-270.32839	1
184	H	74.86259	71.05583	76.24914	2007.69063	-1035.27229	1523.50231	1
185	C	75.93756	71.91390	77.87228	-540.76542	-573.33303	49.50000	1
186	H	76.19377	72.59180	77.02693	-2374.20950	-1036.76023	843.75774	1
187	C	75.14918	72.65957	79.03248	-77.09082	666.87422	-415.84136	1

188	H	74.78817	71.90089	79.78058	-985.81834	617.19825	2463.91927	1
189	O	73.93690	73.37493	78.62851	293.29899	-391.65602	-477.80926	1
190	H	73.26781	72.84283	79.09628	2528.72714	-681.76262	-751.27122	1
191	C	76.26880	73.55916	79.66026	252.47363	-605.14473	440.05134	1
192	H	75.91394	74.06429	80.58874	-2052.65063	1456.49051	-1043.51830	1
193	H	77.17809	72.97141	79.92816	-2152.98800	-1661.97574	-161.70652	1
194	H	76.59225	74.35718	78.95194	-473.12726	-1584.27339	2165.61725	1
195	C	77.26611	71.07899	78.36866	360.36307	488.46713	505.10056	1
196	O	78.13676	70.86486	77.55845	-200.08817	-528.03552	-385.82850	1
197	N	77.24462	70.74712	79.65520	-597.54095	-226.44775	355.20479	1
198	H	76.41720	70.93023	80.22134	2179.23655	-1300.70981	-991.33835	1
199	C	78.36079	70.05570	80.16753	-687.68921	297.39807	-249.45179	1
200	H	79.05085	69.88508	79.30660	-349.16256	-2467.37713	-1101.72831	1
201	C	78.97622	70.83147	81.42965	672.47345	361.54328	-201.62880	1
202	H	78.18492	70.97836	82.20237	1541.41502	582.18425	2169.97026	1
203	H	79.76281	70.19558	81.89817	-2534.67717	60.25153	997.72295	1
204	C	79.57982	72.16954	80.98438	574.26774	-389.43119	-377.02542	1
205	C	80.72702	72.16512	80.13457	688.82679	-287.33580	-257.96133	1
206	H	81.16755	71.21367	79.78522	331.14182	1470.38163	2269.80013	1
207	C	79.01118	73.40124	81.42851	-383.52382	-675.04808	144.24917	1
208	H	78.12318	73.40697	82.08618	4.09847	1517.59662	2262.86397	1
209	C	81.27957	73.38702	79.75416	-134.76730	428.45285	-649.50303	1
210	H	82.16779	73.38416	79.09833	-903.23433	1600.49020	2011.53387	1
211	C	79.60151	74.59907	81.01887	-335.53281	-615.00040	-364.39058	1
212	H	79.15589	75.54625	81.36924	1596.45398	-1369.33862	1732.02659	1
213	C	80.75005	74.64123	80.17571	585.48547	-340.24194	-406.23938	1
214	O	81.35788	75.85341	79.75727	-419.15649	-173.04408	-511.94141	1
215	H	80.78528	76.49970	80.23394	-1071.84350	1559.71507	-1960.13012	1
216	C	77.82848	68.71705	80.96735	291.41878	-183.13091	710.72246	1
217	O	77.48472	68.79323	82.12334	379.87695	523.47396	-222.23622	1
218	N	77.93439	67.66111	80.17570	564.30591	373.09380	277.24371	1
219	H	78.17919	67.75427	79.18655	-120.59931	-2436.07824	-1214.35098	1
220	C	77.39853	66.40598	80.61176	404.07514	-299.37480	608.84009	1
221	H	77.78998	66.20713	81.63477	-1071.07882	-841.69025	2359.66467	1
222	C	75.82359	66.59904	80.63130	-683.12807	68.71770	-390.13096	1
223	H	75.53986	67.41526	81.33489	2068.88918	1596.58590	770.89603	1
224	H	75.46500	66.93709	79.62846	1379.86429	2342.49779	-179.85638	1
225	C	75.16891	65.24514	81.04312	-176.39967	537.49466	550.97268	1
226	H	75.58090	64.40257	80.44367	-396.28051	1942.22168	1869.33314	1
227	H	75.39779	64.99011	82.10158	-94.44700	586.00678	-2659.20016	1
228	C	73.59614	65.40736	80.80982	-291.69381	-718.18079	-150.72929	1
229	H	73.01813	65.82942	81.67074	-2303.38776	1089.76242	964.62032	1
230	H	73.29473	65.97066	79.89111	884.16729	2568.80533	-207.74283	1
231	N	73.21761	64.07471	80.61769	-594.49522	-252.81478	342.29276	1
232	H	73.95760	63.37788	80.70945	-1735.17426	2084.05705	-263.71605	1
233	C	72.03056	63.70934	80.33115	595.23177	-271.52487	442.22352	1
234	N	71.05530	64.69856	80.20019	585.53813	-424.79750	-105.81303	1
235	H	71.14454	65.71005	80.29623	959.88797	1327.56823	-2177.11905	1
236	H	70.07584	64.53290	79.96408	1578.48647	16.27378	-2220.76233	1
237	N	72.01407	62.31602	80.20475	-452.17763	-390.33541	-421.51853	1
238	H	72.79854	61.65592	80.24675	470.26107	1974.25629	-1817.92087	1
239	H	71.18221	61.77419	79.96326	1856.67307	-1573.97321	-1224.35416	1
240	C	77.88518	65.37285	79.45319	-531.47271	-581.45780	-55.06206	1
241	O	78.06604	65.72694	78.31149	-243.00837	192.73507	609.52485	1
242	N	77.92889	64.13670	79.95746	343.49288	-644.25607	38.09164	1
243	H	77.75930	64.05158	80.96095	-1691.16043	-1535.97525	-1484.73099	1
244	C	78.57658	63.04925	79.22930	542.66492	350.14337	454.42563	1
245	H	78.31510	63.20809	78.15725	1209.57979	-2396.95920	463.86744	1
246	C	80.06972	63.11394	79.49951	-737.14309	145.93010	242.71942	1
247	H	80.20629	63.17306	80.60241	-1050.18303	159.36419	-2509.06125	1
248	C	80.78465	61.87312	78.99711	-706.77696	-252.88343	-245.16230	1
249	H	81.88517	61.90521	79.22889	-1624.64039	-1665.49085	1417.86935	1

250	H	80.37140	60.93820	79.46668	2566.10521	598.51109	693.22305	1
251	H	80.68238	61.75868	77.88263	-1972.69758	107.10018	-1876.34312	1
252	C	80.70088	64.35049	78.88659	412.85148	672.58832	-27.69222	1
253	H	81.76977	64.48187	79.21224	1447.02277	1762.76533	-1490.78944	1
254	H	80.69724	64.30091	77.76279	1320.77379	-145.20455	2378.68491	1
255	H	80.13822	65.28547	79.17110	-1512.10848	1470.52031	1724.75147	1
256	C	77.90539	61.69435	79.93583	-607.11113	499.56689	73.73769	1
257	O	78.05467	61.48058	81.11395	357.97126	460.81534	356.68785	1
258	N	77.35189	60.94382	78.99688	536.55407	-368.62270	332.76306	1
259	H	77.41651	61.30714	78.04643	524.38866	2297.69985	1367.20941	1
260	C	76.37861	59.95771	79.31073	46.50277	-774.29190	-147.97904	1
261	H	76.30469	59.36874	78.36988	1676.51875	1883.29066	1032.55549	1
262	C	76.83028	59.08389	80.58862	-559.41456	-34.19198	-556.30433	1
263	H	76.70744	59.71638	81.50321	-64.66664	395.18769	2695.05373	1
264	H	76.14439	58.21370	80.72531	-2703.44278	-60.40056	333.79418	1
265	C	78.26265	58.63147	80.48085	-519.76435	377.31045	459.42366	1
266	H	78.88519	59.53003	80.26034	-1746.74323	1667.50644	-1261.73691	1
267	C	78.72856	58.04479	81.80808	570.95554	16.46261	-545.27700	1
268	H	79.80231	57.72749	81.76757	2391.58273	28.05277	-1305.07271	1
269	H	78.63366	58.78918	82.64067	175.75588	917.63458	2559.43867	1
270	H	78.12679	57.14488	82.09634	-1063.97851	-2155.34650	1283.00462	1
271	C	78.46347	57.61188	79.36913	193.76014	2.62946	-765.53141	1
272	H	79.53072	57.27477	79.30749	507.39394	-846.55087	2539.60089	1
273	H	77.83647	56.69717	79.52912	1337.57841	1818.19054	1526.01994	1
274	H	78.19036	58.03345	78.36768	1100.88635	-1172.91350	-2199.08909	1
275	C	74.99008	60.67670	79.67540	-549.21115	475.64486	-309.38218	1
276	O	74.87567	61.82714	80.04641	556.06106	-390.37755	-78.24250	1
277	O	73.84961	59.84866	79.62083	-572.27940	-310.19032	-209.75862	1
278	H	74.30113	59.00354	79.32060	-1380.08193	2212.14486	790.85944	1

Listing 27: C00027.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	1.1695	4678
		0.2500	300.00	0.00	0.00	0.00	-1293.9452	0.0000	300.0000
3	H	66.79296	76.53065	74.29401	-2043.14101	-1757.64893	399.89339		1
4	N	66.68826	77.51405	74.05073	426.75047	490.45733	-334.42467		1
5	H	66.09303	77.86696	74.80431	442.25559	-1110.30854	-2448.52907		1
6	C	67.90228	78.23254	73.97682	415.32972	-666.39213	83.73172		1
7	H	68.70690	77.53404	73.65516	879.32219	2491.00447	667.35213		1
8	C	67.67988	79.45501	72.94403	31.35357	477.41777	628.23362		1
9	H	66.81731	80.07910	73.28054	1168.38489	2240.25337	-1019.71136		1
10	H	68.57090	80.12832	72.93719	-360.43770	2534.90498	931.67112		1
11	C	67.42055	78.88057	71.57714	463.18208	512.70242	-382.34388		1
12	H	66.65934	78.07379	71.67989	1725.29117	1863.52247	-987.07854		1
13	C	66.86629	79.94534	70.63913	710.42801	-144.27427	-313.15367		1
14	H	66.65025	79.52843	69.62158	364.20195	-1033.13725	2494.72524		1
15	H	65.91074	80.38331	71.02781	2567.61904	335.80679	847.48802		1
16	H	67.58820	80.79153	70.50398	-2587.99029	680.92867	-512.16411		1
17	C	68.69147	78.28700	70.98406	268.17616	741.64379	-40.42634		1
18	H	68.51567	77.86976	69.95892	1283.54314	-1945.37420	-1411.27812		1
19	H	69.50308	79.05501	70.89662	-1258.57796	1317.15249	-2026.02085		1
20	H	69.09806	77.45582	71.61628	-2502.84526	909.80597	575.92391		1
21	C	68.10150	78.82359	75.47362	619.36578	-458.64843	-172.09273		1
22	O	67.17137	79.05395	76.21440	-81.40433	433.87611	522.34594		1
23	N	69.40044	79.07210	75.65005	175.23996	-622.20190	341.55523		1
24	H	70.10597	78.84411	74.90991	-876.57256	-303.22879	-2561.90213		1
25	C	69.79696	79.40022	76.99436	-571.88214	-534.10783	-106.15033		1
26	H	68.85520	79.37780	77.59525	-2713.20841	-16.25800	-248.80809		1
27	C	70.82483	78.24824	77.40608	166.60354	288.16399	-716.09568		1
28	H	71.65144	78.23908	76.63871	-2097.85574	1636.78449	-586.18044		1
29	O	70.33120	76.87182	77.26504	-317.80580	-363.38227	484.43082		1

30	H	70.09199	76.68464	78.19075	1863.74748	-1451.84923	1357.29467	1
31	C	71.37065	78.62685	78.81902	503.80731	517.99032	318.51606	1
32	H	72.17183	77.92163	79.14611	640.61020	-2157.10410	-1536.29104	1
33	H	71.81270	79.66194	78.83964	1687.88455	465.60692	2087.56452	1
34	H	70.56879	78.58558	79.59410	-1293.07895	-1899.88581	-1463.57452	1
35	C	70.46685	80.86167	76.91275	-153.07550	-733.68902	248.70981	1
36	O	70.86464	81.32214	75.84648	186.15459	-480.78787	-449.34387	1
37	N	70.57902	81.42432	78.11249	-487.53139	543.18517	42.03850	1
38	C	71.49434	82.53051	78.26237	-699.35871	69.34393	360.10701	1
39	H	71.31823	83.18205	77.37602	2.81126	-221.99807	-2715.58072	1
40	C	71.06078	83.15189	79.65213	-507.46439	-592.59194	122.07761	1
41	H	71.91652	83.60373	80.20264	-1975.08116	525.87560	-1801.71556	1
42	H	70.31652	83.96737	79.51080	1588.27743	-1913.22100	1113.83566	1
43	C	70.42728	81.93668	80.40041	-613.62442	-457.55993	-194.14490	1
44	H	71.21588	81.26849	80.81314	1707.54637	-721.27992	1996.92523	1
45	H	69.77127	82.22843	81.25108	758.23357	2100.81767	1560.55011	1
46	C	69.64065	81.23727	79.21015	-352.41524	704.96076	49.21465	1
47	H	69.42656	80.15333	79.34685	1714.76886	-2070.42778	443.35792	1
48	H	68.70427	81.75902	78.90005	1224.15040	1801.50881	1636.97633	1
49	C	73.01792	81.94971	78.29605	566.85117	537.05831	117.62814	1
50	O	73.33860	81.01917	79.04289	-550.26779	-406.08867	4.21666	1
51	N	73.74854	82.63407	77.46825	566.34832	-425.77725	180.18749	1
52	H	73.27176	83.34659	76.91957	644.44502	2646.80550	-52.73430	1
53	C	75.15299	82.43141	77.26177	612.34801	-281.48662	411.56221	1
54	H	75.67757	82.90877	78.11791	1667.23498	-1490.75142	1556.16753	1
55	C	75.40187	80.85345	77.27182	-714.45746	-175.43074	286.98927	1
56	H	74.41341	80.37019	77.02618	-787.09484	1763.03619	-1922.46060	1
57	O	75.75323	80.34471	78.55983	-429.46514	516.51932	-128.40526	1
58	H	74.81968	80.35849	79.00652	1981.82785	436.16847	-1818.18182	1
59	C	76.42606	80.60177	76.10988	630.79189	-468.94448	76.03230	1
60	H	76.63634	79.51485	75.97425	-1775.71861	2062.30353	131.89849	1
61	H	76.05310	80.99047	75.13208	-1855.14608	88.94118	1993.53760	1
62	H	77.40244	81.10118	76.31351	-1504.82350	-780.94249	-2132.90992	1
63	C	75.45023	83.17985	75.85427	288.57638	618.62814	-397.00270	1
64	O	74.66000	83.13931	74.94055	321.70495	-185.26452	574.37218	1
65	N	76.70865	83.66095	75.85132	-447.05792	-446.53431	367.76425	1
66	H	77.21040	83.62096	76.73989	350.31316	1975.63644	-1843.31522	1
67	C	76.94700	84.73979	74.92831	-511.23061	374.03917	-471.51480	1
68	H	76.03774	85.37762	74.98130	2234.79579	-898.70890	-1273.45190	1
69	C	78.27377	85.47286	75.41628	529.53781	-159.34528	563.72604	1
70	H	78.38264	86.41026	74.80451	654.59388	2347.94251	1217.51488	1
71	H	78.10576	85.79219	76.47790	-1526.55661	2103.42026	817.87394	1
72	O	79.51927	84.73141	75.26646	-554.84278	14.12789	399.58769	1
73	H	79.48651	84.19594	76.07749	1297.06236	2061.84854	1220.68812	1
74	C	77.14682	84.13419	73.43619	-662.15484	-412.13544	123.62687	1
75	O	77.02210	84.86252	72.47554	-540.01537	-317.05804	274.91456	1
76	N	77.51633	82.85279	73.45212	-202.76299	-690.00100	-131.49145	1
77	H	77.62849	82.39881	74.35731	-702.62132	-2617.37191	281.70413	1
78	C	77.72509	82.19702	72.21204	-491.73914	576.34187	222.73509	1
79	H	77.19761	82.82368	71.45601	1977.17978	-1823.58850	-434.68928	1
80	C	79.30392	82.16587	71.99849	-649.50797	-328.66843	306.11224	1
81	H	79.80452	81.71374	72.88129	2075.07803	1452.16490	-1004.45904	1
82	C	79.63031	81.35989	70.69626	-615.18735	-489.99689	-70.96352	1
83	H	80.71728	81.40259	70.44996	-1226.32661	-1724.38906	-1716.47170	1
84	H	79.35914	80.28386	70.80699	2381.64273	-969.84735	900.46860	1
85	H	79.07299	81.75684	69.81555	2122.74991	1702.23946	-141.36228	1
86	C	79.79675	83.63857	71.79022	-501.86074	-479.61276	-376.42482	1
87	H	80.89610	83.68773	71.60815	993.79261	-2246.95401	-1177.81305	1
88	H	79.29055	84.12052	70.92065	42.71279	-626.15391	-2651.37258	1
89	H	79.57710	84.26721	72.68745	-2026.39012	-1590.33709	-887.82922	1
90	C	77.17986	80.65770	72.38417	-672.89153	382.57394	-156.34072	1
91	O	77.62309	79.90863	73.22239	410.04627	221.86223	500.35950	1

92	N	76.30614	80.39316	71.41479	-378.11782	-443.79414	-441.10984	1
93	H	76.00754	81.15957	70.81225	2404.15973	-568.14894	1149.30085	1
94	C	75.54180	79.19047	71.53181	-544.54484	466.16019	331.29119	1
95	H	76.21437	78.50194	72.09564	-1409.80988	-170.17955	2325.32679	1
96	C	74.21834	79.58680	72.31296	-184.48284	116.78282	-758.89137	1
97	H	74.48924	80.17185	73.22276	1893.78641	1861.14652	611.04528	1
98	H	73.60541	80.27745	71.69026	-2170.79665	-974.19311	1327.50117	1
99	C	73.37197	78.32574	72.69030	389.51668	672.81878	-138.49152	1
100	H	73.00037	77.82021	71.76705	510.64577	1933.03327	1851.02484	1
101	H	74.01497	77.57618	73.20919	-2302.30869	-1105.72939	-948.89774	1
102	C	72.16887	78.74111	73.62467	-559.93427	-126.34590	542.30857	1
103	O	71.03846	78.30836	73.49502	-670.36003	-111.83166	76.36448	1
104	N	72.59017	79.60339	74.56056	-216.06729	-537.07037	446.51379	1
105	H	73.53756	80.00397	74.60494	-1251.96487	1074.12894	-2168.52500	1
106	H	71.94371	80.16857	75.17474	-2451.83023	-720.73851	944.84612	1
107	C	75.06601	78.69262	70.05325	546.24052	-563.88337	-85.11809	1
108	O	73.88049	78.68912	69.84457	71.70702	-307.40463	606.69673	1
109	N	76.07192	78.33561	69.23719	479.90863	-504.50129	222.86849	1
110	C	75.84490	78.05046	67.85898	75.51268	-600.91904	506.73700	1
111	H	74.84606	78.46866	67.59303	-2033.61562	1795.30103	254.89480	1
112	C	77.11883	78.71721	67.17679	523.79067	517.99274	284.45581	1
113	H	77.30797	78.32189	66.15158	1599.61665	-1127.00911	1895.98173	1
114	H	77.01156	79.82124	67.08823	-1881.83093	1275.82488	-1501.55016	1
115	C	78.23053	78.32869	68.20135	-600.05639	-404.05026	316.64485	1
116	H	78.54427	77.27008	68.06264	-2597.05260	496.36221	657.73249	1
117	H	79.15346	78.94500	68.11242	-1666.24518	1294.38985	-1723.90591	1
118	C	77.47631	78.53077	69.58378	493.57570	-129.95376	-602.56394	1
119	H	77.74079	77.79691	70.38043	-1469.08415	-637.84797	2204.22581	1
120	H	77.54237	79.56173	69.99966	-1038.97840	1068.88701	-2280.71789	1
121	C	76.03434	76.46117	67.48557	188.88100	241.05089	-727.87821	1
122	O	76.54725	76.18441	66.42832	531.88613	-49.19943	427.07960	1
123	N	75.57319	75.64837	68.41805	708.14833	26.93417	-179.73509	1
124	H	75.10155	75.96812	69.27954	-2232.69501	-1179.09831	1023.94816	1
125	C	75.55868	74.24315	68.15696	-738.32412	259.92548	104.42456	1
126	H	75.47801	74.07785	67.05858	2028.89123	1260.02983	1311.33324	1
127	C	76.89596	73.63372	68.78491	-258.65678	-345.52513	661.28459	1
128	H	77.12199	74.13268	69.75138	-1826.06090	-1801.46097	-918.64554	1
129	C	76.73989	72.08845	68.97854	-541.23400	531.92970	-218.41428	1
130	H	77.66928	71.62807	69.38853	1311.73218	-2219.18200	882.19023	1
131	H	75.91078	71.84692	69.68648	-1048.71298	1223.58118	-2196.97971	1
132	H	76.51221	71.57502	68.01497	419.06414	1903.92898	1903.44670	1
133	C	78.05564	73.85622	67.75768	-423.86431	152.66566	-648.55262	1
134	H	79.04023	73.52703	68.16580	105.68386	-2342.50080	1387.51238	1
135	H	77.87962	73.28961	66.81313	-1695.63603	-1484.73621	-1531.02793	1
136	H	78.14669	74.93512	67.47943	-1853.57121	-487.39031	1936.59343	1
137	C	74.28427	73.82297	69.07007	539.71428	-510.58232	267.58633	1
138	O	73.97555	74.57775	69.99821	-15.93758	-278.34085	-624.49402	1
139	N	73.74687	72.68117	68.69957	-676.81886	12.05292	276.17960	1
140	H	74.19194	72.18510	67.92801	-1694.44250	-373.84189	-2100.66098	1
141	C	72.79768	72.03867	69.55247	412.33078	-664.70360	108.35451	1
142	H	72.19764	72.89654	69.93437	1765.77476	1294.44366	1621.76594	1
143	C	72.01392	70.98468	68.67481	-179.66635	-721.95667	-264.73915	1
144	H	71.57062	71.46526	67.77374	-607.34922	2587.87032	-598.10018	1
145	H	72.71651	70.21224	68.28890	-359.69332	-1479.13954	-2259.74260	1
146	C	70.90751	70.32041	69.56064	-240.01076	616.02425	431.85322	1
147	H	71.34538	69.95758	70.52041	-1359.17131	782.54425	2227.99181	1
148	H	70.11475	71.05259	69.83338	-820.36667	85.81767	-2596.78715	1
149	C	70.31717	69.11386	68.72571	-513.07015	236.18570	-551.87280	1
150	H	69.96006	69.45969	67.72849	1816.11944	-1183.11722	-1650.94321	1
151	H	71.11082	68.35976	68.51783	-1800.04429	-1361.53473	1526.34643	1
152	C	69.15901	68.47513	69.52649	726.08972	-253.19732	-179.64713	1
153	H	69.44070	68.10373	70.53191	1224.27271	-456.51798	-2390.90304	1

154	H	68.24474	69.09788	69.59424	1206.40339	-1150.93514	-2154.90344	1
155	N	68.71577	67.19057	68.74698	329.70796	-633.68968	-155.67358	1
156	H	67.89654	66.65929	69.16113	1348.31305	1938.76845	1359.00643	1
157	H	68.39720	67.31753	67.74253	2096.92035	1446.54551	-966.48890	1
158	H	69.43714	66.41765	68.65187	-1197.07217	-2303.53719	827.28733	1
159	C	73.61208	71.29086	70.76217	-378.01186	-556.17301	-413.96481	1
160	O	73.59541	70.09433	70.90249	-409.44433	-307.55053	-453.30833	1
161	N	74.26649	72.21322	71.46960	-429.02477	524.70884	274.08502	1
162	H	74.12992	73.21754	71.22587	1706.34263	-1425.96036	1574.38926	1
163	C	74.58055	71.87080	72.82460	-45.25864	-626.22952	478.93267	1
164	H	74.25608	70.81087	72.95515	1988.63164	570.90773	1772.87287	1
165	C	76.15112	72.06096	72.98148	551.77128	-20.49526	-564.54996	1
166	H	76.66895	71.55239	72.13855	1434.61535	-1753.10253	1513.99471	1
167	H	76.42295	73.13520	72.88578	-714.67738	1819.09770	1898.36494	1
168	C	76.65652	71.48453	74.34378	446.99263	-555.77305	338.97221	1
169	H	76.30385	72.10782	75.19554	1953.68466	1892.25957	-161.67766	1
170	H	76.23847	70.46625	74.51066	-403.03785	2688.07032	-188.43591	1
171	C	78.23618	71.42591	74.39630	567.86262	335.74681	434.04421	1
172	H	78.64842	70.78588	73.58297	-1080.02275	1568.26081	-1948.78900	1
173	H	78.68391	72.43594	74.25224	-919.54108	2111.34692	1456.13463	1
174	C	78.57415	70.85370	75.79474	195.81897	173.33862	-745.11536	1
175	H	78.23686	71.48245	76.64630	1405.67949	-2301.21089	-390.08113	1
176	H	78.25896	69.79947	75.94734	-940.37328	-1118.32446	2299.72133	1
177	N	80.13155	70.81852	75.94499	319.26422	656.36007	-42.02424	1
178	H	80.49756	70.35781	76.82785	1961.03633	619.91968	1787.09422	1
179	H	80.67747	70.30011	75.19829	854.14343	-2156.80752	1429.08711	1
180	H	80.63470	71.75290	75.97276	1237.02905	-1378.50857	-1998.28500	1
181	C	73.77522	72.95256	73.71896	532.53319	-268.57236	517.55729	1
182	O	73.11137	73.87715	73.24055	266.16714	-290.73804	-558.88002	1
183	N	73.95926	72.71722	75.05073	-226.25352	640.49678	-270.32839	1
184	H	74.55827	71.87876	75.00521	2007.69063	-1035.27229	1523.50231	1
185	C	74.46732	73.89108	75.75244	-540.76542	-573.33303	49.50000	1
186	H	75.31431	74.24118	75.12391	-2374.20950	-1036.76023	843.75774	1
187	C	73.27240	74.94212	75.68749	-77.09082	666.87422	-415.84136	1
188	H	72.35952	74.35827	75.36487	-985.81834	617.19825	2463.91927	1
189	O	73.41231	75.93838	74.66504	293.29899	-391.65602	-477.80926	1
190	H	73.03985	75.41516	73.86901	2528.72714	-681.76262	-751.27122	1
191	C	73.08955	75.45320	77.15827	252.47363	-605.14473	440.05134	1
192	H	72.12986	76.03751	77.27056	-2052.65063	1456.49051	-1043.51830	1
193	H	73.06306	74.60797	77.88996	-2152.98800	-1661.97574	-161.70652	1
194	H	73.94208	76.10718	77.46789	-473.12726	-1584.27339	2165.61725	1
195	C	74.95917	73.49313	77.22730	360.36307	488.46713	505.10056	1
196	O	75.34257	74.37218	77.97492	-200.08817	-528.03552	-385.82850	1
197	N	74.91702	72.18312	77.47558	-597.54095	-226.44775	355.20479	1
198	H	74.56662	71.53383	76.77417	2179.23655	-1300.70981	-991.33835	1
199	C	75.26177	71.72146	78.76961	-687.68921	297.39807	-249.45179	1
200	H	75.52903	72.62467	79.36860	-349.16256	-2467.37713	-1101.72831	1
201	C	73.97117	70.93270	79.32379	672.47345	361.54328	-201.62880	1
202	H	73.68657	70.11976	78.61815	1541.41502	582.18425	2169.97026	1
203	H	74.19736	70.45540	80.30412	-2534.67717	60.25153	997.72295	1
204	C	72.84342	71.96220	79.45574	574.26774	-389.43119	-377.02542	1
205	C	72.62437	72.63115	80.69855	688.82679	-287.33580	-257.96133	1
206	H	73.22204	72.37066	81.59058	331.14182	1470.38163	2269.80013	1
207	C	72.05947	72.31170	78.31310	-383.52382	-675.04808	144.24917	1
208	H	72.23245	71.81266	77.34277	4.09847	1517.59662	2262.86397	1
209	C	71.65345	73.63163	80.76258	-134.76730	428.45285	-649.50303	1
210	H	71.49202	74.14643	81.72573	-903.23433	1600.49020	2011.53387	1
211	C	71.10075	73.32107	78.42600	-335.53281	-615.00040	-364.39058	1
212	H	70.51594	73.58857	77.52836	1596.45398	-1369.33862	1732.02659	1
213	C	70.86349	74.02547	79.64296	585.48547	-340.24194	-406.23938	1
214	O	69.90227	75.06701	79.75556	-419.15649	-173.04408	-511.94141	1
215	H	69.55706	75.06953	78.82990	-1071.84350	1559.71507	-1960.13012	1

216	C	76.47624	70.66162	78.56547	291.41878	-183.13091	710.72246	1
217	O	76.69826	70.08403	77.49835	379.87695	523.47396	-222.23622	1
218	N	77.08782	70.51915	79.71878	564.30591	373.09380	277.24371	1
219	H	76.73309	71.06797	80.49852	-120.59931	-2436.07824	-1214.35098	1
220	C	78.37325	69.87800	79.75300	404.07514	-299.37480	608.84009	1
221	H	78.84246	70.21637	78.80085	-1071.07882	-841.69025	2359.66467	1
222	C	79.11507	70.33696	81.07453	-683.12807	68.71770	-390.13096	1
223	H	79.21562	71.44493	81.11901	2068.88918	1596.58590	770.89603	1
224	H	78.52490	70.04826	81.97341	1379.86429	2342.49779	-179.85638	1
225	C	80.50978	69.63680	81.07843	-176.39967	537.49466	550.97268	1
226	H	80.38567	68.53389	80.97224	-396.28051	1942.22168	1869.33314	1
227	H	81.11997	69.95787	80.20500	-94.44700	586.00678	-2659.20016	1
228	C	81.24378	69.98482	82.45329	-291.69381	-718.18079	-150.72929	1
229	H	81.52287	71.05781	82.61039	-2303.38776	1089.76242	964.62032	1
230	H	80.72931	69.61770	83.37810	884.16729	2568.80533	-207.74283	1
231	N	82.42000	69.23494	82.28955	-594.49522	-252.81478	342.29276	1
232	H	82.46160	68.62910	81.48415	-1735.17426	2084.05705	-263.71605	1
233	C	83.41433	69.25292	83.08222	595.23177	-271.52487	442.22352	1
234	N	83.34288	70.08687	84.20234	585.53813	-424.79750	-105.81303	1
235	H	82.58452	70.69710	84.50456	959.88797	1327.56823	-2177.11905	1
236	H	84.07078	70.17995	84.91155	1578.48647	16.27378	-2220.76233	1
237	N	84.41958	68.38444	82.63435	-452.17763	-390.33541	-421.51853	1
238	H	84.45427	67.76800	81.82376	470.26107	1974.25629	-1817.92087	1
239	H	85.29948	68.24093	83.13087	1856.67307	-1573.97321	-1224.35416	1
240	C	78.14011	68.27108	79.76136	-531.47271	-581.45780	-55.06206	1
241	O	78.31598	67.59294	80.73430	-243.00837	192.73507	609.52485	1
242	N	77.83954	67.87611	78.49768	343.49288	-644.25607	38.09164	1
243	H	77.58041	68.63474	77.80954	-1691.16043	-1535.97525	-1484.73099	1
244	C	77.16706	66.56642	78.35575	542.66492	350.14337	454.42563	1
245	H	77.48666	66.03306	79.28304	1209.57979	-2396.95920	463.86744	1
246	C	75.67537	66.79559	78.26551	-737.14309	145.93010	242.71942	1
247	H	75.48519	67.44673	77.38194	-1050.18303	159.36419	-2509.06125	1
248	C	74.92398	65.49142	78.06525	-706.77696	-252.88343	-245.16230	1
249	H	73.81392	65.65585	77.99237	-1624.64039	-1665.49085	1417.86935	1
250	H	75.24994	64.97301	77.11895	2566.10521	598.51109	693.22305	1
251	H	75.10108	64.77636	78.91519	-1972.69758	107.10018	-1876.34312	1
252	C	75.13493	67.51813	79.48723	412.85148	672.58832	-27.69222	1
253	H	74.03320	67.72523	79.40024	1447.02277	1762.76533	-1490.78944	1
254	H	75.29071	66.91565	80.42412	1320.77379	-145.20455	2378.68491	1
255	H	75.65290	68.50505	79.64117	-1512.10848	1470.52031	1724.75147	1
256	C	77.78535	65.91330	76.97058	-607.11113	499.56689	73.73769	1
257	O	77.09255	65.69718	76.00110	357.97126	460.81534	356.68785	1
258	N	79.08125	65.68767	77.12113	536.55407	-368.62270	332.76306	1
259	H	79.50872	65.94178	78.01117	524.38866	2297.69985	1367.20941	1
260	C	79.76567	64.93490	76.13650	46.50277	-774.29190	-147.97904	1
261	H	78.96240	64.47385	75.51711	1676.51875	1883.29066	1032.55549	1
262	C	80.72575	65.91458	75.27888	-559.41456	-34.19198	-556.30433	1
263	H	81.49362	66.35933	75.95488	-64.66664	395.18769	2695.05373	1
264	H	81.29304	65.32742	74.51818	-2703.44278	-60.40056	333.79418	1
265	C	79.91910	67.00052	74.62175	-519.76435	377.31045	459.42366	1
266	H	79.35767	67.54874	75.41264	-1746.74323	1667.50644	-1261.73691	1
267	C	80.84203	67.98177	73.90866	570.95554	16.46261	-545.27700	1
268	H	80.26906	68.82518	73.44425	2391.58273	28.05277	-1305.07271	1
269	H	81.58927	68.43121	74.61188	175.75588	917.63458	2559.43867	1
270	H	81.41958	67.48222	73.08896	-1063.97851	-2155.34650	1283.00462	1
271	C	78.91452	66.42908	73.63153	193.76014	2.62946	-765.53141	1
272	H	78.42190	67.23594	73.02964	507.39394	-846.55087	2539.60089	1
273	H	79.39853	65.72339	72.90742	1337.57841	1818.19054	1526.01994	1
274	H	78.09347	65.86701	74.16532	1100.88635	-1172.91350	-2199.08909	1
275	C	80.73083	63.90316	76.91324	-549.21115	475.64486	-309.38218	1
276	O	80.98923	63.99213	78.08502	556.06106	-390.37755	-78.24250	1
277	O	81.35637	62.91955	76.10980	-572.27940	-310.19032	-209.75862	1

278	H	80.93093	63.14148	75.23619	-1380.08193	2212.14486	790.85944	1
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Listing 28: C00028.xmolout

1		276						
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.9687 3875
		0.2500	300.00	0.00	0.00	0.00	-1293.9439	0.0000 300.0000
3	H	65.84523	73.21692	90.01490	-2043.14101	-1757.64893	399.89339	1
4	N	66.67251	72.67887	90.26539	426.75047	490.45733	-334.42467	1
5	H	66.50239	71.80438	89.77243	442.25559	-1110.30854	-2448.52907	1
6	C	67.88179	73.31427	89.90043	415.32972	-666.39213	83.73172	1
7	H	67.71398	74.34169	90.28740	879.32219	2491.00447	667.35213	1
8	C	69.11706	72.57614	90.61870	31.35357	477.41777	628.23362	1
9	H	69.21220	71.53672	90.22135	1168.38489	2240.25337	-1019.71136	1
10	H	70.07717	73.09308	90.37503	-360.43770	2534.90498	931.67112	1
11	C	68.89394	72.54637	92.10968	463.18208	512.70242	-382.34388	1
12	H	67.87822	72.13142	92.29992	1725.29117	1863.52247	-987.07854	1
13	C	69.92247	71.64489	92.78070	710.42801	-144.27427	-313.15367	1
14	H	69.75887	71.58218	93.88754	364.20195	-1033.13725	2494.72524	1
15	H	69.88294	70.59940	92.37929	2567.61904	335.80679	847.48802	1
16	H	70.96578	72.02173	92.62156	-2587.99029	680.92867	-512.16411	1
17	C	68.97078	73.94080	92.71553	268.17616	741.64379	-40.42634	1
18	H	68.83830	73.91563	93.82812	1283.54314	-1945.37420	-1411.27812	1
19	H	69.95982	74.42630	92.51043	-1258.57796	1317.15249	-2026.02085	1
20	H	68.17740	74.61652	92.30442	-2502.84526	909.80597	575.92391	1
21	C	67.91901	73.30041	88.27523	619.36578	-458.64843	-172.09273	1
22	O	66.97344	73.69005	87.62379	-81.40433	433.87611	522.34594	1
23	N	69.10286	72.90122	87.81355	175.23996	-622.20190	341.55523	1
24	H	69.82762	72.56132	88.44153	-876.57256	-303.22879	-2561.90213	1
25	C	69.25252	72.85674	86.39121	-571.88214	-534.10783	-106.15033	1
26	H	68.59261	73.67315	86.01097	-2713.20841	-16.25800	-248.80809	1
27	C	70.81817	73.01453	86.07647	166.60354	288.16399	-716.09568	1
28	H	71.35281	72.13591	86.53157	-2097.85574	1636.78449	-586.18044	1
29	O	71.44795	74.18856	86.61352	-317.80580	-363.38227	484.43082	1
30	H	72.11295	73.78874	87.21068	1863.74748	-1451.84923	1357.29467	1
31	C	70.85734	72.87520	84.51045	503.80731	517.99032	318.51606	1
32	H	71.90524	72.84395	84.13171	640.61020	-2157.10410	-1536.29104	1
33	H	70.35269	71.94206	84.15667	1687.88455	465.60692	2087.56452	1
34	H	70.35264	73.73446	84.01107	-1293.07895	-1899.88581	-1463.57452	1
35	C	68.82029	71.37759	85.88496	-153.07550	-733.68902	248.70981	1
36	O	69.29435	70.37407	86.40068	186.15459	-480.78787	-449.34387	1
37	N	68.03051	71.47187	84.81905	-487.53139	543.18517	42.03850	1
38	C	67.65608	70.30977	84.06170	-699.35871	69.34393	360.10701	1
39	H	67.40250	69.51011	84.79354	2.81126	-221.99807	-2715.58072	1
40	C	66.44987	70.84709	83.18617	-507.46439	-592.59194	122.07761	1
41	H	66.29479	70.25511	82.25582	-1975.08116	525.87560	-1801.71556	1
42	H	65.48903	70.81787	83.74736	1588.27743	-1913.22100	1113.83566	1
43	C	66.90471	72.31477	82.91435	-613.62442	-457.55993	-194.14490	1
44	H	67.72456	72.33997	82.16010	1707.54637	-721.27992	1996.92523	1
45	H	66.09244	72.97705	82.53817	758.23357	2100.81767	1560.55011	1
46	C	67.43778	72.72086	84.35404	-352.41524	704.96076	49.21465	1
47	H	68.21327	73.52324	84.36465	1714.76886	-2070.42778	443.35792	1
48	H	66.64063	72.96830	85.09612	1224.15040	1801.50881	1636.97633	1
49	C	68.91445	69.90498	83.09512	566.85117	537.05831	117.62814	1
50	O	69.50829	70.71192	82.42428	-550.26779	-406.08867	4.21666	1
51	N	68.99832	68.56750	83.07922	566.34832	-425.77725	180.18749	1
52	H	68.34962	68.08307	83.70272	644.44502	2646.80550	-52.73430	1
53	C	70.31342	68.00324	82.97987	612.34801	-281.48662	411.56221	1
54	H	70.89187	68.67296	82.30562	1667.23498	-1490.75142	1556.16753	1
55	C	70.88242	67.97254	84.47332	-714.45746	-175.43074	286.98927	1
56	H	70.04955	67.64402	85.15704	-787.09484	1763.03619	-1922.46060	1
57	O	71.31822	69.22831	84.99501	-429.46514	516.51932	-128.40526	1

58	H	70.55379	69.47595	85.60710	1981.82785	436.16847	-1818.18182	1
59	C	71.96517	66.83934	84.38507	630.79189	-468.94448	76.03230	1
60	H	72.44163	66.65324	85.37582	-1775.71861	2062.30353	131.89849	1
61	H	71.52268	65.87137	84.04322	-1855.14608	88.94118	1993.53760	1
62	H	72.77816	67.10561	83.66975	-1504.82350	-780.94249	-2132.90992	1
63	C	70.04025	66.50487	82.40400	288.57638	618.62814	-397.00270	1
64	O	69.47135	65.66396	83.05651	321.70495	-185.26452	574.37218	1
65	N	70.55567	66.39431	81.15779	-447.05792	-446.53431	367.76425	1
66	H	70.98072	67.25616	80.80399	350.31316	1975.63644	-1843.31522	1
67	C	69.64008	65.75211	80.22783	-511.23061	374.03917	-471.51480	1
68	H	69.55266	64.70705	80.59991	2234.79579	-898.70890	-1273.45190	1
69	C	68.28351	66.55493	80.34966	529.53781	-159.34528	563.72604	1
70	H	67.54706	66.10003	79.64067	654.59388	2347.94251	1217.51488	1
71	H	67.87270	66.40797	81.38050	-1526.55661	2103.42026	817.87394	1
72	O	68.35844	68.02187	80.05130	-554.84278	14.12789	399.58769	1
73	H	68.59845	68.32878	80.93855	1297.06236	2061.84854	1220.68812	1
74	C	70.32449	65.86441	78.75959	-662.15484	-412.13544	123.62687	1
75	O	70.75214	64.89145	78.19708	-540.01537	-317.05804	274.91456	1
76	N	70.27393	67.12971	78.32080	-202.76299	-690.00100	-131.49145	1
77	H	69.84193	67.84313	78.93553	-702.62132	-2617.37191	281.70413	1
78	C	70.98867	67.51320	77.10619	-491.73914	576.34187	222.73509	1
79	H	70.95784	66.60349	76.46006	1977.17978	-1823.58850	-434.68928	1
80	C	70.26847	68.72232	76.53963	-649.50797	-328.66843	306.11224	1
81	H	70.38584	69.55926	77.26472	2075.07803	1452.16490	-1004.45904	1
82	C	70.84926	69.16336	75.21010	-615.18735	-489.99689	-70.96352	1
83	H	70.28003	70.03200	74.77816	-1226.32661	-1724.38906	-1716.47170	1
84	H	71.93558	69.49406	75.30855	2381.64273	-969.84735	900.46860	1
85	H	70.81799	68.33551	74.44931	2122.74991	1702.23946	-141.36228	1
86	C	68.77904	68.46454	76.38395	-501.86074	-479.61276	-376.42482	1
87	H	68.23374	69.37462	76.01236	993.79261	-2246.95401	-1177.81305	1
88	H	68.57879	67.63348	75.65390	42.71279	-626.15391	-2651.37258	1
89	H	68.30857	68.16677	77.36176	-2026.39012	-1590.33709	-887.82922	1
90	C	72.54141	67.91236	77.55967	-672.89153	382.57394	-156.34072	1
91	O	72.82144	68.32620	78.65787	410.04627	221.86223	500.35950	1
92	N	73.34899	67.72595	76.51930	-378.11782	-443.79414	-441.10984	1
93	H	72.87925	67.45329	75.65920	2404.15973	-568.14894	1149.30085	1
94	C	74.61697	68.40065	76.53814	-544.54484	466.16019	331.29119	1
95	H	75.04440	68.18009	77.54031	-1409.80988	-170.17955	2325.32679	1
96	C	75.44586	67.85847	75.30430	-184.48284	116.78282	-758.89137	1
97	H	75.53009	66.74822	75.32311	1893.78641	1861.14652	611.04528	1
98	H	74.92016	68.11092	74.35534	-2170.79665	-974.19311	1327.50117	1
99	C	76.84976	68.53986	75.35820	389.51668	672.81878	-138.49152	1
100	H	76.74330	69.61868	75.60668	510.64577	1933.03327	1851.02484	1
101	H	77.44487	68.12768	76.20201	-2302.30869	-1105.72939	-948.89774	1
102	C	77.65579	68.40244	74.01177	-559.93427	-126.34590	542.30857	1
103	O	78.66856	69.03834	73.86138	-670.36003	-111.83166	76.36448	1
104	N	77.10845	67.54850	73.12085	-216.06729	-537.07037	446.51379	1
105	H	76.27659	66.95416	73.21458	-1251.96487	1074.12894	-2168.52500	1
106	H	77.53415	67.31139	72.21808	-2451.83023	-720.73851	944.84612	1
107	C	74.35064	69.98451	76.26895	546.24052	-563.88337	-85.11809	1
108	O	73.74891	70.32047	75.27318	71.70702	-307.40463	606.69673	1
109	N	74.94314	70.75070	77.19008	479.90863	-504.50129	222.86849	1
110	C	74.58150	72.13478	77.30913	75.51268	-600.91904	506.73700	1
111	H	73.48085	72.14535	77.14560	-2033.61562	1795.30103	254.89480	1
112	C	75.03822	72.49997	78.77866	523.79067	517.99274	284.45581	1
113	H	75.34673	73.56503	78.87876	1599.61665	-1127.00911	1895.98173	1
114	H	74.20367	72.35003	79.50006	-1881.83093	1275.82488	-1501.55016	1
115	C	76.20244	71.49989	79.07098	-600.05639	-404.05026	316.64485	1
116	H	77.16488	71.85427	78.63901	-2597.05260	496.36221	657.73249	1
117	H	76.38789	71.33737	80.15674	-1666.24518	1294.38985	-1723.90591	1
118	C	75.66516	70.20158	78.33169	493.57570	-129.95376	-602.56394	1
119	H	76.45507	69.50784	77.95901	-1469.08415	-637.84797	2204.22581	1

120	H	74.90085	69.62455	78.90822	-1038.97840	1068.88701	-2280.71789	1
121	C	75.31557	73.06441	76.17523	188.88100	241.05089	-727.87821	1
122	O	74.64018	73.94294	75.63562	531.88613	-49.19943	427.07960	1
123	N	76.60203	72.81795	76.05984	708.14833	26.93417	-179.73509	1
124	H	76.84942	72.02847	76.65591	-2232.69501	-1179.09831	1023.94816	1
125	C	77.41325	73.22326	74.96804	-738.32412	259.92548	104.42456	1
126	H	78.32869	72.60114	75.08317	2028.89123	1260.02983	1311.33324	1
127	C	76.60322	72.91850	73.63206	-258.65678	-345.52513	661.28459	1
128	H	75.65685	73.50575	73.61629	-1826.06090	-1801.46097	-918.64554	1
129	C	77.53240	73.28993	72.42691	-541.23400	531.92970	-218.41428	1
130	H	77.02628	73.12188	71.44752	1311.73218	-2219.18200	882.19023	1
131	H	77.84169	74.36168	72.46401	-1048.71298	1223.58118	-2196.97971	1
132	H	78.46421	72.67649	72.42946	419.06414	1903.92898	1903.44670	1
133	C	76.28425	71.38800	73.54276	-423.86431	152.66566	-648.55262	1
134	H	75.78016	71.12679	72.58265	105.68386	-2342.50080	1387.51238	1
135	H	77.21394	70.77088	73.61066	-1695.63603	-1484.73621	-1531.02793	1
136	H	75.60182	71.06753	74.37067	-1853.57121	-487.39031	1936.59343	1
137	C	77.75448	74.82380	74.95416	539.71428	-510.58232	267.58633	1
138	O	78.92795	75.15417	74.88496	-15.93758	-278.34085	-624.49402	1
139	N	76.67061	75.55213	74.94219	-676.81886	12.05292	276.17960	1
140	H	75.73009	75.07945	75.01449	-1694.44250	-373.84189	-2100.66098	1
141	C	76.68992	76.97307	74.98454	412.33078	-664.70360	108.35451	1
142	H	75.62070	77.21570	75.18090	1765.77476	1294.44366	1621.76594	1
143	C	77.65865	77.43570	76.15391	-179.66635	-721.95667	-264.73915	1
144	H	77.40027	76.91510	77.10297	-607.34922	2587.87032	-598.10018	1
145	H	78.71601	77.15593	75.94004	-359.69332	-1479.13954	-2259.74260	1
146	C	77.50280	78.98448	76.29455	-240.01076	616.02425	431.85322	1
147	H	77.88777	79.50829	75.38700	-1359.17131	782.54425	2227.99181	1
148	H	76.42825	79.26352	76.37508	-820.36667	85.81767	-2596.78715	1
149	C	78.28972	79.44362	77.58802	-513.07015	236.18570	-551.87280	1
150	H	77.92574	78.90120	78.49065	1816.11944	-1183.11722	-1650.94321	1
151	H	79.37444	79.20232	77.50497	-1800.04429	-1361.53473	1526.34643	1
152	C	78.06817	80.96726	77.73173	726.08972	-253.19732	-179.64713	1
153	H	78.55718	81.57822	76.94509	1224.27271	-456.51798	-2390.90304	1
154	H	77.00700	81.26867	77.83976	1206.40339	-1150.93514	-2154.90344	1
155	N	78.73005	81.41693	79.07745	329.70796	-633.68968	-155.67358	1
156	H	78.62621	82.44488	79.31790	1348.31305	1938.76845	1359.00643	1
157	H	78.37239	80.96075	79.96706	2096.92035	1446.54551	-966.48890	1
158	H	79.77913	81.28593	79.17037	-1197.07217	-2303.53719	827.28733	1
159	C	77.18443	77.62148	73.56332	-378.01186	-556.17301	-413.96481	1
160	O	76.39592	78.34424	72.97226	-409.44433	-307.55053	-453.30833	1
161	N	78.41314	77.28349	73.27567	-429.02477	524.70884	274.08502	1
162	H	78.91713	76.62403	73.91350	1706.34263	-1425.96036	1574.38926	1
163	C	79.02221	77.64074	72.04377	-45.25864	-626.22952	478.93267	1
164	H	79.95122	77.02843	72.05335	1988.63164	570.90773	1772.87287	1
165	C	78.03124	77.23889	70.87702	551.77128	-20.49526	-564.54996	1
166	H	77.68055	76.19403	71.03212	1434.61535	-1753.10253	1513.99471	1
167	H	77.10704	77.86206	70.89243	-714.67738	1819.09770	1898.36494	1
168	C	78.77673	77.38125	69.50931	446.99263	-555.77305	338.97221	1
169	H	78.63435	78.41424	69.06351	1953.68466	1892.25957	-161.67766	1
170	H	79.87431	77.24765	69.64268	-403.03785	2688.07032	-188.43591	1
171	C	78.20152	76.26164	68.55507	567.86262	335.74681	434.04421	1
172	H	78.24402	75.26133	69.04415	-1080.02275	1568.26081	-1948.78900	1
173	H	77.12580	76.44392	68.32919	-919.54108	2111.34692	1456.13463	1
174	C	79.06252	76.27062	67.26505	195.81897	173.33862	-745.11536	1
175	H	79.00645	77.21155	66.67585	1405.67949	-2301.21089	-390.08113	1
176	H	80.12429	75.98247	67.41137	-940.37328	-1118.32446	2299.72133	1
177	N	78.48713	75.24239	66.26476	319.26422	656.36007	-42.02424	1
178	H	79.18507	74.53599	65.89492	1961.03633	619.91968	1787.09422	1
179	H	77.69028	74.60456	66.55464	854.14343	-2156.80752	1429.08711	1
180	H	78.11774	75.76301	65.33204	1237.02905	-1378.50857	-1998.28500	1
181	C	79.38260	79.25281	72.00226	532.53319	-268.57236	517.55729	1

182	O	80.54658	79.53680	71.89716	266.16714	-290.73804	-558.88002	1
183	N	78.30467	80.01209	72.05671	-226.25352	640.49678	-270.32839	1
184	H	77.37314	79.54660	72.18250	2007.69063	-1035.27229	1523.50231	1
185	C	78.36937	81.42169	72.18228	-540.76542	-573.33303	49.50000	1
186	H	77.31557	81.67219	72.43540	-2374.20950	-1036.76023	843.75774	1
187	C	79.40222	81.81818	73.33007	-77.09082	666.87422	-415.84136	1
188	H	80.43151	81.51005	72.99319	-985.81834	617.19825	2463.91927	1
189	O	79.18793	81.20661	74.62014	293.29899	-391.65602	-477.80926	1
190	H	79.97441	80.62790	74.67713	2528.72714	-681.76262	-751.27122	1
191	C	79.28879	83.38720	73.31272	252.47363	-605.14473	440.05134	1
192	H	80.03078	83.85668	73.99895	-2052.65063	1456.49051	-1043.51830	1
193	H	79.46894	83.80459	72.29383	-2152.98800	-1661.97574	-161.70652	1
194	H	78.27793	83.72764	73.63626	-473.12726	-1584.27339	2165.61725	1
195	C	78.83212	82.06832	70.73496	360.36307	488.46713	505.10056	1
196	O	79.96851	82.42790	70.53949	-200.08817	-528.03552	-385.82850	1
197	N	77.75874	82.19371	69.96888	-597.54095	-226.44775	355.20479	1
198	H	76.88571	81.82265	70.34208	2179.23655	-1300.70981	-991.33835	1
199	C	77.85577	82.55514	68.59944	-687.68921	297.39807	-249.45179	1
200	H	76.79055	82.71485	68.32238	-349.16256	-2467.37713	-1101.72831	1
201	C	78.74804	83.87410	68.43781	672.47345	361.54328	-201.62880	1
202	H	79.80430	83.65132	68.72736	1541.41502	582.18425	2169.97026	1
203	H	78.76242	84.19435	67.36998	-2534.67717	60.25153	997.72295	1
204	C	78.18834	85.00537	69.31267	574.26774	-389.43119	-377.02542	1
205	C	76.91441	85.58015	69.02371	688.82679	-287.33580	-257.96133	1
206	H	76.30885	85.21565	68.17422	331.14182	1470.38163	2269.80013	1
207	C	78.96639	85.48221	70.41013	-383.52382	-675.04808	144.24917	1
208	H	79.95379	85.03670	70.63010	4.09847	1517.59662	2262.86397	1
209	C	76.45219	86.61372	69.83775	-134.76730	428.45285	-649.50303	1
210	H	75.46775	87.06133	69.61554	-903.23433	1600.49020	2011.53387	1
211	C	78.46007	86.51961	71.19657	-335.53281	-615.00040	-364.39058	1
212	H	79.07083	86.88095	72.04242	1596.45398	-1369.33862	1732.02659	1
213	C	77.19394	87.12343	70.94280	585.48547	-340.24194	-406.23938	1
214	O	76.66922	88.17801	71.73455	-419.15649	-173.04408	-511.94141	1
215	H	77.41894	88.30318	72.36299	-1071.84350	1559.71507	-1960.13012	1
216	C	78.49985	81.28861	67.80494	291.41878	-183.13091	710.72246	1
217	O	78.34028	80.14941	68.21153	379.87695	523.47396	-222.23622	1
218	N	79.07723	81.70528	66.69638	564.30591	373.09380	277.24371	1
219	H	79.07475	82.70699	66.51860	-120.59931	-2436.07824	-1214.35098	1
220	C	79.66904	80.84590	65.72260	404.07514	-299.37480	608.84009	1
221	H	80.52125	81.44973	65.33693	-1071.07882	-841.69025	2359.66467	1
222	C	80.11991	79.52455	66.47368	-683.12807	68.71770	-390.13096	1
223	H	80.48178	79.80623	67.49108	2068.88918	1596.58590	770.89603	1
224	H	79.22296	78.88283	66.65048	1379.86429	2342.49779	-179.85638	1
225	C	81.22586	78.71823	65.73104	-176.39967	537.49466	550.97268	1
226	H	80.79861	77.85958	65.16569	-396.28051	1942.22168	1869.33314	1
227	H	81.75888	79.34379	64.98141	-94.44700	586.00678	-2659.20016	1
228	C	82.23196	78.22565	66.88145	-291.69381	-718.18079	-150.72929	1
229	H	82.90801	79.04673	67.23532	-2303.38776	1089.76242	964.62032	1
230	H	81.76650	77.70121	67.75364	884.16729	2568.80533	-207.74283	1
231	N	82.98261	77.31282	66.13786	-594.49522	-252.81478	342.29276	1
232	H	83.29410	77.62980	65.23046	-1735.17426	2084.05705	-263.71605	1
233	C	83.32744	76.14547	66.52111	595.23177	-271.52487	442.22352	1
234	N	82.92337	75.71513	67.78672	585.53813	-424.79750	-105.81303	1
235	H	82.41885	76.22650	68.51042	959.88797	1327.56823	-2177.11905	1
236	H	83.18063	74.82325	68.21151	1578.48647	16.27378	-2220.76233	1
237	N	84.08709	75.51463	65.53021	-452.17763	-390.33541	-421.51853	1
238	H	84.38188	75.83812	64.60968	470.26107	1974.25629	-1817.92087	1
239	H	84.47585	74.57610	65.63071	1856.67307	-1573.97321	-1224.35416	1
240	C	78.56556	80.61343	64.55231	-531.47271	-581.45780	-55.06206	1
241	O	77.51034	81.20306	64.48667	-243.00837	192.73507	609.52485	1
242	N	79.08860	79.78764	63.62069	343.49288	-644.25607	38.09164	1
243	H	79.95164	79.33396	63.91532	-1691.16043	-1535.97525	-1484.73099	1

244	C	78.09440	79.01643	62.90920	542.66492	350.14337	454.42563	1
245	H	77.31823	79.75547	62.60697	1209.57979	-2396.95920	463.86744	1
246	C	78.81973	78.26692	61.71683	-737.14309	145.93010	242.71942	1
247	H	79.53920	77.51924	62.11599	-1050.18303	159.36419	-2509.06125	1
248	C	77.70665	77.57134	60.85926	-706.77696	-252.88343	-245.16230	1
249	H	78.14178	76.99785	60.00752	-1624.64039	-1665.49085	1417.86935	1
250	H	77.10695	76.85562	61.47074	2566.10521	598.51109	693.22305	1
251	H	76.99619	78.31585	60.42948	-1972.69758	107.10018	-1876.34312	1
252	C	79.56354	79.30115	60.80329	412.85148	672.58832	-27.69222	1
253	H	80.05322	78.80538	59.93228	1447.02277	1762.76533	-1490.78944	1
254	H	78.86220	80.06895	60.40060	1320.77379	-145.20455	2378.68491	1
255	H	80.35731	79.84376	61.36863	-1512.10848	1470.52031	1724.75147	1
256	C	77.56212	77.90907	63.96746	-607.11113	499.56689	73.73769	1
257	O	78.32668	77.08889	64.49948	357.97126	460.81534	356.68785	1
258	N	76.26349	78.00837	64.09505	536.55407	-368.62270	332.76306	1
259	H	75.77833	78.71155	63.53732	524.38866	2297.69985	1367.20941	1
260	C	75.67574	77.51243	65.29610	46.50277	-774.29190	-147.97904	1
261	H	76.50784	77.50095	66.03415	1676.51875	1883.29066	1032.55549	1
262	C	74.43223	78.46515	65.66767	-559.41456	-34.19198	-556.30433	1
263	H	73.72848	78.50166	64.80126	-64.66664	395.18769	2695.05373	1
264	H	73.84991	78.03806	66.51973	-2703.44278	-60.40056	333.79418	1
265	C	74.93862	79.84628	66.00222	-519.76435	377.31045	459.42366	1
266	H	75.75048	80.12286	65.28599	-1746.74323	1667.50644	-1261.73691	1
267	C	73.81602	80.86656	65.86707	570.95554	16.46261	-545.27700	1
268	H	74.16948	81.90357	66.10210	2391.58273	28.05277	-1305.07271	1
269	H	73.39902	80.88742	64.82682	175.75588	917.63458	2559.43867	1
270	H	72.96525	80.63904	66.55991	-1063.97851	-2155.34650	1283.00462	1
271	C	75.51066	79.87861	67.41242	193.76014	2.62946	-765.53141	1
272	H	75.86974	80.90311	67.68795	507.39394	-846.55087	2539.60089	1
273	H	74.75083	79.57500	68.17848	1337.57841	1818.19054	1526.01994	1
274	H	76.38768	79.18592	67.51862	1100.88635	-1172.91350	-2199.08909	1
275	C	75.10805	76.03329	64.98401	-549.21115	475.64486	-309.38218	1
276	O	74.28584	75.80077	64.13853	556.06106	-390.37755	-78.24250	1
277	O	75.55607	75.02106	65.86626	-572.27940	-310.19032	-209.75862	1
278	H	76.26294	75.52927	66.34885	-1380.08193	2212.14486	790.85944	1

Listing 29: C00029.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.9222	0.0000	300.0000
3	H	73.83440	70.01963	87.99284	-2043.14101	-1757.64893	399.89339		1
4	N	74.78120	69.79032	87.69688	426.75047	490.45733	-334.42467		1
5	H	75.14626	69.30328	88.51221	442.25559	-1110.30854	-2448.52907		1
6	C	75.54966	70.88451	87.25121	415.32972	-666.39213	83.73172		1
7	H	74.82964	71.51831	86.69253	879.32219	2491.00447	667.35213		1
8	C	76.19753	71.66164	88.50589	31.35357	477.41777	628.23362		1
9	H	76.70398	70.93351	89.18436	1168.38489	2240.25337	-1019.71136		1
10	H	76.99833	72.34949	88.14062	-360.43770	2534.90498	931.67112		1
11	C	75.13385	72.43230	89.24405	463.18208	512.70242	-382.34388		1
12	H	74.29215	71.74408	89.48125	1725.29117	1863.52247	-987.07854		1
13	C	75.69353	72.97892	90.55172	710.42801	-144.27427	-313.15367		1
14	H	74.91991	73.55142	91.12576	364.20195	-1033.13725	2494.72524		1
15	H	76.06501	72.15898	91.21915	2567.61904	335.80679	847.48802		1
16	H	76.55375	73.67422	90.37108	-2587.99029	680.92867	-512.16411		1
17	C	74.60375	73.58495	88.40182	268.17616	741.64379	-40.42634		1
18	H	73.85450	74.19836	88.96568	1283.54314	-1945.37420	-1411.27812		1
19	H	75.42802	74.27603	88.08688	-1258.57796	1317.15249	-2026.02085		1
20	H	74.09974	73.22507	87.46851	-2502.84526	909.80597	575.92391		1
21	C	76.78977	70.38921	86.33298	619.36578	-458.64843	-172.09273		1
22	O	77.64726	71.19038	86.01652	-81.40433	433.87611	522.34594		1
23	N	76.69998	69.10797	85.96637	175.23996	-622.20190	341.55523		1

24	H	75.89340	68.57875	86.29661	-876.57256	-303.22879	-2561.90213	1
25	C	77.63604	68.60542	85.02724	-571.88214	-534.10783	-106.15033	1
26	H	78.39594	69.41934	84.93387	-2713.20841	-16.25800	-248.80809	1
27	C	78.18424	67.19936	85.56670	166.60354	288.16399	-716.09568	1
28	H	77.33681	66.46044	85.51265	-2097.85574	1636.78449	-586.18044	1
29	O	78.66401	67.19451	86.92187	-317.80580	-363.38227	484.43082	1
30	H	78.03126	66.58075	87.34652	1863.74748	-1451.84923	1357.29467	1
31	C	79.25741	66.82810	84.47785	503.80731	517.99032	318.51606	1
32	H	79.68677	65.81562	84.66027	640.61020	-2157.10410	-1536.29104	1
33	H	78.82104	66.82371	83.44988	1687.88455	465.60692	2087.56452	1
34	H	80.10572	67.55138	84.47856	-1293.07895	-1899.88581	-1463.57452	1
35	C	76.81650	68.25862	83.65244	-153.07550	-733.68902	248.70981	1
36	O	76.55261	67.10302	83.44458	186.15459	-480.78787	-449.34387	1
37	N	76.48598	69.34624	82.94217	-487.53139	543.18517	42.03850	1
38	C	75.99671	69.24300	81.60262	-699.35871	69.34393	360.10701	1
39	H	75.61298	68.20761	81.44860	2.81126	-221.99807	-2715.58072	1
40	C	74.90877	70.41137	81.61574	-507.46439	-592.59194	122.07761	1
41	H	74.59098	70.71984	80.59533	-1975.08116	525.87560	-1801.71556	1
42	H	73.98849	70.10640	82.16131	1588.27743	-1913.22100	1113.83566	1
43	C	75.68374	71.52481	82.38212	-613.62442	-457.55993	-194.14490	1
44	H	76.43090	72.01548	81.71416	1707.54637	-721.27992	1996.92523	1
45	H	75.02968	72.33232	82.78348	758.23357	2100.81767	1560.55011	1
46	C	76.41108	70.68369	83.51652	-352.41524	704.96076	49.21465	1
47	H	77.45375	71.01362	83.74610	1714.76886	-2070.42778	443.35792	1
48	H	75.84325	70.57797	84.47336	1224.15040	1801.50881	1636.97633	1
49	C	77.17998	69.68466	80.57545	566.85117	537.05831	117.62814	1
50	O	77.97970	70.58166	80.83983	-550.26779	-406.08867	4.21666	1
51	N	77.07949	68.98197	79.46436	566.34832	-425.77725	180.18749	1
52	H	76.31772	68.30502	79.43255	644.44502	2646.80550	-52.73430	1
53	C	77.53432	69.62677	78.25874	612.34801	-281.48662	411.56221	1
54	H	77.37079	70.71419	78.43534	1667.23498	-1490.75142	1556.16753	1
55	C	79.08333	69.30362	78.11339	-714.45746	-175.43074	286.98927	1
56	H	79.26040	68.18967	78.06255	-787.09484	1763.03619	-1922.46060	1
57	O	79.92935	69.67437	79.22044	-429.46514	516.51932	-128.40526	1
58	H	79.23668	70.07157	79.85408	1981.82785	436.16847	-1818.18182	1
59	C	79.42154	69.93545	76.71902	630.79189	-468.94448	76.03230	1
60	H	80.47810	69.73093	76.42641	-1775.71861	2062.30353	131.89849	1
61	H	78.76653	69.53413	75.90996	-1855.14608	88.94118	1993.53760	1
62	H	79.28949	71.04280	76.73036	-1504.82350	-780.94249	-2132.90992	1
63	C	76.65850	69.03256	77.02238	288.57638	618.62814	-397.00270	1
64	O	76.05801	69.80845	76.29380	321.70495	-185.26452	574.37218	1
65	N	76.62841	67.67114	76.98182	-447.05792	-446.53431	367.76425	1
66	H	77.21849	67.43864	77.79601	350.31316	1975.63644	-1843.31522	1
67	C	77.02009	67.04442	75.73363	-511.23061	374.03917	-471.51480	1
68	H	78.02873	67.44578	75.49688	2234.79579	-898.70890	-1273.45190	1
69	C	77.03776	65.49060	76.06727	529.53781	-159.34528	563.72604	1
70	H	77.34135	64.93963	75.13603	654.59388	2347.94251	1217.51488	1
71	H	77.84566	65.31991	76.82500	-1526.55661	2103.42026	817.87394	1
72	O	75.76715	64.91267	76.50840	-554.84278	14.12789	399.58769	1
73	H	75.73957	65.27759	77.40872	1297.06236	2061.84854	1220.68812	1
74	C	75.97780	67.23985	74.52642	-662.15484	-412.13544	123.62687	1
75	O	76.17964	66.66700	73.47690	-540.01537	-317.05804	274.91456	1
76	N	74.94770	68.02373	74.85700	-202.76299	-690.00100	-131.49145	1
77	H	74.95178	68.52390	75.76888	-702.62132	-2617.37191	281.70413	1
78	C	73.85861	68.11998	73.95269	-491.73914	576.34187	222.73509	1
79	H	74.19462	67.51863	73.07513	1977.17978	-1823.58850	-434.68928	1
80	C	72.62300	67.48107	74.71717	-649.50797	-328.66843	306.11224	1
81	H	72.42375	68.02616	75.66481	2075.07803	1452.16490	-1004.45904	1
82	C	71.36124	67.47449	73.78844	-615.18735	-489.99689	-70.96352	1
83	H	70.47654	67.03178	74.30377	-1226.32661	-1724.38906	-1716.47170	1
84	H	71.07750	68.50365	73.46659	2381.64273	-969.84735	900.46860	1
85	H	71.53907	66.87823	72.86326	2122.74991	1702.23946	-141.36228	1

86	C	72.97347	65.98451	75.02940	-501.86074	-479.61276	-376.42482	1
87	H	72.16944	65.48554	75.61993	993.79261	-2246.95401	-1177.81305	1
88	H	73.11422	65.39437	74.09363	42.71279	-626.15391	-2651.37258	1
89	H	73.92403	65.89635	75.61460	-2026.39012	-1590.33709	-887.82922	1
90	C	73.74990	69.73244	73.62437	-672.89153	382.57394	-156.34072	1
91	O	74.58977	70.23138	72.91286	410.04627	221.86223	500.35950	1
92	N	72.70358	70.30556	74.20067	-378.11782	-443.79414	-441.10984	1
93	H	72.11697	69.71625	74.78891	2404.15973	-568.14894	1149.30085	1
94	C	72.58555	71.72540	74.28509	-544.54484	466.16019	331.29119	1
95	H	71.69964	71.85925	74.94693	-1409.80988	-170.17955	2325.32679	1
96	C	73.93801	72.29037	74.90164	-184.48284	116.78282	-758.89137	1
97	H	74.20314	71.74957	75.83925	1893.78641	1861.14652	611.04528	1
98	H	74.78883	72.10886	74.20291	-2170.79665	-974.19311	1327.50117	1
99	C	73.69451	73.80899	75.16848	389.51668	672.81878	-138.49152	1
100	H	73.82064	74.38407	74.22119	510.64577	1933.03327	1851.02484	1
101	H	72.63644	73.98012	75.46539	-2302.30869	-1105.72939	-948.89774	1
102	C	74.62654	74.39330	76.30880	-559.93427	-126.34590	542.30857	1
103	O	74.28329	75.30987	77.01384	-670.36003	-111.83166	76.36448	1
104	N	75.85159	73.74894	76.37652	-216.06729	-537.07037	446.51379	1
105	H	76.26003	73.39304	75.49747	-1251.96487	1074.12894	-2168.52500	1
106	H	76.59851	74.31070	76.79914	-2451.83023	-720.73851	944.84612	1
107	C	72.41155	72.38313	72.80962	546.24052	-563.88337	-85.11809	1
108	O	73.28974	73.12464	72.39141	71.70702	-307.40463	606.69673	1
109	N	71.22608	72.10160	72.27706	479.90863	-504.50129	222.86849	1
110	C	70.95161	72.29597	70.87952	75.51268	-600.91904	506.73700	1
111	H	71.81736	71.87398	70.32108	-2033.61562	1795.30103	254.89480	1
112	C	69.58799	71.50859	70.69621	523.79067	517.99274	284.45581	1
113	H	69.01122	71.84757	69.80625	1599.61665	-1127.00911	1895.98173	1
114	H	69.75945	70.41619	70.57110	-1881.83093	1275.82488	-1501.55016	1
115	C	68.87273	71.81618	72.04987	-600.05639	-404.05026	316.64485	1
116	H	68.45706	72.84870	72.05504	-2597.05260	496.36221	657.73249	1
117	H	68.02469	71.13081	72.27447	-1666.24518	1294.38985	-1723.90591	1
118	C	70.07912	71.67439	73.07154	493.57570	-129.95376	-602.56394	1
119	H	70.01381	72.32286	73.97629	-1469.08415	-637.84797	2204.22581	1
120	H	70.30301	70.62696	73.38212	-1038.97840	1068.88701	-2280.71789	1
121	C	70.72803	73.87821	70.54317	188.88100	241.05089	-727.87821	1
122	O	70.37627	74.22196	69.44180	531.88613	-49.19943	427.07960	1
123	N	70.95353	74.64630	71.61132	708.14833	26.93417	-179.73509	1
124	H	71.30086	74.13600	72.43017	-2232.69501	-1179.09831	1023.94816	1
125	C	70.80465	76.09419	71.56929	-738.32412	259.92548	104.42456	1
126	H	70.00759	76.26184	70.80545	2028.89123	1260.02983	1311.33324	1
127	C	70.43352	76.55858	72.96784	-258.65678	-345.52513	661.28459	1
128	H	71.25357	76.25604	73.65722	-1826.06090	-1801.46097	-918.64554	1
129	C	70.28819	78.06725	73.04408	-541.23400	531.92970	-218.41428	1
130	H	69.99516	78.40807	74.07501	1311.73218	-2219.18200	882.19023	1
131	H	71.25231	78.58291	72.78091	-1048.71298	1223.58118	-2196.97971	1
132	H	69.50517	78.44608	72.33102	419.06414	1903.92898	1903.44670	1
133	C	69.15810	75.89138	73.45177	-423.86431	152.66566	-648.55262	1
134	H	68.90881	76.18155	74.50890	105.68386	-2342.50080	1387.51238	1
135	H	68.27834	76.17483	72.81137	-1695.63603	-1484.73621	-1531.02793	1
136	H	69.24101	74.77039	73.41963	-1853.57121	-487.39031	1936.59343	1
137	C	72.24321	76.77610	71.07638	539.71428	-510.58232	267.58633	1
138	O	72.25388	77.95769	70.82344	-15.93758	-278.34085	-624.49402	1
139	N	73.29067	75.93191	71.14338	-676.81886	12.05292	276.17960	1
140	H	72.86375	75.04151	71.42743	-1694.44250	-373.84189	-2100.66098	1
141	C	74.24656	75.87814	70.04378	412.33078	-664.70360	108.35451	1
142	H	73.83907	75.02995	69.45049	1765.77476	1294.44366	1621.76594	1
143	C	74.19322	77.22506	69.23313	-179.66635	-721.95667	-264.73915	1
144	H	73.16635	77.37957	68.82559	-607.34922	2587.87032	-598.10018	1
145	H	74.35613	78.07767	69.93421	-359.69332	-1479.13954	-2259.74260	1
146	C	75.21478	77.25672	68.04472	-240.01076	616.02425	431.85322	1
147	H	76.25464	77.10523	68.41510	-1359.17131	782.54425	2227.99181	1

148	H	75.02425	76.43419	67.31983	-820.36667	85.81767	-2596.78715	1
149	C	75.04614	78.67286	67.36089	-513.07015	236.18570	-551.87280	1
150	H	74.07326	78.73538	66.82155	1816.11944	-1183.11722	-1650.94321	1
151	H	75.00905	79.48091	68.12595	-1800.04429	-1361.53473	1526.34643	1
152	C	76.23117	78.91553	66.39689	726.08972	-253.19732	-179.64713	1
153	H	77.23295	78.77721	66.85000	1224.27271	-456.51798	-2390.90304	1
154	H	76.17111	78.36957	65.43411	1206.40339	-1150.93514	-2154.90344	1
155	N	76.21082	80.43450	66.02027	329.70796	-633.68968	-155.67358	1
156	H	76.98292	80.75306	65.36667	1348.31305	1938.76845	1359.00643	1
157	H	75.34679	80.81561	65.53530	2096.92035	1446.54551	-966.48890	1
158	H	76.33330	81.11289	66.82662	-1197.07217	-2303.53719	827.28733	1
159	C	75.66952	75.47564	70.66215	-378.01186	-556.17301	-413.96481	1
160	O	76.72425	75.96385	70.23815	-409.44433	-307.55053	-453.30833	1
161	N	75.50396	74.51371	71.53366	-429.02477	524.70884	274.08502	1
162	H	74.53604	74.18572	71.76972	1706.34263	-1425.96036	1574.38926	1
163	C	76.56662	73.85403	72.20096	-45.25864	-626.22952	478.93267	1
164	H	76.02842	73.06328	72.77055	1988.63164	570.90773	1772.87287	1
165	C	77.60765	73.26966	71.15738	551.77128	-20.49526	-564.54996	1
166	H	77.15516	72.45496	70.54903	1434.61535	-1753.10253	1513.99471	1
167	H	77.92932	74.04702	70.42692	-714.67738	1819.09770	1898.36494	1
168	C	78.81531	72.75034	72.00590	446.99263	-555.77305	338.97221	1
169	H	79.21034	73.57314	72.64813	1953.68466	1892.25957	-161.67766	1
170	H	78.48321	71.95226	72.70718	-403.03785	2688.07032	-188.43591	1
171	C	79.96838	72.21683	71.06532	567.86262	335.74681	434.04421	1
172	H	79.63493	71.33050	70.47825	-1080.02275	1568.26081	-1948.78900	1
173	H	80.26844	72.98614	70.31708	-919.54108	2111.34692	1456.13463	1
174	C	81.14749	71.86407	72.00327	195.81897	173.33862	-745.11536	1
175	H	81.58791	72.73300	72.53416	1405.67949	-2301.21089	-390.08113	1
176	H	80.93207	71.05169	72.72587	-940.37328	-1118.32446	2299.72133	1
177	N	82.31616	71.30412	71.12659	319.26422	656.36007	-42.02424	1
178	H	83.18284	71.00716	71.66176	1961.03633	619.91968	1787.09422	1
179	H	82.11727	70.43277	70.55363	854.14343	-2156.80752	1429.08711	1
180	H	82.73564	71.95513	70.40076	1237.02905	-1378.50857	-1998.28500	1
181	C	77.38962	74.86861	73.20547	532.53319	-268.57236	517.55729	1
182	O	77.34117	74.67143	74.39800	266.16714	-290.73804	-558.88002	1
183	N	78.09845	75.73651	72.50921	-226.25352	640.49678	-270.32839	1
184	H	77.99774	75.75361	71.47160	2007.69063	-1035.27229	1523.50231	1
185	C	78.93246	76.65196	73.19818	-540.76542	-573.33303	49.50000	1
186	H	78.83181	76.38270	74.27628	-2374.20950	-1036.76023	843.75774	1
187	C	80.41312	76.42384	72.61456	-77.09082	666.87422	-415.84136	1
188	H	80.39534	76.65057	71.51326	-985.81834	617.19825	2463.91927	1
189	O	80.91740	75.07878	72.72569	293.29899	-391.65602	-477.80926	1
190	H	81.05092	74.85838	71.78115	2528.72714	-681.76262	-751.27122	1
191	C	81.27913	77.51299	73.34231	252.47363	-605.14473	440.05134	1
192	H	82.35491	77.42808	73.06193	-2052.65063	1456.49051	-1043.51830	1
193	H	80.95701	78.55094	73.08358	-2152.98800	-1661.97574	-161.70652	1
194	H	81.21709	77.41205	74.45104	-473.12726	-1584.27339	2165.61725	1
195	C	78.45790	78.17401	72.85502	360.36307	488.46713	505.10056	1
196	O	78.85441	79.08836	73.53686	-200.08817	-528.03552	-385.82850	1
197	N	77.75376	78.24786	71.72210	-597.54095	-226.44775	355.20479	1
198	H	77.39248	77.39467	71.26655	2179.23655	-1300.70981	-991.33835	1
199	C	77.02373	79.45798	71.53337	-687.68921	297.39807	-249.45179	1
200	H	77.63768	80.26423	71.99924	-349.16256	-2467.37713	-1101.72831	1
201	C	76.72152	79.62519	69.97270	672.47345	361.54328	-201.62880	1
202	H	76.01186	78.82025	69.68508	1541.41502	582.18425	2169.97026	1
203	H	76.21039	80.59598	69.78080	-2534.67717	60.25153	997.72295	1
204	C	77.97802	79.49940	69.10236	574.26774	-389.43119	-377.02542	1
205	C	78.57277	80.66871	68.53915	688.82679	-287.33580	-257.96133	1
206	H	78.18407	81.67489	68.77939	331.14182	1470.38163	2269.80013	1
207	C	78.49224	78.19914	68.80691	-383.52382	-675.04808	144.24917	1
208	H	78.03606	77.29277	69.26577	4.09847	1517.59662	2262.86397	1
209	C	79.64156	80.50697	67.65876	-134.76730	428.45285	-649.50303	1

210	H	80.09842	81.40696	67.21146	-903.23433	1600.49020	2011.53387	1
211	C	79.56137	78.09375	67.91466	-335.53281	-615.00040	-364.39058	1
212	H	79.94336	77.08617	67.67508	1596.45398	-1369.33862	1732.02659	1
213	C	80.16812	79.23108	67.30429	585.48547	-340.24194	-406.23938	1
214	O	81.24818	79.13312	66.38904	-419.15649	-173.04408	-511.94141	1
215	H	81.35280	78.15285	66.35976	-1071.84350	1559.71507	-1960.13012	1
216	C	75.57889	79.22279	72.24958	291.41878	-183.13091	710.72246	1
217	O	75.25995	78.21185	72.83117	379.87695	523.47396	-222.23622	1
218	N	74.85353	80.31895	72.05507	564.30591	373.09380	277.24371	1
219	H	75.22571	81.15242	71.59977	-120.59931	-2436.07824	-1214.35098	1
220	C	73.54126	80.35906	72.64101	404.07514	-299.37480	608.84009	1
221	H	73.03752	79.40426	72.35880	-1071.07882	-841.69025	2359.66467	1
222	C	73.83918	80.44252	74.19849	-683.12807	68.71770	-390.13096	1
223	H	74.54672	79.62703	74.47886	2068.88918	1596.58590	770.89603	1
224	H	74.37300	81.39078	74.43140	1379.86429	2342.49779	-179.85638	1
225	C	72.53309	80.32623	75.03857	-176.39967	537.49466	550.97268	1
226	H	71.82637	81.16167	74.83563	-396.28051	1942.22168	1869.33314	1
227	H	71.97683	79.38956	74.81377	-94.44700	586.00678	-2659.20016	1
228	C	73.07760	80.34335	76.54304	-291.69381	-718.18079	-150.72929	1
229	H	73.63766	79.41792	76.83572	-2303.38776	1089.76242	964.62032	1
230	H	73.70960	81.23185	76.82235	884.16729	2568.80533	-207.74283	1
231	N	71.91545	80.38144	77.32044	-594.49522	-252.81478	342.29276	1
232	H	71.05549	80.13141	76.85734	-1735.17426	2084.05705	-263.71605	1
233	C	71.88637	80.67532	78.55741	595.23177	-271.52487	442.22352	1
234	N	73.09634	81.00448	79.17887	585.53813	-424.79750	-105.81303	1
235	H	74.04267	80.99638	78.80047	959.88797	1327.56823	-2177.11905	1
236	H	73.20124	81.21906	80.17090	1578.48647	16.27378	-2220.76233	1
237	N	70.57951	80.60770	79.05787	-452.17763	-390.33541	-421.51853	1
238	H	69.70306	80.34731	78.60794	470.26107	1974.25629	-1817.92087	1
239	H	70.34902	80.78342	80.03678	1856.67307	-1573.97321	-1224.35416	1
240	C	72.87322	81.71432	72.06387	-531.47271	-581.45780	-55.06206	1
241	O	73.54541	82.70991	71.80742	-243.00837	192.73507	609.52485	1
242	N	71.55968	81.57864	72.01003	343.49288	-644.25607	38.09164	1
243	H	71.20411	80.67341	72.31054	-1691.16043	-1535.97525	-1484.73099	1
244	C	70.73777	82.53251	71.26411	542.66492	350.14337	454.42563	1
245	H	71.45170	82.92185	70.49869	1209.57979	-2396.95920	463.86744	1
246	C	69.54155	81.79727	70.68606	-737.14309	145.93010	242.71942	1
247	H	68.93259	81.41366	71.53457	-1050.18303	159.36419	-2509.06125	1
248	C	68.67037	82.72417	69.85831	-706.77696	-252.88343	-245.16230	1
249	H	67.74840	82.20292	69.47908	-1624.64039	-1665.49085	1417.86935	1
250	H	68.33213	83.61335	70.46106	2566.10521	598.51109	693.22305	1
251	H	69.22099	83.11932	68.96014	-1972.69758	107.10018	-1876.34312	1
252	C	69.97339	80.60700	69.84798	412.85148	672.58832	-27.69222	1
253	H	69.09501	79.99985	69.49662	1447.02277	1762.76533	-1490.78944	1
254	H	70.53974	80.93334	68.93298	1320.77379	-145.20455	2378.68491	1
255	H	70.65186	79.91457	70.41988	-1512.10848	1470.52031	1724.75147	1
256	C	70.37304	83.70583	72.38659	-607.11113	499.56689	73.73769	1
257	O	69.24555	83.95714	72.72138	357.97126	460.81534	356.68785	1
258	N	71.50828	84.26996	72.75851	536.55407	-368.62270	332.76306	1
259	H	72.41216	83.94094	72.34521	524.38866	2297.69985	1367.20941	1
260	C	71.48211	85.23256	73.79790	46.50277	-774.29190	-147.97904	1
261	H	70.52707	85.03757	74.33702	1676.51875	1883.29066	1032.55549	1
262	C	72.82837	85.11938	74.67975	-559.41456	-34.19198	-556.30433	1
263	H	73.71100	85.25207	74.00863	-64.66664	395.18769	2695.05373	1
264	H	72.87492	85.95943	75.41378	-2703.44278	-60.40056	333.79418	1
265	C	72.90709	83.79187	75.38601	-519.76435	377.31045	459.42366	1
266	H	72.75539	82.98617	74.63320	-1746.74323	1667.50644	-1261.73691	1
267	C	74.28112	83.61616	76.02009	570.95554	16.46261	-545.27700	1
268	H	74.35546	82.64759	76.59239	2391.58273	28.05277	-1305.07271	1
269	H	75.09529	83.61450	75.24995	175.75588	917.63458	2559.43867	1
270	H	74.51004	84.44395	76.73998	-1063.97851	-2155.34650	1283.00462	1
271	C	71.83774	83.66772	76.46309	193.76014	2.62946	-765.53141	1

272	H	71.94236	82.71414	77.04292	507.39394	-846.55087	2539.60089	1
273	H	71.89623	84.50950	77.20060	1337.57841	1818.19054	1526.01994	1
274	H	70.80582	83.67734	76.02720	1100.88635	-1172.91350	-2199.08909	1
275	C	71.49093	86.66643	73.05543	-549.21115	475.64486	-309.38218	1
276	O	72.38312	87.46463	73.16343	556.06106	-390.37755	-78.24250	1
277	O	70.34789	86.94607	72.27252	-572.27940	-310.19032	-209.75862	1
278	H	69.88056	86.06195	72.35948	-1380.08193	2212.14486	790.85944	1

Listing 30: C00030.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.7397	2959
		0.2500	300.00	0.00	0.00	0.00	-1293.9175	0.0000	300.0000
3	H	78.62264	63.84704	87.94986	-2043.14101	-1757.64893	399.89339		1
4	N	78.80462	64.55328	87.23881	426.75047	490.45733	-334.42467		1
5	H	77.97384	65.13605	87.32135	442.25559	-1110.30854	-2448.52907		1
6	C	80.02957	65.23756	87.40265	415.32972	-666.39213	83.73172		1
7	H	80.65037	64.57071	88.03759	879.32219	2491.00447	667.35213		1
8	C	80.66873	65.48275	85.94383	31.35357	477.41777	628.23362		1
9	H	80.00100	66.13560	85.33121	1168.38489	2240.25337	-1019.71136		1
10	H	81.64006	66.02772	86.02156	-360.43770	2534.90498	931.67112		1
11	C	80.84798	64.14299	85.27530	463.18208	512.70242	-382.34388		1
12	H	79.95403	63.51880	85.50195	1725.29117	1863.52247	-987.07854		1
13	C	80.94098	64.31424	83.76495	710.42801	-144.27427	-313.15367		1
14	H	81.07976	63.33318	83.24118	364.20195	-1033.13725	2494.72524		1
15	H	80.01350	64.78934	83.34534	2567.61904	335.80679	847.48802		1
16	H	81.80065	64.97304	83.47507	-2587.99029	680.92867	-512.16411		1
17	C	82.08888	63.43087	85.79501	268.17616	741.64379	-40.42634		1
18	H	82.22175	62.42742	85.31394	1283.54314	-1945.37420	-1411.27812		1
19	H	83.01884	64.02211	85.59024	-1258.57796	1317.15249	-2026.02085		1
20	H	82.03890	63.26436	86.90190	-2502.84526	909.80597	575.92391		1
21	C	79.69309	66.66772	88.11414	619.36578	-458.64843	-172.09273		1
22	O	80.20702	66.96994	89.19762	-81.40433	433.87611	522.34594		1
23	N	78.87909	67.34351	87.35504	175.23996	-622.20190	341.55523		1
24	H	78.57444	66.84374	86.52174	-876.57256	-303.22879	-2561.90213		1
25	C	78.45684	68.70215	87.54243	-571.88214	-534.10783	-106.15033		1
26	H	77.36795	68.60161	87.74491	-2713.20841	-16.25800	-248.80809		1
27	C	79.22574	69.39868	88.76163	166.60354	288.16399	-716.09568		1
28	H	80.32794	69.17174	88.65973	-2097.85574	1636.78449	-586.18044		1
29	O	78.86735	68.91134	90.05247	-317.80580	-363.38227	484.43082		1
30	H	79.52871	68.11441	90.11419	1863.74748	-1451.84923	1357.29467		1
31	C	78.97679	70.92629	88.49403	503.80731	517.99032	318.51606		1
32	H	79.49466	71.56042	89.25029	640.61020	-2157.10410	-1536.29104		1
33	H	79.34559	71.23889	87.48909	1687.88455	465.60692	2087.56452		1
34	H	77.89149	71.17584	88.54238	-1293.07895	-1899.88581	-1463.57452		1
35	C	78.61735	69.39211	86.09339	-153.07550	-733.68902	248.70981		1
36	O	77.54996	69.61358	85.50258	186.15459	-480.78787	-449.34387		1
37	N	79.84785	69.63009	85.68120	-487.53139	543.18517	42.03850		1
38	C	80.12171	70.44205	84.51955	-699.35871	69.34393	360.10701		1
39	H	79.44303	71.32288	84.58983	2.81126	-221.99807	-2715.58072		1
40	C	81.67854	70.72156	84.62562	-507.46439	-592.59194	122.07761		1
41	H	82.13626	70.92433	83.62872	-1975.08116	525.87560	-1801.71556		1
42	H	81.90337	71.59761	85.27464	1588.27743	-1913.22100	1113.83566		1
43	C	82.18325	69.38811	85.26463	-613.62442	-457.55993	-194.14490		1
44	H	82.22632	68.57688	84.50315	1707.54637	-721.27992	1996.92523		1
45	H	83.20038	69.46216	85.71150	758.23357	2100.81767	1560.55011		1
46	C	81.04579	69.11512	86.33715	-352.41524	704.96076	49.21465		1
47	H	80.86962	68.04469	86.58973	1714.76886	-2070.42778	443.35792		1
48	H	81.16162	69.70412	87.27785	1224.15040	1801.50881	1636.97633		1
49	C	79.93027	69.59125	83.14938	566.85117	537.05831	117.62814		1
50	O	80.89033	69.44944	82.39681	-550.26779	-406.08867	4.21666		1
51	N	78.69246	69.17712	82.99052	566.34832	-425.77725	180.18749		1

52	H	77.99311	69.33588	83.73924	644.44502	2646.80550	-52.73430	1
53	C	78.38218	68.52665	81.75072	612.34801	-281.48662	411.56221	1
54	H	78.99422	69.13007	81.04032	1667.23498	-1490.75142	1556.16753	1
55	C	78.89653	67.01900	81.79693	-714.45746	-175.43074	286.98927	1
56	H	78.20548	66.37928	82.41403	-787.09484	1763.03619	-1922.46060	1
57	O	80.18786	66.79610	82.39308	-429.46514	516.51932	-128.40526	1
58	H	80.56168	67.72812	82.34858	1981.82785	436.16847	-1818.18182	1
59	C	78.75512	66.57453	80.29905	630.79189	-468.94448	76.03230	1
60	H	79.01239	65.49760	80.16887	-1775.71861	2062.30353	131.89849	1
61	H	77.71427	66.71541	79.91790	-1855.14608	88.94118	1993.53760	1
62	H	79.43482	67.15798	79.63484	-1504.82350	-780.94249	-2132.90992	1
63	C	76.77177	68.61099	81.52598	288.57638	618.62814	-397.00270	1
64	O	76.13418	67.63289	81.21143	321.70495	-185.26452	574.37218	1
65	N	76.32884	69.88555	81.62111	-447.05792	-446.53431	367.76425	1
66	H	77.04956	70.50945	81.99042	350.31316	1975.63644	-1843.31522	1
67	C	74.98348	69.99534	82.12054	-511.23061	374.03917	-471.51480	1
68	H	74.48960	69.03704	81.83378	2234.79579	-898.70890	-1273.45190	1
69	C	75.10437	70.17757	83.70317	529.53781	-159.34528	563.72604	1
70	H	74.05419	70.31281	84.07836	654.59388	2347.94251	1217.51488	1
71	H	75.47416	69.21387	84.14688	-1526.55661	2103.42026	817.87394	1
72	O	75.92405	71.26292	84.16615	-554.84278	14.12789	399.58769	1
73	H	76.62395	70.73598	84.67744	1297.06236	2061.84854	1220.68812	1
74	C	74.22632	71.30189	81.55090	-662.15484	-412.13544	123.62687	1
75	O	73.08199	71.51039	81.88006	-540.01537	-317.05804	274.91456	1
76	N	74.96346	72.03886	80.69424	-202.76299	-690.00100	-131.49145	1
77	H	75.90940	71.67891	80.56321	-702.62132	-2617.37191	281.70413	1
78	C	74.64662	73.46783	80.56891	-491.73914	576.34187	222.73509	1
79	H	73.72195	73.59308	81.18206	1977.17978	-1823.58850	-434.68928	1
80	C	75.83600	74.27082	81.05348	-649.50797	-328.66843	306.11224	1
81	H	76.71324	73.98489	80.43084	2075.07803	1452.16490	-1004.45904	1
82	C	75.60593	75.76274	80.88893	-615.18735	-489.99689	-70.96352	1
83	H	76.50229	76.35991	81.21261	-1226.32661	-1724.38906	-1716.47170	1
84	H	75.39132	76.03207	79.81802	2381.64273	-969.84735	900.46860	1
85	H	74.73162	76.11638	81.50135	2122.74991	1702.23946	-141.36228	1
86	C	76.17379	73.95807	82.49998	-501.86074	-479.61276	-376.42482	1
87	H	77.12143	74.46527	82.83133	993.79261	-2246.95401	-1177.81305	1
88	H	75.35552	74.28960	83.19706	42.71279	-626.15391	-2651.37258	1
89	H	76.30845	72.85124	82.66011	-2026.39012	-1590.33709	-887.82922	1
90	C	74.41708	73.76022	78.94923	-672.89153	382.57394	-156.34072	1
91	O	75.31791	73.67970	78.14932	410.04627	221.86223	500.35950	1
92	N	73.17728	74.19428	78.75464	-378.11782	-443.79414	-441.10984	1
93	H	72.56484	74.20186	79.56872	2404.15973	-568.14894	1149.30085	1
94	C	72.64035	74.11072	77.43388	-544.54484	466.16019	331.29119	1
95	H	73.53311	73.94809	76.78635	-1409.80988	-170.17955	2325.32679	1
96	C	71.62090	72.89552	77.45396	-184.48284	116.78282	-758.89137	1
97	H	72.12345	71.97112	77.81993	1893.78641	1861.14652	611.04528	1
98	H	70.78931	73.09344	78.16716	-2170.79665	-974.19311	1327.50117	1
99	C	71.07883	72.70885	76.00368	389.51668	672.81878	-138.49152	1
100	H	70.56554	73.64232	75.67418	510.64577	1933.03327	1851.02484	1
101	H	71.92184	72.59172	75.28745	-2302.30869	-1105.72939	-948.89774	1
102	C	70.09661	71.48514	75.86141	-559.93427	-126.34590	542.30857	1
103	O	69.64394	71.21633	74.77864	-670.36003	-111.83166	76.36448	1
104	N	69.84958	70.82993	77.01601	-216.06729	-537.07037	446.51379	1
105	H	70.19438	71.01515	77.96505	-1251.96487	1074.12894	-2168.52500	1
106	H	69.22362	70.02100	77.09172	-2451.83023	-720.73851	944.84612	1
107	C	71.82209	75.49413	77.13567	546.24052	-563.88337	-85.11809	1
108	O	70.62297	75.46773	77.04734	71.70702	-307.40463	606.69673	1
109	N	72.65999	76.53099	76.97020	479.90863	-504.50129	222.86849	1
110	C	72.22630	77.87522	77.17436	75.51268	-600.91904	506.73700	1
111	H	71.36439	77.84305	77.87918	-2033.61562	1795.30103	254.89480	1
112	C	73.56060	78.53705	77.73485	523.79067	517.99274	284.45581	1
113	H	73.55186	79.64759	77.66891	1599.61665	-1127.00911	1895.98173	1

114	H	73.72912	78.27668	78.80352	-1881.83093	1275.82488	-1501.55016	1
115	C	74.62706	77.86800	76.81453	-600.05639	-404.05026	316.64485	1
116	H	74.62214	78.32455	75.79844	-2597.05260	496.36221	657.73249	1
117	H	75.66851	77.95716	77.19791	-1666.24518	1294.38985	-1723.90591	1
118	C	74.09767	76.37082	76.78471	493.57570	-129.95376	-602.56394	1
119	H	74.26348	75.82831	75.82422	-1469.08415	-637.84797	2204.22581	1
120	H	74.45333	75.73199	77.62957	-1038.97840	1068.88701	-2280.71789	1
121	C	71.85853	78.64885	75.77724	188.88100	241.05089	-727.87821	1
122	O	71.45431	79.79531	75.83091	531.88613	-49.19943	427.07960	1
123	N	72.19130	77.96064	74.67117	708.14833	26.93417	-179.73509	1
124	H	72.45818	77.03006	74.99563	-2232.69501	-1179.09831	1023.94816	1
125	C	71.54208	78.16173	73.37103	-738.32412	259.92548	104.42456	1
126	H	71.73162	77.20872	72.82225	2028.89123	1260.02983	1311.33324	1
127	C	70.06304	78.42310	73.58898	-258.65678	-345.52513	661.28459	1
128	H	69.97416	79.32121	74.24617	-1826.06090	-1801.46097	-918.64554	1
129	C	69.35288	78.72161	72.28104	-541.23400	531.92970	-218.41428	1
130	H	68.26241	78.94731	72.43708	1311.73218	-2219.18200	882.19023	1
131	H	69.80964	79.61058	71.76164	-1048.71298	1223.58118	-2196.97971	1
132	H	69.41706	77.85402	71.56803	419.06414	1903.92898	1903.44670	1
133	C	69.38317	77.26745	74.30029	-423.86431	152.66566	-648.55262	1
134	H	68.30704	77.49748	74.53239	105.68386	-2342.50080	1387.51238	1
135	H	69.39626	76.33176	73.67648	-1695.63603	-1484.73621	-1531.02793	1
136	H	69.89077	77.02094	75.27554	-1853.57121	-487.39031	1936.59343	1
137	C	72.24301	79.45225	72.61461	539.71428	-510.58232	267.58633	1
138	O	72.06828	79.61634	71.42526	-15.93758	-278.34085	-624.49402	1
139	N	72.88968	80.22294	73.46319	-676.81886	12.05292	276.17960	1
140	H	72.88218	79.95713	74.45497	-1694.44250	-373.84189	-2100.66098	1
141	C	73.58684	81.35927	72.96660	412.33078	-664.70360	108.35451	1
142	H	73.11367	81.56390	71.97821	1765.77476	1294.44366	1621.76594	1
143	C	73.44962	82.49080	74.06200	-179.66635	-721.95667	-264.73915	1
144	H	72.38046	82.72399	74.26645	-607.34922	2587.87032	-598.10018	1
145	H	73.87165	82.14407	75.03239	-359.69332	-1479.13954	-2259.74260	1
146	C	74.22104	83.74861	73.54238	-240.01076	616.02425	431.85322	1
147	H	75.28236	83.47775	73.33213	-1359.17131	782.54425	2227.99181	1
148	H	73.79476	84.11025	72.58069	-820.36667	85.81767	-2596.78715	1
149	C	74.15143	84.88137	74.64512	-513.07015	236.18570	-551.87280	1
150	H	73.09845	85.18957	74.84192	1816.11944	-1183.11722	-1650.94321	1
151	H	74.54907	84.51584	75.61991	-1800.04429	-1361.53473	1526.34643	1
152	C	74.99415	86.06189	74.11018	726.08972	-253.19732	-179.64713	1
153	H	76.07189	85.83572	73.98729	1224.27271	-456.51798	-2390.90304	1
154	H	74.59916	86.52862	73.18574	1206.40339	-1150.93514	-2154.90344	1
155	N	74.95773	87.20952	75.17453	329.70796	-633.68968	-155.67358	1
156	H	75.52016	88.07438	74.92746	1348.31305	1938.76845	1359.00643	1
157	H	74.01162	87.63467	75.40057	2096.92035	1446.54551	-966.48890	1
158	H	75.33640	86.98565	76.14060	-1197.07217	-2303.53719	827.28733	1
159	C	75.18740	80.98189	72.84770	-378.01186	-556.17301	-413.96481	1
160	O	75.96341	81.32740	73.70904	-409.44433	-307.55053	-453.30833	1
161	N	75.43349	80.30229	71.73770	-429.02477	524.70884	274.08502	1
162	H	74.65637	80.04557	71.13065	1706.34263	-1425.96036	1574.38926	1
163	C	76.81694	80.11560	71.39271	-45.25864	-626.22952	478.93267	1
164	H	77.28013	81.11708	71.53727	1988.63164	570.90773	1772.87287	1
165	C	77.37727	79.06880	72.43406	551.77128	-20.49526	-564.54996	1
166	H	77.23718	79.44395	73.47608	1434.61535	-1753.10253	1513.99471	1
167	H	76.81292	78.11153	72.37294	-714.67738	1819.09770	1898.36494	1
168	C	78.89063	78.86241	72.09054	446.99263	-555.77305	338.97221	1
169	H	79.00770	78.55265	71.02785	1953.68466	1892.25957	-161.67766	1
170	H	79.45924	79.81345	72.19592	-403.03785	2688.07032	-188.43591	1
171	C	79.45726	77.75236	73.06303	567.86262	335.74681	434.04421	1
172	H	79.38995	78.08037	74.12599	-1080.02275	1568.26081	-1948.78900	1
173	H	78.85489	76.81708	72.99488	-919.54108	2111.34692	1456.13463	1
174	C	80.92539	77.49328	72.65158	195.81897	173.33862	-745.11536	1
175	H	81.04974	77.04595	71.64546	1405.67949	-2301.21089	-390.08113	1

176	H	81.59756	78.36766	72.76105	-940.37328	-1118.32446	2299.72133	1
177	N	81.49810	76.42312	73.63979	319.26422	656.36007	-42.02424	1
178	H	82.50137	76.12604	73.46564	1961.03633	619.91968	1787.09422	1
179	H	81.53425	76.68847	74.66705	854.14343	-2156.80752	1429.08711	1
180	H	81.00420	75.48408	73.67387	1237.02905	-1378.50857	-1998.28500	1
181	C	76.94805	79.50240	69.88169	532.53319	-268.57236	517.55729	1
182	O	76.52801	78.37453	69.59443	266.16714	-290.73804	-558.88002	1
183	N	77.58638	80.37426	69.14825	-226.25352	640.49678	-270.32839	1
184	H	77.81367	81.22067	69.67154	2007.69063	-1035.27229	1523.50231	1
185	C	78.13631	80.21395	67.85398	-540.76542	-573.33303	49.50000	1
186	H	78.45625	81.25217	67.61094	-2374.20950	-1036.76023	843.75774	1
187	C	79.38217	79.20376	67.90609	-77.09082	666.87422	-415.84136	1
188	H	79.01632	78.17240	68.16186	-985.81834	617.19825	2463.91927	1
189	O	80.42284	79.51119	68.84334	293.29899	-391.65602	-477.80926	1
190	H	80.46240	78.68215	69.36395	2528.72714	-681.76262	-751.27122	1
191	C	79.77059	79.26053	66.38201	252.47363	-605.14473	440.05134	1
192	H	80.56937	78.52620	66.12844	-2052.65063	1456.49051	-1043.51830	1
193	H	78.88689	79.04123	65.72868	-2152.98800	-1661.97574	-161.70652	1
194	H	80.14952	80.26888	66.09468	-473.12726	-1584.27339	2165.61725	1
195	C	77.09693	79.59328	66.74512	360.36307	488.46713	505.10056	1
196	O	76.90410	80.22673	65.73683	-200.08817	-528.03552	-385.82850	1
197	N	76.68152	78.37012	67.05419	-597.54095	-226.44775	355.20479	1
198	H	76.89884	77.93503	67.98466	2179.23655	-1300.70981	-991.33835	1
199	C	75.88658	77.70287	66.08434	-687.68921	297.39807	-249.45179	1
200	H	75.98716	78.29845	65.14553	-349.16256	-2467.37713	-1101.72831	1
201	C	76.41979	76.18596	65.96923	672.47345	361.54328	-201.62880	1
202	H	76.51158	75.72059	66.97644	1541.41502	582.18425	2169.97026	1
203	H	75.69205	75.57645	65.38701	-2534.67717	60.25153	997.72295	1
204	C	77.77610	76.23874	65.25936	574.26774	-389.43119	-377.02542	1
205	C	77.77931	76.42470	63.84343	688.82679	-287.33580	-257.96133	1
206	H	76.85815	76.49058	63.26831	331.14182	1470.38163	2269.80013	1
207	C	78.99688	76.15716	65.99616	-383.52382	-675.04808	144.24917	1
208	H	78.98489	76.01951	67.09201	4.09847	1517.59662	2262.86397	1
209	C	79.03251	76.53383	63.20394	-134.76730	428.45285	-649.50303	1
210	H	79.04764	76.68200	62.10999	-903.23433	1600.49020	2011.53387	1
211	C	80.20728	76.26707	65.30835	-335.53281	-615.00040	-364.39058	1
212	H	81.14505	76.20434	65.88788	1596.45398	-1369.33862	1732.02659	1
213	C	80.27547	76.46510	63.89801	585.48547	-340.24194	-406.23938	1
214	O	81.49889	76.59383	63.19097	-419.15649	-173.04408	-511.94141	1
215	H	82.13495	76.49018	63.93773	-1071.84350	1559.71507	-1960.13012	1
216	C	74.35064	77.58737	66.59472	291.41878	-183.13091	710.72246	1
217	O	73.48794	77.33546	65.76047	379.87695	523.47396	-222.23622	1
218	N	74.25503	77.70669	67.89652	564.30591	373.09380	277.24371	1
219	H	75.11020	77.91060	68.44270	-120.59931	-2436.07824	-1214.35098	1
220	C	73.00431	77.89865	68.55313	404.07514	-299.37480	608.84009	1
221	H	73.31411	78.21495	69.57684	-1071.07882	-841.69025	2359.66467	1
222	C	72.20185	79.02501	67.77044	-683.12807	68.71770	-390.13096	1
223	H	72.82344	79.94092	67.65308	2068.88918	1596.58590	770.89603	1
224	H	71.93975	78.70323	66.73593	1379.86429	2342.49779	-179.85638	1
225	C	70.93021	79.29974	68.62678	-176.39967	537.49466	550.97268	1
226	H	70.23152	78.43286	68.59628	-396.28051	1942.22168	1869.33314	1
227	H	71.22004	79.42640	69.71527	-94.44700	586.00678	-2659.20016	1
228	C	70.24205	80.63038	68.06885	-291.69381	-718.18079	-150.72929	1
229	H	70.83714	81.55997	68.25888	-2303.38776	1089.76242	964.62032	1
230	H	69.91804	80.61818	66.99900	884.16729	2568.80533	-207.74283	1
231	N	69.11203	80.65836	68.89907	-594.49522	-252.81478	342.29276	1
232	H	69.20294	80.20741	69.79680	-1735.17426	2084.05705	-263.71605	1
233	C	68.00995	81.23571	68.62615	595.23177	-271.52487	442.22352	1
234	N	67.89163	81.88476	67.39324	585.53813	-424.79750	-105.81303	1
235	H	68.58682	82.00861	66.65896	959.88797	1327.56823	-2177.11905	1
236	H	67.07084	82.40461	67.08214	1578.48647	16.27378	-2220.76233	1
237	N	67.10438	81.09048	69.68561	-452.17763	-390.33541	-421.51853	1

238	H	67.20138	80.63032	70.58956	470.26107	1974.25629	-1817.92087	1
239	H	66.16823	81.49687	69.67904	1856.67307	-1573.97321	-1224.35416	1
240	C	72.10246	76.53454	68.59867	-531.47271	-581.45780	-55.06206	1
241	O	71.77185	76.13230	69.67740	-243.00837	192.73507	609.52485	1
242	N	71.75579	76.09722	67.38064	343.49288	-644.25607	38.09164	1
243	H	72.18230	76.60578	66.55445	-1691.16043	-1535.97525	-1484.73099	1
244	C	71.44638	74.66771	67.16768	542.66492	350.14337	454.42563	1
245	H	71.59403	74.56972	66.06668	1209.57979	-2396.95920	463.86744	1
246	C	72.39672	73.80830	67.97460	-737.14309	145.93010	242.71942	1
247	H	72.21399	74.02629	69.05406	-1050.18303	159.36419	-2509.06125	1
248	C	72.12870	72.33155	67.74251	-706.77696	-252.88343	-245.16230	1
249	H	72.79917	71.68202	68.36897	-1624.64039	-1665.49085	1417.86935	1
250	H	71.06520	72.06790	68.00411	2566.10521	598.51109	693.22305	1
251	H	72.29325	72.04251	66.66792	-1972.69758	107.10018	-1876.34312	1
252	C	73.84897	74.12896	67.67040	412.85148	672.58832	-27.69222	1
253	H	74.55284	73.52570	68.30590	1447.02277	1762.76533	-1490.78944	1
254	H	74.10305	73.91768	66.59573	1320.77379	-145.20455	2378.68491	1
255	H	74.07722	75.21497	67.85534	-1512.10848	1470.52031	1724.75147	1
256	C	69.88182	74.44300	67.61869	-607.11113	499.56689	73.73769	1
257	O	69.60770	73.85443	68.66700	357.97126	460.81534	356.68785	1
258	N	69.02184	74.87180	66.68276	536.55407	-368.62270	332.76306	1
259	H	69.65739	75.29325	65.98820	524.38866	2297.69985	1367.20941	1
260	C	67.91139	75.70047	67.10916	46.50277	-774.29190	-147.97904	1
261	H	68.36755	76.39848	67.84465	1676.51875	1883.29066	1032.55549	1
262	C	67.30955	76.42724	65.80451	-559.41456	-34.19198	-556.30433	1
263	H	67.14403	75.64612	65.02251	-64.66664	395.18769	2695.05373	1
264	H	66.29637	76.84208	66.03994	-2703.44278	-60.40056	333.79418	1
265	C	68.19061	77.52573	65.25854	-519.76435	377.31045	459.42366	1
266	H	69.24521	77.17318	65.23172	-1746.74323	1667.50644	-1261.73691	1
267	C	67.75854	77.86639	63.83781	570.95554	16.46261	-545.27700	1
268	H	68.38097	78.68875	63.39885	2391.58273	28.05277	-1305.07271	1
269	H	67.84559	76.98228	63.15408	175.75588	917.63458	2559.43867	1
270	H	66.69014	78.20557	63.80337	-1063.97851	-2155.34650	1283.00462	1
271	C	68.11369	78.77723	66.12127	193.76014	2.62946	-765.53141	1
272	H	68.68620	79.62601	65.66582	507.39394	-846.55087	2539.60089	1
273	H	67.05690	79.12920	66.24937	1337.57841	1818.19054	1526.01994	1
274	H	68.52933	78.60803	67.14816	1100.88635	-1172.91350	-2199.08909	1
275	C	66.70924	74.86141	67.70429	-549.21115	475.64486	-309.38218	1
276	O	65.58573	75.21232	67.44433	556.06106	-390.37755	-78.24250	1
277	O	66.97158	73.81782	68.56465	-572.27940	-310.19032	-209.75862	1
278	H	68.03754	73.85633	68.56446	-1380.08193	2212.14486	790.85944	1

Listing 31: C00031.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.9028	0.0000	300.0000
3	H	88.06052	71.69157	76.34736	-2043.14101	-1757.64893	399.89339		1
4	N	88.33511	71.92573	75.39598	426.75047	490.45733	-334.42467		1
5	H	87.45597	72.21694	74.97664	442.25559	-1110.30854	-2448.52907		1
6	C	89.41160	72.82548	75.27339	415.32972	-666.39213	83.73172		1
7	H	90.15425	72.45848	76.01249	879.32219	2491.00447	667.35213		1
8	C	89.96395	72.77494	73.76276	31.35357	477.41777	628.23362		1
9	H	89.22069	73.24324	73.07432	1168.38489	2240.25337	-1019.71136		1
10	H	90.89088	73.39092	73.66708	-360.43770	2534.90498	931.67112		1
11	C	90.21046	71.34184	73.35902	463.18208	512.70242	-382.34388		1
12	H	89.34149	70.73231	73.69577	1725.29117	1863.52247	-987.07854		1
13	C	90.31690	71.23003	71.84383	710.42801	-144.27427	-313.15367		1
14	H	90.47483	70.16974	71.51732	364.20195	-1033.13725	2494.72524		1
15	H	89.38932	71.60007	71.33498	2567.61904	335.80679	847.48802		1
16	H	91.17526	71.83076	71.44627	-2587.99029	680.92867	-512.16411		1
17	C	91.47115	70.79267	74.01116	268.17616	741.64379	-40.42634		1

18	H	91.65780	69.72728	73.71734	1283.54314	-1945.37420	-1411.27812	1
19	H	92.37777	71.38211	73.71661	-1258.57796	1317.15249	-2026.02085	1
20	H	91.40434	70.82210	75.12941	-2502.84526	909.80597	575.92391	1
21	C	88.95983	74.35894	75.56220	619.36578	-458.64843	-172.09273	1
22	O	89.76845	75.24612	75.39406	-81.40433	433.87611	522.34594	1
23	N	87.67999	74.46231	75.91861	175.23996	-622.20190	341.55523	1
24	H	87.16548	73.60084	76.08873	-876.57256	-303.22879	-2561.90213	1
25	C	87.05139	75.71084	76.17669	-571.88214	-534.10783	-106.15033	1
26	H	86.02975	75.40539	76.49609	-2713.20841	-16.25800	-248.80809	1
27	C	87.89205	76.35109	77.38856	166.60354	288.16399	-716.09568	1
28	H	88.89672	76.64438	76.97394	-2097.85574	1636.78449	-586.18044	1
29	O	88.14692	75.45504	78.48662	-317.80580	-363.38227	484.43082	1
30	H	89.11399	75.33551	78.39868	1863.74748	-1451.84923	1357.29467	1
31	C	87.10553	77.64602	77.80322	503.80731	517.99032	318.51606	1
32	H	87.62785	78.18529	78.62824	640.61020	-2157.10410	-1536.29104	1
33	H	86.99359	78.37512	76.95030	1687.88455	465.60692	2087.56452	1
34	H	86.08207	77.39970	78.17107	-1293.07895	-1899.88581	-1463.57452	1
35	C	87.02529	76.64479	74.85112	-153.07550	-733.68902	248.70981	1
36	O	87.10163	77.83734	75.05026	186.15459	-480.78787	-449.34387	1
37	N	86.81760	76.03712	73.67007	-487.53139	543.18517	42.03850	1
38	C	86.83510	76.82762	72.48123	-699.35871	69.34393	360.10701	1
39	H	87.49910	77.69712	72.69546	2.81126	-221.99807	-2715.58072	1
40	C	87.37092	75.78139	71.41572	-507.46439	-592.59194	122.07761	1
41	H	87.12981	76.07086	70.36842	-1975.08116	525.87560	-1801.71556	1
42	H	88.47792	75.68080	71.47301	1588.27743	-1913.22100	1113.83566	1
43	C	86.66813	74.46302	71.86828	-613.62442	-457.55993	-194.14490	1
44	H	85.60983	74.43107	71.52554	1707.54637	-721.27992	1996.92523	1
45	H	87.15262	73.54065	71.47570	758.23357	2100.81767	1560.55011	1
46	C	86.77649	74.59787	73.44788	-352.41524	704.96076	49.21465	1
47	H	85.92357	74.17494	74.02964	1714.76886	-2070.42778	443.35792	1
48	H	87.73149	74.21311	73.87033	1224.15040	1801.50881	1636.97633	1
49	C	85.31195	77.31448	72.07237	566.85117	537.05831	117.62814	1
50	O	85.17231	78.34888	71.46828	-550.26779	-406.08867	4.21666	1
51	N	84.40750	76.41926	72.43061	566.34832	-425.77725	180.18749	1
52	H	84.73106	75.61354	72.96339	644.44502	2646.80550	-52.73430	1
53	C	83.04081	76.52617	72.06902	612.34801	-281.48662	411.56221	1
54	H	82.82435	77.60364	71.88760	1667.23498	-1490.75142	1556.16753	1
55	C	82.82148	75.62397	70.75418	-714.45746	-175.43074	286.98927	1
56	H	83.17330	74.57941	70.97630	-787.09484	1763.03619	-1922.46060	1
57	O	83.53324	76.04377	69.58155	-429.46514	516.51932	-128.40526	1
58	H	84.11214	75.26990	69.42261	1981.82785	436.16847	-1818.18182	1
59	C	81.25532	75.61632	70.61244	630.79189	-468.94448	76.03230	1
60	H	80.93628	75.07522	69.68839	-1775.71861	2062.30353	131.89849	1
61	H	80.75910	75.11278	71.47946	-1855.14608	88.94118	1993.53760	1
62	H	80.84156	76.64922	70.54399	-1504.82350	-780.94249	-2132.90992	1
63	C	82.25235	75.80580	73.29541	288.57638	618.62814	-397.00270	1
64	O	82.70638	74.81025	73.85132	321.70495	-185.26452	574.37218	1
65	N	81.10045	76.41069	73.51272	-447.05792	-446.53431	367.76425	1
66	H	80.81569	77.19197	72.92426	350.31316	1975.63644	-1843.31522	1
67	C	80.18702	75.76263	74.40205	-511.23061	374.03917	-471.51480	1
68	H	80.86412	75.37087	75.19650	2234.79579	-898.70890	-1273.45190	1
69	C	79.09053	76.82596	74.85930	529.53781	-159.34528	563.72604	1
70	H	78.52512	76.34829	75.70445	654.59388	2347.94251	1217.51488	1
71	H	79.59482	77.72663	75.29782	-1526.55661	2103.42026	817.87394	1
72	O	78.17116	77.23475	73.83276	-554.84278	14.12789	399.58769	1
73	H	77.91360	76.31509	73.46924	1297.06236	2061.84854	1220.68812	1
74	C	79.42917	74.56691	73.58876	-662.15484	-412.13544	123.62687	1
75	O	78.25905	74.68062	73.25247	-540.01537	-317.05804	274.91456	1
76	N	80.28089	73.58655	73.42882	-202.76299	-690.00100	-131.49145	1
77	H	81.26373	73.71603	73.75402	-702.62132	-2617.37191	281.70413	1
78	C	79.91112	72.38826	72.76176	-491.73914	576.34187	222.73509	1
79	H	80.78451	71.73580	72.98433	1977.17978	-1823.58850	-434.68928	1

80	C	78.55412	71.83578	73.37461	-649.50797	-328.66843	306.11224	1
81	H	77.71593	72.54124	73.17132	2075.07803	1452.16490	-1004.45904	1
82	C	78.27350	70.41587	72.77301	-615.18735	-489.99689	-70.96352	1
83	H	77.31847	69.98886	73.15854	-1226.32661	-1724.38906	-1716.47170	1
84	H	78.20083	70.44157	71.66037	2381.64273	-969.84735	900.46860	1
85	H	79.08621	69.69756	73.03184	2122.74991	1702.23946	-141.36228	1
86	C	78.73516	71.65557	74.92114	-501.86074	-479.61276	-376.42482	1
87	H	77.81656	71.24129	75.39850	993.79261	-2246.95401	-1177.81305	1
88	H	79.57661	70.96306	75.15729	42.71279	-626.15391	-2651.37258	1
89	H	78.95892	72.62984	75.41593	-2026.39012	-1590.33709	-887.82922	1
90	C	79.84270	72.72622	71.15564	-672.89153	382.57394	-156.34072	1
91	O	80.86772	73.01469	70.57703	410.04627	221.86223	500.35950	1
92	N	78.62899	72.60627	70.64719	-378.11782	-443.79414	-441.10984	1
93	H	77.84060	72.39821	71.25470	2404.15973	-568.14894	1149.30085	1
94	C	78.46643	72.80153	69.23363	-544.54484	466.16019	331.29119	1
95	H	79.27519	73.53957	69.02284	-1409.80988	-170.17955	2325.32679	1
96	C	78.81946	71.41144	68.54976	-184.48284	116.78282	-758.89137	1
97	H	79.86284	71.10761	68.79332	1893.78641	1861.14652	611.04528	1
98	H	78.18397	70.59714	68.96506	-2170.79665	-974.19311	1327.50117	1
99	C	78.63408	71.57250	67.00766	389.51668	672.81878	-138.49152	1
100	H	77.73632	72.19248	66.78705	510.64577	1933.03327	1851.02484	1
101	H	79.47278	72.16620	66.58190	-2302.30869	-1105.72939	-948.89774	1
102	C	78.50846	70.19888	66.24501	-559.93427	-126.34590	542.30857	1
103	O	78.25138	70.19868	65.06965	-670.36003	-111.83166	76.36448	1
104	N	78.70070	69.11094	67.02235	-216.06729	-537.07037	446.51379	1
105	H	78.98838	69.05457	68.00613	-1251.96487	1074.12894	-2168.52500	1
106	H	78.70643	68.14885	66.66587	-2451.83023	-720.73851	944.84612	1
107	C	76.97698	73.41291	69.04389	546.24052	-563.88337	-85.11809	1
108	O	76.86496	74.59266	69.36024	71.70702	-307.40463	606.69673	1
109	N	76.02616	72.59798	68.59802	479.90863	-504.50129	222.86849	1
110	C	74.79404	73.12769	68.07111	75.51268	-600.91904	506.73700	1
111	H	75.08344	74.04060	67.50077	-2033.61562	1795.30103	254.89480	1
112	C	74.26488	71.90025	67.21045	523.79067	517.99274	284.45581	1
113	H	73.17529	71.96521	66.99205	1599.61665	-1127.00911	1895.98173	1
114	H	74.78903	71.82496	66.23124	-1881.83093	1275.82488	-1501.55016	1
115	C	74.63436	70.70683	68.14405	-600.05639	-404.05026	316.64485	1
116	H	73.92341	70.63456	68.99770	-2597.05260	496.36221	657.73249	1
117	H	74.62061	69.71812	67.63211	-1666.24518	1294.38985	-1723.90591	1
118	C	76.08704	71.14272	68.62006	493.57570	-129.95376	-602.56394	1
119	H	76.37558	70.81608	69.64712	-1469.08415	-637.84797	2204.22581	1
120	H	76.89428	70.85682	67.90058	-1038.97840	1068.88701	-2280.71789	1
121	C	73.76072	73.45222	69.28205	188.88100	241.05089	-727.87821	1
122	O	72.67969	72.93431	69.30541	531.88613	-49.19943	427.07960	1
123	N	74.25826	74.36916	70.13624	708.14833	26.93417	-179.73509	1
124	H	75.23400	74.72609	69.96327	-2232.69501	-1179.09831	1023.94816	1
125	C	73.76899	74.30230	71.52360	-738.32412	259.92548	104.42456	1
126	H	72.69797	74.00601	71.42553	2028.89123	1260.02983	1311.33324	1
127	C	74.60795	73.29394	72.28530	-258.65678	-345.52513	661.28459	1
128	H	75.65366	73.67821	72.30928	-1826.06090	-1801.46097	-918.64554	1
129	C	74.12349	73.14286	73.71622	-541.23400	531.92970	-218.41428	1
130	H	74.74364	72.39956	74.28896	1311.73218	-2219.18200	882.19023	1
131	H	74.17046	74.11939	74.27348	-1048.71298	1223.58118	-2196.97971	1
132	H	73.05657	72.78768	73.75576	419.06414	1903.92898	1903.44670	1
133	C	74.64107	71.93356	71.61325	-423.86431	152.66566	-648.55262	1
134	H	75.26530	71.19307	72.18581	105.68386	-2342.50080	1387.51238	1
135	H	73.60807	71.49868	71.51019	-1695.63603	-1484.73621	-1531.02793	1
136	H	75.07000	72.00760	70.57760	-1853.57121	-487.39031	1936.59343	1
137	C	74.03182	75.77766	72.22794	539.71428	-510.58232	267.58633	1
138	O	75.05739	76.38908	72.05124	-15.93758	-278.34085	-624.49402	1
139	N	73.04405	76.06096	73.06862	-676.81886	12.05292	276.17960	1
140	H	72.22618	75.45552	73.04905	-1694.44250	-373.84189	-2100.66098	1
141	C	73.15611	77.23550	73.86999	412.33078	-664.70360	108.35451	1

142	H	74.24357	77.49037	73.83928	1765.77476	1294.44366	1621.76594	1
143	C	72.26452	78.36062	73.17999	-179.66635	-721.95667	-264.73915	1
144	H	72.41891	78.36675	72.07836	-607.34922	2587.87032	-598.10018	1
145	H	71.18229	78.15254	73.33565	-359.69332	-1479.13954	-2259.74260	1
146	C	72.67007	79.72766	73.81634	-240.01076	616.02425	431.85322	1
147	H	72.54870	79.69017	74.92903	-1359.17131	782.54425	2227.99181	1
148	H	73.74780	79.94139	73.63408	-820.36667	85.81767	-2596.78715	1
149	C	71.76254	80.86712	73.19953	-513.07015	236.18570	-551.87280	1
150	H	71.92518	80.95965	72.10139	1816.11944	-1183.11722	-1650.94321	1
151	H	70.68039	80.63426	73.32615	-1800.04429	-1361.53473	1526.34643	1
152	C	72.14479	82.17333	73.93509	726.08972	-253.19732	-179.64713	1
153	H	71.96349	82.15785	75.02843	1224.27271	-456.51798	-2390.90304	1
154	H	73.17454	82.52939	73.73241	1206.40339	-1150.93514	-2154.90344	1
155	N	71.21866	83.30920	73.39112	329.70796	-633.68968	-155.67358	1
156	H	71.40180	84.27709	73.78699	1348.31305	1938.76845	1359.00643	1
157	H	71.27403	83.50202	72.34907	2096.92035	1446.54551	-966.48890	1
158	H	70.16993	83.21171	73.55009	-1197.07217	-2303.53719	827.28733	1
159	C	72.54137	77.02505	75.35807	-378.01186	-556.17301	-413.96481	1
160	O	72.52797	77.98418	76.13999	-409.44433	-307.55053	-453.30833	1
161	N	72.10608	75.81076	75.56505	-429.02477	524.70884	274.08502	1
162	H	72.21938	75.15271	74.79746	1706.34263	-1425.96036	1574.38926	1
163	C	71.37596	75.47090	76.74568	-45.25864	-626.22952	478.93267	1
164	H	71.15772	74.38619	76.61701	1988.63164	570.90773	1772.87287	1
165	C	72.40390	75.76405	77.92517	551.77128	-20.49526	-564.54996	1
166	H	73.42428	75.50172	77.56778	1434.61535	-1753.10253	1513.99471	1
167	H	72.44770	76.85987	78.12489	-714.67738	1819.09770	1898.36494	1
168	C	72.11119	74.99247	79.24926	446.99263	-555.77305	338.97221	1
169	H	71.27609	75.45532	79.82501	1953.68466	1892.25957	-161.67766	1
170	H	71.79787	73.94311	79.04841	-403.03785	2688.07032	-188.43591	1
171	C	73.44422	75.02739	80.10383	567.86262	335.74681	434.04421	1
172	H	74.27234	74.49875	79.57860	-1080.02275	1568.26081	-1948.78900	1
173	H	73.79613	76.07463	80.25110	-919.54108	2111.34692	1456.13463	1
174	C	73.12299	74.35604	81.45930	195.81897	173.33862	-745.11536	1
175	H	72.43687	74.93932	82.10804	1405.67949	-2301.21089	-390.08113	1
176	H	72.76458	73.30851	81.38080	-940.37328	-1118.32446	2299.72133	1
177	N	74.44942	74.24177	82.28318	319.26422	656.36007	-42.02424	1
178	H	74.33877	73.84456	83.26041	1961.03633	619.91968	1787.09422	1
179	H	75.20875	73.61229	81.89129	854.14343	-2156.80752	1429.08711	1
180	H	74.98358	75.13722	82.48076	1237.02905	-1378.50857	-1998.28500	1
181	C	70.03886	76.38305	76.73919	532.53319	-268.57236	517.55729	1
182	O	69.55897	76.85196	75.71012	266.16714	-290.73804	-558.88002	1
183	N	69.54455	76.41365	77.96401	-226.25352	640.49678	-270.32839	1
184	H	69.98900	75.77718	78.63529	2007.69063	-1035.27229	1523.50231	1
185	C	69.06705	77.63177	78.54086	-540.76542	-573.33303	49.50000	1
186	H	69.21260	77.47263	79.63201	-2374.20950	-1036.76023	843.75774	1
187	C	69.97333	78.82792	77.98610	-77.09082	666.87422	-415.84136	1
188	H	69.99888	78.77101	76.85960	-985.81834	617.19825	2463.91927	1
189	O	71.33675	78.80018	78.38715	293.29899	-391.65602	-477.80926	1
190	H	71.80511	78.54325	77.49534	2528.72714	-681.76262	-751.27122	1
191	C	69.14329	80.08632	78.42843	252.47363	-605.14473	440.05134	1
192	H	69.60181	81.03040	78.05208	-2052.65063	1456.49051	-1043.51830	1
193	H	68.09681	80.05184	78.04308	-2152.98800	-1661.97574	-161.70652	1
194	H	69.08628	80.16502	79.53928	-473.12726	-1584.27339	2165.61725	1
195	C	67.48245	77.80488	78.19820	360.36307	488.46713	505.10056	1
196	O	66.71742	78.15767	79.07142	-200.08817	-528.03552	-385.82850	1
197	N	67.22086	77.56691	76.91964	-597.54095	-226.44775	355.20479	1
198	H	67.98711	77.26927	76.26666	2179.23655	-1300.70981	-991.33835	1
199	C	65.92851	77.91933	76.43791	-687.68921	297.39807	-249.45179	1
200	H	65.57593	78.68842	77.16331	-349.16256	-2467.37713	-1101.72831	1
201	C	66.09061	78.42921	74.93197	672.47345	361.54328	-201.62880	1
202	H	66.62061	77.66218	74.32211	1541.41502	582.18425	2169.97026	1
203	H	65.09083	78.58806	74.46663	-2534.67717	60.25153	997.72295	1

204	C	66.89280	79.73897	74.98318	574.26774	-389.43119	-377.02542	1
205	C	66.19884	80.98536	74.97478	688.82679	-287.33580	-257.96133	1
206	H	65.09731	81.01879	74.89344	331.14182	1470.38163	2269.80013	1
207	C	68.31494	79.70328	75.10183	-383.52382	-675.04808	144.24917	1
208	H	68.85319	78.72915	75.13008	4.09847	1517.59662	2262.86397	1
209	C	66.94212	82.16295	75.07585	-134.76730	428.45285	-649.50303	1
210	H	66.40644	83.12848	75.06439	-903.23433	1600.49020	2011.53387	1
211	C	69.01206	80.91101	75.21590	-335.53281	-615.00040	-364.39058	1
212	H	70.10916	80.87166	75.33287	1596.45398	-1369.33862	1732.02659	1
213	C	68.36049	82.17733	75.19661	585.48547	-340.24194	-406.23938	1
214	O	69.05862	83.41945	75.29768	-419.15649	-173.04408	-511.94141	1
215	H	69.98254	83.08245	75.33102	-1071.84350	1559.71507	-1960.13012	1
216	C	65.01199	76.57108	76.49942	291.41878	-183.13091	710.72246	1
217	O	64.25932	76.25282	75.61240	379.87695	523.47396	-222.23622	1
218	N	65.17651	76.01259	77.70484	564.30591	373.09380	277.24371	1
219	H	65.89339	76.44284	78.30690	-120.59931	-2436.07824	-1214.35098	1
220	C	64.83993	74.61234	77.83023	404.07514	-299.37480	608.84009	1
221	H	63.73962	74.63588	77.66588	-1071.07882	-841.69025	2359.66467	1
222	C	65.56774	73.79337	76.69277	-683.12807	68.71770	-390.13096	1
223	H	65.40272	74.27493	75.69912	2068.88918	1596.58590	770.89603	1
224	H	66.67017	73.77521	76.85151	1379.86429	2342.49779	-179.85638	1
225	C	64.95723	72.35665	76.74151	-176.39967	537.49466	550.97268	1
226	H	65.17517	71.87886	77.72574	-396.28051	1942.22168	1869.33314	1
227	H	63.84800	72.39842	76.66418	-94.44700	586.00678	-2659.20016	1
228	C	65.57262	71.51001	75.53577	-291.69381	-718.18079	-150.72929	1
229	H	65.45945	71.95494	74.51452	-2303.38776	1089.76242	964.62032	1
230	H	66.64291	71.20783	75.66797	884.16729	2568.80533	-207.74283	1
231	N	64.78088	70.35204	75.58434	-594.49522	-252.81478	342.29276	1
232	H	64.20130	70.23106	76.40059	-1735.17426	2084.05705	-263.71605	1
233	C	64.75043	69.45358	74.68589	595.23177	-271.52487	442.22352	1
234	N	65.56833	69.62110	73.56323	585.53813	-424.79750	-105.81303	1
235	H	66.22201	70.37147	73.34320	959.88797	1327.56823	-2177.11905	1
236	H	65.63208	68.96374	72.78518	1578.48647	16.27378	-2220.76233	1
237	N	63.85694	68.42795	75.02662	-452.17763	-390.33541	-421.51853	1
238	H	63.25526	68.30664	75.83993	470.26107	1974.25629	-1817.92087	1
239	H	63.68572	67.61689	74.43096	1856.67307	-1573.97321	-1224.35416	1
240	C	65.28252	74.13198	79.31068	-531.47271	-581.45780	-55.06206	1
241	O	65.96197	73.11861	79.47644	-243.00837	192.73507	609.52485	1
242	N	64.80686	74.96389	80.22100	343.49288	-644.25607	38.09164	1
243	H	64.31352	75.74505	79.78684	-1691.16043	-1535.97525	-1484.73099	1
244	C	64.59585	74.63334	81.62044	542.66492	350.14337	454.42563	1
245	H	63.86189	75.39891	81.96968	1209.57979	-2396.95920	463.86744	1
246	C	64.08940	73.20241	81.74196	-737.14309	145.93010	242.71942	1
247	H	64.85807	72.53072	81.29061	-1050.18303	159.36419	-2509.06125	1
248	C	63.90745	72.80125	83.19311	-706.77696	-252.88343	-245.16230	1
249	H	63.54771	71.73976	83.28929	-1624.64039	-1665.49085	1417.86935	1
250	H	64.87579	72.88330	83.77228	2566.10521	598.51109	693.22305	1
251	H	63.15447	73.45622	83.71185	-1972.69758	107.10018	-1876.34312	1
252	C	62.79903	72.98658	80.97311	412.85148	672.58832	-27.69222	1
253	H	62.45575	71.91701	81.02836	1447.02277	1762.76533	-1490.78944	1
254	H	61.96579	73.62595	81.37448	1320.77379	-145.20455	2378.68491	1
255	H	62.92159	73.24307	79.88486	-1512.10848	1470.52031	1724.75147	1
256	C	66.05046	74.76532	82.42287	-607.11113	499.56689	73.73769	1
257	O	66.10131	75.39677	83.44653	357.97126	460.81534	356.68785	1
258	N	66.99388	74.06633	81.82045	536.55407	-368.62270	332.76306	1
259	H	66.77125	73.51154	80.95744	524.38866	2297.69985	1367.20941	1
260	C	68.26009	74.00937	82.46300	46.50277	-774.29190	-147.97904	1
261	H	68.24112	74.85929	83.18571	1676.51875	1883.29066	1032.55549	1
262	C	68.42717	72.56967	83.19133	-559.41456	-34.19198	-556.30433	1
263	H	68.25053	71.75613	82.44873	-64.66664	395.18769	2695.05373	1
264	H	69.47990	72.44579	83.53929	-2703.44278	-60.40056	333.79418	1
265	C	67.46935	72.45103	84.34133	-519.76435	377.31045	459.42366	1

266	H	66.42760	72.60324	83.95956	-1746.74323	1667.50644	-1261.73691	1
267	C	67.56561	71.05871	84.95447	570.95554	16.46261	-545.27700	1
268	H	66.85808	70.93467	85.81405	2391.58273	28.05277	-1305.07271	1
269	H	67.32395	70.26075	84.20596	175.75588	917.63458	2559.43867	1
270	H	68.59667	70.84987	85.34001	-1063.97851	-2155.34650	1283.00462	1
271	C	67.75218	73.50149	85.40685	193.76014	2.62946	-765.53141	1
272	H	67.16018	73.31584	86.33966	507.39394	-846.55087	2539.60089	1
273	H	68.83468	73.51572	85.69706	1337.57841	1818.19054	1526.01994	1
274	H	67.48498	74.53169	85.04750	1100.88635	-1172.91350	-2199.08909	1
275	C	69.42728	74.09140	81.36620	-549.21115	475.64486	-309.38218	1
276	O	70.55327	73.74016	81.61468	556.06106	-390.37755	-78.24250	1
277	O	69.13475	74.72082	80.12417	-572.27940	-310.19032	-209.75862	1
278	H	68.14849	74.81136	80.23576	-1380.08193	2212.14486	790.85944	1

Listing 32: C00032.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.8923	0.0000	300.0000
3	H	75.92431	66.32038	83.84679	-2043.14101	-1757.64893	399.89339		1
4	N	76.30681	66.42121	82.90814	426.75047	490.45733	-334.42467		1
5	H	75.47084	66.58558	82.34694	442.25559	-1110.30854	-2448.52907		1
6	C	77.23606	67.47390	82.76453	415.32972	-666.39213	83.73172		1
7	H	77.83959	67.51467	83.69615	879.32219	2491.00447	667.35213		1
8	C	78.10009	67.16860	81.44120	31.35357	477.41777	628.23362		1
9	H	77.43072	67.22582	80.54873	1168.38489	2240.25337	-1019.71136		1
10	H	78.88367	67.95014	81.28944	-360.43770	2534.90498	931.67112		1
11	C	78.70873	65.79222	81.55144	463.18208	512.70242	-382.34388		1
12	H	77.90940	65.08979	81.88058	1725.29117	1863.52247	-987.07854		1
13	C	79.23045	65.32350	80.19968	710.42801	-144.27427	-313.15367		1
14	H	79.65889	64.28931	80.25769	364.20195	-1033.13725	2494.72524		1
15	H	78.41917	65.30382	79.42641	2567.61904	335.80679	847.48802		1
16	H	80.03964	65.99620	79.81420	-2587.99029	680.92867	-512.16411		1
17	C	79.83439	65.75898	82.57529	268.17616	741.64379	-40.42634		1
18	H	80.28456	64.73590	82.66077	1283.54314	-1945.37420	-1411.27812		1
19	H	80.66192	66.46362	82.30173	-1258.57796	1317.15249	-2026.02085		1
20	H	79.47415	66.04850	83.59608	-2502.84526	909.80597	575.92391		1
21	C	76.30241	68.79353	82.50561	619.36578	-458.64843	-172.09273		1
22	O	75.41442	68.77615	81.67636	-81.40433	433.87611	522.34594		1
23	N	76.68021	69.77483	83.30827	175.23996	-622.20190	341.55523		1
24	H	77.48696	69.61887	83.91053	-876.57256	-303.22879	-2561.90213		1
25	C	76.07206	71.06127	83.20234	-571.88214	-534.10783	-106.15033		1
26	H	75.00387	70.87963	82.95100	-2713.20841	-16.25800	-248.80809		1
27	C	76.32167	71.75734	84.62172	166.60354	288.16399	-716.09568		1
28	H	77.42683	71.74458	84.82704	-2097.85574	1636.78449	-586.18044		1
29	O	75.70638	71.08144	85.73713	-317.80580	-363.38227	484.43082		1
30	H	76.49012	70.83797	86.26592	1863.74748	-1451.84923	1357.29467		1
31	C	75.86924	73.24718	84.41326	503.80731	517.99032	318.51606		1
32	H	76.08150	73.86322	85.31851	640.61020	-2157.10410	-1536.29104		1
33	H	76.39401	73.74599	83.54394	1687.88455	465.60692	2087.56452		1
34	H	74.76996	73.31549	84.22643	-1293.07895	-1899.88581	-1463.57452		1
35	C	76.86784	71.85845	82.02852	-153.07550	-733.68902	248.70981		1
36	O	78.05458	71.69952	81.91231	186.15459	-480.78787	-449.34387		1
37	N	76.06215	72.70355	81.36449	-487.53139	543.18517	42.03850		1
38	C	76.58825	73.58375	80.36910	-699.35871	69.34393	360.10701		1
39	H	77.50685	73.08667	79.97759	2.81126	-221.99807	-2715.58072		1
40	C	75.34695	73.67409	79.37598	-507.46439	-592.59194	122.07761		1
41	H	75.40753	74.51488	78.65200	-1975.08116	525.87560	-1801.71556		1
42	H	75.24029	72.74563	78.77304	1588.27743	-1913.22100	1113.83566		1
43	C	74.19526	73.83236	80.41442	-613.62442	-457.55993	-194.14490		1
44	H	74.16276	74.86878	80.81953	1707.54637	-721.27992	1996.92523		1
45	H	73.18270	73.62971	79.99202	758.23357	2100.81767	1560.55011		1

46	C	74.61987	72.79466	81.54111	-352.41524	704.96076	49.21465	1
47	H	74.40652	73.13351	82.58237	1714.76886	-2070.42778	443.35792	1
48	H	74.20682	71.76390	81.41088	1224.15040	1801.50881	1636.97633	1
49	C	76.89437	75.03484	81.07342	566.85117	537.05831	117.62814	1
50	O	77.12453	75.10994	82.26098	-550.26779	-406.08867	4.21666	1
51	N	76.87925	75.99895	80.16971	566.34832	-425.77725	180.18749	1
52	H	76.69909	75.75646	79.19875	644.44502	2646.80550	-52.73430	1
53	C	77.07892	77.34703	80.60510	612.34801	-281.48662	411.56221	1
54	H	77.95436	77.30605	81.29215	1667.23498	-1490.75142	1556.16753	1
55	C	77.28473	78.24270	79.30179	-714.45746	-175.43074	286.98927	1
56	H	76.39968	78.08588	78.62755	-787.09484	1763.03619	-1922.46060	1
57	O	78.45467	77.94413	78.50958	-429.46514	516.51932	-128.40526	1
58	H	78.04797	77.63869	77.67777	1981.82785	436.16847	-1818.18182	1
59	C	77.22172	79.69938	79.88943	630.79189	-468.94448	76.03230	1
60	H	77.24407	80.46853	79.08319	-1775.71861	2062.30353	131.89849	1
61	H	76.29175	79.87008	80.48340	-1855.14608	88.94118	1993.53760	1
62	H	78.08526	79.90046	80.56516	-1504.82350	-780.94249	-2132.90992	1
63	C	75.74296	77.85319	81.39596	288.57638	618.62814	-397.00270	1
64	O	75.87447	78.59946	82.33784	321.70495	-185.26452	574.37218	1
65	N	74.60700	77.44184	80.81210	-447.05792	-446.53431	367.76425	1
66	H	74.72149	76.85903	79.98131	350.31316	1975.63644	-1843.31522	1
67	C	73.53078	78.38515	80.88277	-511.23061	374.03917	-471.51480	1
68	H	73.98401	79.30674	81.31559	2234.79579	-898.70890	-1273.45190	1
69	C	72.99004	78.55262	79.39034	529.53781	-159.34528	563.72604	1
70	H	72.18868	79.33508	79.42647	654.59388	2347.94251	1217.51488	1
71	H	73.82963	78.97909	78.77804	-1526.55661	2103.42026	817.87394	1
72	O	72.54078	77.33942	78.71657	-554.84278	14.12789	399.58769	1
73	H	71.64874	77.26779	79.10188	1297.06236	2061.84854	1220.68812	1
74	C	72.36939	77.80151	81.86843	-662.15484	-412.13544	123.62687	1
75	O	72.00329	78.50240	82.78484	-540.01537	-317.05804	274.91456	1
76	N	71.83480	76.62581	81.45679	-202.76299	-690.00100	-131.49145	1
77	H	72.42511	76.25041	80.70816	-702.62132	-2617.37191	281.70413	1
78	C	71.40720	75.77427	82.54682	-491.73914	576.34187	222.73509	1
79	H	72.09129	76.00284	83.39254	1977.17978	-1823.58850	-434.68928	1
80	C	69.89097	76.07065	82.88013	-649.50797	-328.66843	306.11224	1
81	H	69.26455	75.90102	81.97762	2075.07803	1452.16490	-1004.45904	1
82	C	69.49553	75.07982	84.03023	-615.18735	-489.99689	-70.96352	1
83	H	68.41387	75.15753	84.29008	-1226.32661	-1724.38906	-1716.47170	1
84	H	69.69721	74.01931	83.73821	2381.64273	-969.84735	900.46860	1
85	H	70.07751	75.27907	84.96026	2122.74991	1702.23946	-141.36228	1
86	C	69.65166	77.52149	83.42669	-501.86074	-479.61276	-376.42482	1
87	H	68.62985	77.63944	83.85873	993.79261	-2246.95401	-1177.81305	1
88	H	70.38859	77.78326	84.22530	42.71279	-626.15391	-2651.37258	1
89	H	69.75926	78.28414	82.61721	-2026.39012	-1590.33709	-887.82922	1
90	C	71.42079	74.22236	82.06461	-672.89153	382.57394	-156.34072	1
91	O	71.68715	73.33416	82.84516	410.04627	221.86223	500.35950	1
92	N	70.99817	74.11079	80.80315	-378.11782	-443.79414	-441.10984	1
93	H	70.82100	74.96624	80.27774	2404.15973	-568.14894	1149.30085	1
94	C	70.54188	72.83774	80.36871	-544.54484	466.16019	331.29119	1
95	H	70.43825	72.21815	81.29066	-1409.80988	-170.17955	2325.32679	1
96	C	69.21462	73.11597	79.55304	-184.48284	116.78282	-758.89137	1
97	H	68.42479	73.53018	80.21975	1893.78641	1861.14652	611.04528	1
98	H	69.40218	73.89748	78.78249	-2170.79665	-974.19311	1327.50117	1
99	C	68.73176	71.79452	78.87426	389.51668	672.81878	-138.49152	1
100	H	69.54042	71.39441	78.21869	510.64577	1933.03327	1851.02484	1
101	H	68.57063	71.00246	79.64144	-2302.30869	-1105.72939	-948.89774	1
102	C	67.42341	71.95835	78.01056	-559.93427	-126.34590	542.30857	1
103	O	66.95035	70.98709	77.48104	-670.36003	-111.83166	76.36448	1
104	N	66.95507	73.22196	77.93647	-216.06729	-537.07037	446.51379	1
105	H	67.34197	74.08608	78.33355	-1251.96487	1074.12894	-2168.52500	1
106	H	66.14520	73.49920	77.37069	-2451.83023	-720.73851	944.84612	1
107	C	71.67498	72.26252	79.31547	546.24052	-563.88337	-85.11809	1

108	O	71.87839	72.94721	78.28559	71.70702	-307.40463	606.69673	1
109	N	72.25988	71.12905	79.64931	479.90863	-504.50129	222.86849	1
110	C	73.53364	70.51029	79.43135	75.51268	-600.91904	506.73700	1
111	H	74.27553	71.19821	79.89774	-2033.61562	1795.30103	254.89480	1
112	C	73.29493	69.15986	80.22576	523.79067	517.99274	284.45581	1
113	H	74.00566	68.35067	79.92665	1599.61665	-1127.00911	1895.98173	1
114	H	73.44179	69.31927	81.32666	-1881.83093	1275.82488	-1501.55016	1
115	C	71.80460	68.85397	79.92593	-600.05639	-404.05026	316.64485	1
116	H	71.66800	68.48418	78.88869	-2597.05260	496.36221	657.73249	1
117	H	71.36679	68.08555	80.59644	-1666.24518	1294.38985	-1723.90591	1
118	C	71.12111	70.32901	80.12521	493.57570	-129.95376	-602.56394	1
119	H	70.19756	70.52698	79.51225	-1469.08415	-637.84797	2204.22581	1
120	H	70.94009	70.60177	81.20239	-1038.97840	1068.88701	-2280.71789	1
121	C	73.88130	70.31447	77.85661	188.88100	241.05089	-727.87821	1
122	O	74.19385	69.24702	77.39129	531.88613	-49.19943	427.07960	1
123	N	73.88663	71.52443	77.28875	708.14833	26.93417	-179.73509	1
124	H	73.47172	72.30963	77.83059	-2232.69501	-1179.09831	1023.94816	1
125	C	73.92073	71.59874	75.85691	-738.32412	259.92548	104.42456	1
126	H	74.74884	70.92573	75.54041	2028.89123	1260.02983	1311.33324	1
127	C	72.50874	71.13529	75.28858	-258.65678	-345.52513	661.28459	1
128	H	71.68931	71.74363	75.72955	-1826.06090	-1801.46097	-918.64554	1
129	C	72.57595	71.33367	73.73629	-541.23400	531.92970	-218.41428	1
130	H	71.62518	71.02945	73.23896	1311.73218	-2219.18200	882.19023	1
131	H	72.76229	72.40257	73.47079	-1048.71298	1223.58118	-2196.97971	1
132	H	73.39866	70.73348	73.28119	419.06414	1903.92898	1903.44670	1
133	C	72.27049	69.61690	75.59482	-423.86431	152.66566	-648.55262	1
134	H	71.41898	69.20521	75.00269	105.68386	-2342.50080	1387.51238	1
135	H	73.17494	69.00405	75.35916	-1695.63603	-1484.73621	-1531.02793	1
136	H	72.03295	69.45236	76.67410	-1853.57121	-487.39031	1936.59343	1
137	C	74.09727	73.16178	75.45692	539.71428	-510.58232	267.58633	1
138	O	74.93826	73.47921	74.62734	-15.93758	-278.34085	-624.49402	1
139	N	73.22259	73.90678	76.09266	-676.81886	12.05292	276.17960	1
140	H	72.55506	73.49774	76.79032	-1694.44250	-373.84189	-2100.66098	1
141	C	73.08825	75.28872	75.79099	412.33078	-664.70360	108.35451	1
142	H	72.37880	75.64668	76.57212	1765.77476	1294.44366	1621.76594	1
143	C	74.52518	75.94799	75.89189	-179.66635	-721.95667	-264.73915	1
144	H	75.06876	75.56686	76.78483	-607.34922	2587.87032	-598.10018	1
145	H	75.15888	75.66864	75.01806	-359.69332	-1479.13954	-2259.74260	1
146	C	74.33555	77.49826	75.97290	-240.01076	616.02425	431.85322	1
147	H	73.71916	77.88414	75.13093	-1359.17131	782.54425	2227.99181	1
148	H	73.79977	77.78229	76.90999	-820.36667	85.81767	-2596.78715	1
149	C	75.80181	78.08903	75.92997	-513.07015	236.18570	-551.87280	1
150	H	76.45222	77.54128	76.64666	1816.11944	-1183.11722	-1650.94321	1
151	H	76.26198	77.92466	74.92839	-1800.04429	-1361.53473	1526.34643	1
152	C	75.76408	79.59530	76.27596	726.08972	-253.19732	-179.64713	1
153	H	75.31216	80.23968	75.49505	1224.27271	-456.51798	-2390.90304	1
154	H	75.32629	79.83468	77.26538	1206.40339	-1150.93514	-2154.90344	1
155	N	77.25739	80.05635	76.38759	329.70796	-633.68968	-155.67358	1
156	H	77.41012	81.08389	76.60102	1348.31305	1938.76845	1359.00643	1
157	H	77.85161	79.59368	77.13828	2096.92035	1446.54551	-966.48890	1
158	H	77.86207	79.93327	75.52422	-1197.07217	-2303.53719	827.28733	1
159	C	72.47076	75.45856	74.27277	-378.01186	-556.17301	-413.96481	1
160	O	71.34403	75.87833	74.18191	-409.44433	-307.55053	-453.30833	1
161	N	73.32901	75.12669	73.32640	-429.02477	524.70884	274.08502	1
162	H	74.25994	74.70967	73.55631	1706.34263	-1425.96036	1574.38926	1
163	C	72.93464	75.32041	71.95431	-45.25864	-626.22952	478.93267	1
164	H	72.05124	74.66498	71.78683	1988.63164	570.90773	1772.87287	1
165	C	72.56112	76.84711	71.80294	551.77128	-20.49526	-564.54996	1
166	H	71.74672	77.12966	72.51494	1434.61535	-1753.10253	1513.99471	1
167	H	73.43900	77.48346	72.07421	-714.67738	1819.09770	1898.36494	1
168	C	72.10872	77.12524	70.33088	446.99263	-555.77305	338.97221	1
169	H	72.90526	76.83778	69.60815	1953.68466	1892.25957	-161.67766	1

170	H	71.21103	76.52682	70.05780	-403.03785	2688.07032	-188.43591	1
171	C	71.81248	78.67667	70.26345	567.86262	335.74681	434.04421	1
172	H	70.87383	78.93194	70.80726	-1080.02275	1568.26081	-1948.78900	1
173	H	72.61476	79.25713	70.77163	-919.54108	2111.34692	1456.13463	1
174	C	71.72331	79.04858	68.76483	195.81897	173.33862	-745.11536	1
175	H	72.64357	78.84148	68.18231	1405.67949	-2301.21089	-390.08113	1
176	H	70.84049	78.63298	68.23911	-940.37328	-1118.32446	2299.72133	1
177	N	71.54781	80.60129	68.68491	319.26422	656.36007	-42.02424	1
178	H	71.43700	80.99933	67.70789	1961.03633	619.91968	1787.09422	1
179	H	70.70371	81.01617	69.17689	854.14343	-2156.80752	1429.08711	1
180	H	72.33889	81.19787	69.06579	1237.02905	-1378.50857	-1998.28500	1
181	C	74.21515	75.00122	71.00625	532.53319	-268.57236	517.55729	1
182	O	75.34265	75.20518	71.38053	266.16714	-290.73804	-558.88002	1
183	N	73.78014	74.74635	69.74760	-226.25352	640.49678	-270.32839	1
184	H	72.77239	74.56683	69.73743	2007.69063	-1035.27229	1523.50231	1
185	C	74.56919	73.81610	68.96802	-540.76542	-573.33303	49.50000	1
186	H	74.94998	73.08225	69.71113	-2374.20950	-1036.76023	843.75774	1
187	C	73.53197	73.21462	67.93307	-77.09082	666.87422	-415.84136	1
188	H	73.12294	74.03528	67.28035	-985.81834	617.19825	2463.91927	1
189	O	72.35257	72.61367	68.52312	293.29899	-391.65602	-477.80926	1
190	H	71.64205	73.12290	68.09006	2528.72714	-681.76262	-751.27122	1
191	C	74.44753	72.27400	67.06654	252.47363	-605.14473	440.05134	1
192	H	73.88080	71.82267	66.21914	-2052.65063	1456.49051	-1043.51830	1
193	H	75.31264	72.82561	66.62668	-2152.98800	-1661.97574	-161.70652	1
194	H	74.86064	71.43460	67.67255	-473.12726	-1584.27339	2165.61725	1
195	C	75.78904	74.59778	68.22285	360.36307	488.46713	505.10056	1
196	O	76.91705	74.43182	68.62910	-200.08817	-528.03552	-385.82850	1
197	N	75.39490	75.33210	67.18391	-597.54095	-226.44775	355.20479	1
198	H	74.40034	75.43247	66.98868	2179.23655	-1300.70981	-991.33835	1
199	C	76.38337	76.06849	66.47280	-687.68921	297.39807	-249.45179	1
200	H	77.33814	75.54459	66.71735	-349.16256	-2467.37713	-1101.72831	1
201	C	76.01758	76.09575	64.91374	672.47345	361.54328	-201.62880	1
202	H	75.01440	76.55184	64.75485	1541.41502	582.18425	2169.97026	1
203	H	76.75718	76.73186	64.37136	-2534.67717	60.25153	997.72295	1
204	C	76.05317	74.65397	64.38842	574.26774	-389.43119	-377.02542	1
205	C	77.31074	74.04376	64.09907	688.82679	-287.33580	-257.96133	1
206	H	78.25732	74.60394	64.24446	331.14182	1470.38163	2269.80013	1
207	C	74.83938	73.92266	64.21586	-383.52382	-675.04808	144.24917	1
208	H	73.86521	74.38670	64.45250	4.09847	1517.59662	2262.86397	1
209	C	77.32401	72.72866	63.63492	-134.76730	428.45285	-649.50303	1
210	H	78.29751	72.25733	63.41151	-903.23433	1600.49020	2011.53387	1
211	C	74.90460	72.60962	63.74337	-335.53281	-615.00040	-364.39058	1
212	H	73.95911	72.05628	63.60701	1596.45398	-1369.33862	1732.02659	1
213	C	76.13760	71.96456	63.43417	585.48547	-340.24194	-406.23938	1
214	O	76.21280	70.63075	62.95459	-419.15649	-173.04408	-511.94141	1
215	H	75.25142	70.41501	62.91040	-1071.84350	1559.71507	-1960.13012	1
216	C	76.33938	77.58550	67.05237	291.41878	-183.13091	710.72246	1
217	O	76.40127	78.58067	66.33545	379.87695	523.47396	-222.23622	1
218	N	76.26707	77.53885	68.36847	564.30591	373.09380	277.24371	1
219	H	76.27289	76.61980	68.81681	-120.59931	-2436.07824	-1214.35098	1
220	C	76.10526	78.78645	69.05580	404.07514	-299.37480	608.84009	1
221	H	75.47504	79.37049	68.34442	-1071.07882	-841.69025	2359.66467	1
222	C	75.45580	78.48980	70.46858	-683.12807	68.71770	-390.13096	1
223	H	74.57882	77.81231	70.36743	2068.88918	1596.58590	770.89603	1
224	H	76.18010	77.94345	71.11564	1379.86429	2342.49779	-179.85638	1
225	C	75.04990	79.85106	71.10926	-176.39967	537.49466	550.97268	1
226	H	75.87071	80.59409	71.00569	-396.28051	1942.22168	1869.33314	1
227	H	74.17922	80.30316	70.58650	-94.44700	586.00678	-2659.20016	1
228	C	74.73627	79.57596	72.66154	-291.69381	-718.18079	-150.72929	1
229	H	74.07322	78.69726	72.88220	-2303.38776	1089.76242	964.62032	1
230	H	75.67378	79.53577	73.27442	884.16729	2568.80533	-207.74283	1
231	N	74.04970	80.75558	72.94854	-594.49522	-252.81478	342.29276	1

232	H	74.54054	81.61287	72.73368	-1735.17426	2084.05705	-263.71605	1
233	C	72.88949	80.84597	73.47534	595.23177	-271.52487	442.22352	1
234	N	72.20353	79.67643	73.80337	585.53813	-424.79750	-105.81303	1
235	H	72.47998	78.70192	73.69749	959.88797	1327.56823	-2177.11905	1
236	H	71.28029	79.64122	74.23790	1578.48647	16.27378	-2220.76233	1
237	N	72.53100	82.18954	73.63015	-452.17763	-390.33541	-421.51853	1
238	H	73.02902	83.04673	73.39331	470.26107	1974.25629	-1817.92087	1
239	H	71.64506	82.48986	74.03921	1856.67307	-1573.97321	-1224.35416	1
240	C	77.59480	79.43860	69.22120	-531.47271	-581.45780	-55.06206	1
241	O	78.18065	79.40809	70.26990	-243.00837	192.73507	609.52485	1
242	N	77.93716	79.98957	68.05667	343.49288	-644.25607	38.09164	1
243	H	77.30657	79.82105	67.23456	-1691.16043	-1535.97525	-1484.73099	1
244	C	79.20753	80.68962	67.84469	542.66492	350.14337	454.42563	1
245	H	78.91642	81.48936	67.12298	1209.57979	-2396.95920	463.86744	1
246	C	79.74911	81.25794	69.13952	-737.14309	145.93010	242.71942	1
247	H	79.93458	80.40573	69.84457	-1050.18303	159.36419	-2509.06125	1
248	C	81.06503	81.99200	68.95327	-706.77696	-252.88343	-245.16230	1
249	H	81.43631	82.42979	69.92056	-1624.64039	-1665.49085	1417.86935	1
250	H	81.87284	81.30942	68.56551	2566.10521	598.51109	693.22305	1
251	H	80.96667	82.83867	68.22014	-1972.69758	107.10018	-1876.34312	1
252	C	78.74946	82.18845	69.80590	412.85148	672.58832	-27.69222	1
253	H	79.14209	82.59864	70.77591	1447.02277	1762.76533	-1490.78944	1
254	H	78.49464	83.06467	69.14961	1320.77379	-145.20455	2378.68491	1
255	H	77.78886	81.64867	70.03618	-1512.10848	1470.52031	1724.75147	1
256	C	80.27127	79.65148	67.11704	-607.11113	499.56689	73.73769	1
257	O	81.35105	80.07758	66.75760	357.97126	460.81534	356.68785	1
258	N	79.78983	78.43206	66.95680	536.55407	-368.62270	332.76306	1
259	H	78.86478	78.27062	67.35021	524.38866	2297.69985	1367.20941	1
260	C	80.66036	77.40331	66.50203	46.50277	-774.29190	-147.97904	1
261	H	81.48818	77.95842	66.00284	1676.51875	1883.29066	1032.55549	1
262	C	81.17604	76.49700	67.73632	-559.41456	-34.19198	-556.30433	1
263	H	80.29825	76.03013	68.24410	-64.66664	395.18769	2695.05373	1
264	H	81.78291	75.64903	67.33808	-2703.44278	-60.40056	333.79418	1
265	C	81.97974	77.30694	68.71629	-519.76435	377.31045	459.42366	1
266	H	81.31972	78.09473	69.14619	-1746.74323	1667.50644	-1261.73691	1
267	C	82.47530	76.40844	69.84395	570.95554	16.46261	-545.27700	1
268	H	83.04982	76.98621	70.61282	2391.58273	28.05277	-1305.07271	1
269	H	81.62628	75.90243	70.37203	175.75588	917.63458	2559.43867	1
270	H	83.15330	75.60307	69.45998	-1063.97851	-2155.34650	1283.00462	1
271	C	83.16830	77.98653	68.05258	193.76014	2.62946	-765.53141	1
272	H	83.85680	78.44736	68.80729	507.39394	-846.55087	2539.60089	1
273	H	83.77598	77.26578	67.44637	1337.57841	1818.19054	1526.01994	1
274	H	82.82972	78.81676	67.36162	1100.88635	-1172.91350	-2199.08909	1
275	C	79.81407	76.44563	65.53158	-549.21115	475.64486	-309.38218	1
276	O	79.91079	75.24566	65.55038	556.06106	-390.37755	-78.24250	1
277	O	79.00618	77.08614	64.55868	-572.27940	-310.19032	-209.75862	1
278	H	79.10265	78.02774	64.88013	-1380.08193	2212.14486	790.85944	1

Listing 33: C00033.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.8604	0.0000	300.0000
3	H	74.98776	63.11486	86.00369	-2043.14101	-1757.64893	399.89339		1
4	N	75.69024	62.95080	85.28496	426.75047	490.45733	-334.42467		1
5	H	75.11769	62.71686	84.47580	442.25559	-1110.30854	-2448.52907		1
6	C	76.55752	64.03842	85.04698	415.32972	-666.39213	83.73172		1
7	H	76.76710	64.50496	86.03344	879.32219	2491.00447	667.35213		1
8	C	77.86406	63.46844	84.29594	31.35357	477.41777	628.23362		1
9	H	77.55714	63.04980	83.30707	1168.38489	2240.25337	-1019.71136		1
10	H	78.58148	64.29476	84.07205	-360.43770	2534.90498	931.67112		1
11	C	78.51001	62.39876	85.14051	463.18208	512.70242	-382.34388		1

12	H	77.71229	61.69925	85.47909	1725.29117	1863.52247	-987.07854	1
13	C	79.52496	61.61222	84.32127	710.42801	-144.27427	-313.15367	1
14	H	79.99472	60.79097	84.92206	364.20195	-1033.13725	2494.72524	1
15	H	79.05334	61.13789	83.42190	2567.61904	335.80679	847.48802	1
16	H	80.35467	62.26921	83.95267	-2587.99029	680.92867	-512.16411	1
17	C	79.19049	62.99296	86.36554	268.17616	741.64379	-40.42634	1
18	H	79.67512	62.20109	86.99361	1283.54314	-1945.37420	-1411.27812	1
19	H	79.99001	63.72422	86.07869	-1258.57796	1317.15249	-2026.02085	1
20	H	78.46241	63.53681	87.02100	-2502.84526	909.80597	575.92391	1
21	C	75.77734	65.01149	83.99498	619.36578	-458.64843	-172.09273	1
22	O	75.42135	64.62963	82.89395	-81.40433	433.87611	522.34594	1
23	N	75.61879	66.21055	84.54110	175.23996	-622.20190	341.55523	1
24	H	76.02900	66.39982	85.45465	-876.57256	-303.22879	-2561.90213	1
25	C	75.20500	67.25915	83.66587	-571.88214	-534.10783	-106.15033	1
26	H	74.55620	66.75515	82.91459	-2713.20841	-16.25800	-248.80809	1
27	C	74.49391	68.40419	84.52780	166.60354	288.16399	-716.09568	1
28	H	75.23390	68.78957	85.28135	-2097.85574	1636.78449	-586.18044	1
29	O	73.33257	67.99992	85.27225	-317.80580	-363.38227	484.43082	1
30	H	73.62250	68.17796	86.18926	1863.74748	-1451.84923	1357.29467	1
31	C	74.24912	69.50509	83.43030	503.80731	517.99032	318.51606	1
32	H	73.86321	70.44921	83.88001	640.61020	-2157.10410	-1536.29104	1
33	H	75.18276	69.76288	82.86728	1687.88455	465.60692	2087.56452	1
34	H	73.49822	69.16855	82.67837	-1293.07895	-1899.88581	-1463.57452	1
35	C	76.58689	67.88446	83.04676	-153.07550	-733.68902	248.70981	1
36	O	77.41336	68.34931	83.78449	186.15459	-480.78787	-449.34387	1
37	N	76.58140	67.81001	81.70443	-487.53139	543.18517	42.03850	1
38	C	77.55351	68.49052	80.91524	-699.35871	69.34393	360.10701	1
39	H	78.40285	68.72500	81.59916	2.81126	-221.99807	-2715.58072	1
40	C	77.81936	67.38166	79.80320	-507.46439	-592.59194	122.07761	1
41	H	78.35533	67.76628	78.90832	-1975.08116	525.87560	-1801.71556	1
42	H	78.43083	66.54485	80.20704	1588.27743	-1913.22100	1113.83566	1
43	C	76.36006	66.92218	79.50044	-613.62442	-457.55993	-194.14490	1
44	H	75.85407	67.63731	78.81301	1707.54637	-721.27992	1996.92523	1
45	H	76.30491	65.92453	79.01029	758.23357	2100.81767	1560.55011	1
46	C	75.69189	66.94477	80.94056	-352.41524	704.96076	49.21465	1
47	H	74.67774	67.40973	80.96873	1714.76886	-2070.42778	443.35792	1
48	H	75.66732	65.95406	81.48994	1224.15040	1801.50881	1636.97633	1
49	C	76.82953	69.82675	80.29064	566.85117	537.05831	117.62814	1
50	O	75.86181	70.32463	80.81787	-550.26779	-406.08867	4.21666	1
51	N	77.49094	70.22177	79.21161	566.34832	-425.77725	180.18749	1
52	H	78.31181	69.69278	78.92544	644.44502	2646.80550	-52.73430	1
53	C	77.13979	71.46235	78.61153	612.34801	-281.48662	411.56221	1
54	H	76.26200	71.80723	79.20818	1667.23498	-1490.75142	1556.16753	1
55	C	78.42877	72.39591	78.78360	-714.45746	-175.43074	286.98927	1
56	H	79.29822	71.93677	78.23850	-787.09484	1763.03619	-1922.46060	1
57	O	78.89319	72.60782	80.13078	-429.46514	516.51932	-128.40526	1
58	H	79.78270	72.20796	80.09234	1981.82785	436.16847	-1818.18182	1
59	C	77.93902	73.68606	78.03459	630.79189	-468.94448	76.03230	1
60	H	78.79335	74.36795	77.79722	-1775.71861	2062.30353	131.89849	1
61	H	77.41812	73.44881	77.07929	-1855.14608	88.94118	1993.53760	1
62	H	77.21512	74.25487	78.66153	-1504.82350	-780.94249	-2132.90992	1
63	C	76.75392	71.14081	77.04837	288.57638	618.62814	-397.00270	1
64	O	75.55515	71.01754	76.79483	321.70495	-185.26452	574.37218	1
65	N	77.79148	71.01807	76.26269	-447.05792	-446.53431	367.76425	1
66	H	78.69015	71.10372	76.73425	350.31316	1975.63644	-1843.31522	1
67	C	77.72591	70.79093	74.86518	-511.23061	374.03917	-471.51480	1
68	H	78.79711	70.59196	74.63648	2234.79579	-898.70890	-1273.45190	1
69	C	76.81121	69.51017	74.60549	529.53781	-159.34528	563.72604	1
70	H	77.10766	69.03623	73.62756	654.59388	2347.94251	1217.51488	1
71	H	77.08689	68.77875	75.41318	-1526.55661	2103.42026	817.87394	1
72	O	75.38612	69.67114	74.55523	-554.84278	14.12789	399.58769	1
73	H	75.24971	70.20786	75.42677	1297.06236	2061.84854	1220.68812	1

74	C	77.19222	72.10217	74.05257	-662.15484	-412.13544	123.62687	1
75	O	76.64878	72.00075	72.97437	-540.01537	-317.05804	274.91456	1
76	N	77.46104	73.25808	74.72489	-202.76299	-690.00100	-131.49145	1
77	H	78.03173	72.91858	75.50832	-702.62132	-2617.37191	281.70413	1
78	C	77.94996	74.41571	74.01048	-491.73914	576.34187	222.73509	1
79	H	79.05704	74.33717	74.05393	1977.17978	-1823.58850	-434.68928	1
80	C	77.42757	74.46929	72.52303	-649.50797	-328.66843	306.11224	1
81	H	76.38090	74.08905	72.46653	2075.07803	1452.16490	-1004.45904	1
82	C	77.53804	75.95893	72.03771	-615.18735	-489.99689	-70.96352	1
83	H	77.05793	76.10619	71.04150	-1226.32661	-1724.38906	-1716.47170	1
84	H	77.05004	76.65559	72.76434	2381.64273	-969.84735	900.46860	1
85	H	78.60082	76.28302	71.94621	2122.74991	1702.23946	-141.36228	1
86	C	78.36862	73.70482	71.52283	-501.86074	-479.61276	-376.42482	1
87	H	77.97104	73.74797	70.48185	993.79261	-2246.95401	-1177.81305	1
88	H	79.39438	74.14089	71.50546	42.71279	-626.15391	-2651.37258	1
89	H	78.47343	72.62630	71.78854	-2026.39012	-1590.33709	-887.82922	1
90	C	77.43714	75.70060	74.85473	-672.89153	382.57394	-156.34072	1
91	O	78.07213	76.74351	74.80576	410.04627	221.86223	500.35950	1
92	N	76.22197	75.51769	75.41952	-378.11782	-443.79414	-441.10984	1
93	H	75.96269	74.55131	75.19750	2404.15973	-568.14894	1149.30085	1
94	C	76.00885	75.92549	76.79411	-544.54484	466.16019	331.29119	1
95	H	75.72795	74.96297	77.27269	-1409.80988	-170.17955	2325.32679	1
96	C	77.33223	76.53685	77.40268	-184.48284	116.78282	-758.89137	1
97	H	78.17951	75.81010	77.37872	1893.78641	1861.14652	611.04528	1
98	H	77.69536	77.40722	76.80666	-2170.79665	-974.19311	1327.50117	1
99	C	76.99242	76.97923	78.86250	389.51668	672.81878	-138.49152	1
100	H	75.97443	77.42497	78.88079	510.64577	1933.03327	1851.02484	1
101	H	76.90740	76.09798	79.53472	-2302.30869	-1105.72939	-948.89774	1
102	C	78.02113	78.00802	79.45842	-559.93427	-126.34590	542.30857	1
103	O	77.82661	78.46544	80.55701	-670.36003	-111.83166	76.36448	1
104	N	79.04860	78.31320	78.63766	-216.06729	-537.07037	446.51379	1
105	H	79.30036	77.91914	77.72352	-1251.96487	1074.12894	-2168.52500	1
106	H	79.81619	78.94365	78.89541	-2451.83023	-720.73851	944.84612	1
107	C	74.74528	76.92503	76.87851	546.24052	-563.88337	-85.11809	1
108	O	73.84813	76.64109	77.67178	71.70702	-307.40463	606.69673	1
109	N	74.87995	78.04717	76.19451	479.90863	-504.50129	222.86849	1
110	C	73.73320	78.78650	75.71184	75.51268	-600.91904	506.73700	1
111	H	72.88337	78.56376	76.39144	-2033.61562	1795.30103	254.89480	1
112	C	74.31266	80.26245	75.90523	523.79067	517.99274	284.45581	1
113	H	73.71029	81.05655	75.40372	1599.61665	-1127.00911	1895.98173	1
114	H	74.33624	80.53770	76.98390	-1881.83093	1275.82488	-1501.55016	1
115	C	75.75227	80.10206	75.33356	-600.05639	-404.05026	316.64485	1
116	H	75.74152	79.98298	74.22582	-2597.05260	496.36221	657.73249	1
117	H	76.43264	80.95243	75.56474	-1666.24518	1294.38985	-1723.90591	1
118	C	76.15247	78.75319	76.06978	493.57570	-129.95376	-602.56394	1
119	H	76.85239	78.07520	75.48561	-1469.08415	-637.84797	2204.22581	1
120	H	76.53165	78.88639	77.11141	-1038.97840	1068.88701	-2280.71789	1
121	C	73.40102	78.31675	74.23039	188.88100	241.05089	-727.87821	1
122	O	72.35318	79.28659	73.21895	531.88613	-49.19943	427.07960	1
123	N	74.62636	78.08804	73.55669	708.14833	26.93417	-179.73509	1
124	H	75.09076	77.46005	74.23439	-2232.69501	-1179.09831	1023.94816	1
125	C	74.59918	77.59181	72.21120	-738.32412	259.92548	104.42456	1
126	H	75.45986	76.89238	72.23170	2028.89123	1260.02983	1311.33324	1
127	C	73.26944	76.80818	71.86053	-258.65678	-345.52513	661.28459	1
128	H	72.39502	77.21282	72.41356	-1826.06090	-1801.46097	-918.64554	1
129	C	72.93673	76.79665	70.35757	-541.23400	531.92970	-218.41428	1
130	H	71.95289	76.31011	70.19378	1311.73218	-2219.18200	882.19023	1
131	H	72.83286	77.83531	69.97284	-1048.71298	1223.58118	-2196.97971	1
132	H	75.08663	76.59199	69.55682	419.06414	1903.92898	1903.44670	1
133	C	73.54034	75.28369	72.22096	-423.86431	152.66566	-648.55262	1
134	H	72.98056	74.63699	71.49924	105.68386	-2342.50080	1387.51238	1
135	H	74.61567	75.02924	72.07569	-1695.63603	-1484.73621	-1531.02793	1

136	H	72.31661	75.52879	74.19839	-1853.57121	-487.39031	1936.59343	1
137	C	74.93423	78.89275	71.28029	539.71428	-510.58232	267.58633	1
138	O	74.08152	79.57823	70.76431	-15.93758	-278.34085	-624.49402	1
139	N	76.26108	78.95602	71.11949	-676.81886	12.05292	276.17960	1
140	H	76.82563	78.33063	71.69262	-1694.44250	-373.84189	-2100.66098	1
141	C	76.84876	80.15348	70.57077	412.33078	-664.70360	108.35451	1
142	H	76.39498	80.98186	71.15989	1765.77476	1294.44366	1621.76594	1
143	C	78.40427	80.01114	70.79335	-179.66635	-721.95667	-264.73915	1
144	H	78.63731	79.74926	71.85015	-607.34922	2587.87032	-598.10018	1
145	H	78.79857	79.16615	70.18533	-359.69332	-1479.13954	-2259.74260	1
146	C	79.09949	81.35371	70.38468	-240.01076	616.02425	431.85322	1
147	H	78.72738	81.69194	69.38432	-1359.17131	782.54425	2227.99181	1
148	H	78.84449	82.17028	71.09694	-820.36667	85.81767	-2596.78715	1
149	C	80.66092	81.10949	70.33661	-513.07015	236.18570	-551.87280	1
150	H	81.06707	80.91071	71.35501	1816.11944	-1183.11722	-1650.94321	1
151	H	80.90277	80.20517	69.73218	-1800.04429	-1361.53473	1526.34643	1
152	C	81.30913	82.36633	69.71034	726.08972	-253.19732	-179.64713	1
153	H	81.03053	82.54839	68.65300	1224.27271	-456.51798	-2390.90304	1
154	H	81.18073	83.29578	70.29993	1206.40339	-1150.93514	-2154.90344	1
155	N	82.85698	82.13285	69.67019	329.70796	-633.68968	-155.67358	1
156	H	83.42668	82.91755	69.24009	1348.31305	1938.76845	1359.00643	1
157	H	83.35137	82.00218	70.60031	2096.92035	1446.54551	-966.48890	1
158	H	83.20495	81.29662	69.11671	-1197.07217	-2303.53719	827.28733	1
159	C	76.51349	80.30636	68.99569	-378.01186	-556.17301	-413.96481	1
160	O	76.96249	81.23438	68.35895	-409.44433	-307.55053	-453.30833	1
161	N	75.80589	79.26096	68.51164	-429.02477	524.70884	274.08502	1
162	H	75.45541	78.65876	69.26125	1706.34263	-1425.96036	1574.38926	1
163	C	74.87852	79.62914	67.45647	-45.25864	-626.22952	478.93267	1
164	H	74.54691	80.66803	67.67596	1988.63164	570.90773	1772.87287	1
165	C	75.77882	79.52900	66.17250	551.77128	-20.49526	-564.54996	1
166	H	76.54639	80.33805	66.18742	1434.61535	-1753.10253	1513.99471	1
167	H	76.35533	78.57668	66.18687	-714.67738	1819.09770	1898.36494	1
168	C	74.89463	79.60798	64.88237	446.99263	-555.77305	338.97221	1
169	H	74.08547	78.84252	64.90245	1953.68466	1892.25957	-161.67766	1
170	H	74.39052	80.59564	64.78786	-403.03785	2688.07032	-188.43591	1
171	C	75.90727	79.34608	63.69607	567.86262	335.74681	434.04421	1
172	H	76.70815	80.12079	63.68668	-1080.02275	1568.26081	-1948.78900	1
173	H	76.43189	78.37335	63.83895	-919.54108	2111.34692	1456.13463	1
174	C	75.13223	79.34631	62.35886	195.81897	173.33862	-745.11536	1
175	H	74.39291	78.52751	62.25187	1405.67949	-2301.21089	-390.08113	1
176	H	74.66654	80.31615	62.09328	-940.37328	-1118.32446	2299.72133	1
177	N	76.18975	79.08351	61.23318	319.26422	656.36007	-42.02424	1
178	H	75.81425	79.05860	60.24181	1961.03633	619.91968	1787.09422	1
179	H	76.97884	79.78749	61.14064	854.14343	-2156.80752	1429.08711	1
180	H	76.72124	78.16575	61.27809	1237.02905	-1378.50857	-1998.28500	1
181	C	73.67159	78.53808	67.50837	532.53319	-268.57236	517.55729	1
182	O	72.51686	78.89730	67.53514	266.16714	-290.73804	-558.88002	1
183	N	74.16164	77.29087	67.46419	-226.25352	640.49678	-270.32839	1
184	H	75.17729	77.19603	67.42442	2007.69063	-1035.27229	1523.50231	1
185	C	73.35194	76.26932	67.99540	-540.76542	-573.33303	49.50000	1
186	H	72.33565	76.71688	68.06182	-2374.20950	-1036.76023	843.75774	1
187	C	73.43986	75.00427	67.05589	-77.09082	666.87422	-415.84136	1
188	H	74.48475	74.59434	67.09237	-985.81834	617.19825	2463.91927	1
189	O	73.14713	75.23571	65.65411	293.29899	-391.65602	-477.80926	1
190	H	74.00143	75.02189	65.24092	2528.72714	-681.76262	-751.27122	1
191	C	72.44538	74.01280	67.76778	252.47363	-605.14473	440.05134	1
192	H	72.44209	73.01425	67.27177	-2052.65063	1456.49051	-1043.51830	1
193	H	72.70616	73.84603	68.84113	-2152.98800	-1661.97574	-161.70652	1
194	H	71.39895	74.39619	67.74084	-473.12726	-1584.27339	2165.61725	1
195	C	74.10534	75.97983	69.49897	360.36307	488.46713	505.10056	1
196	O	74.49788	74.83226	69.80204	-200.08817	-528.03552	-385.82850	1
197	N	71.44721	73.26443	70.58358	-597.54095	-226.44775	355.20479	2

198	H	70.52172	73.60837	70.85780	2179.23655	-1300.70981	-991.33835	2
199	C	72.02747	72.74412	71.53329	-687.68921	297.39807	-249.45179	2
200	H	71.47921	72.74543	72.50004	-349.16256	-2467.37713	-1101.72831	2
201	C	73.50421	72.19518	71.32290	672.47345	361.54328	-201.62880	2
202	H	74.21944	73.04236	71.19577	1541.41502	582.18425	2169.97026	2
203	H	73.82815	71.64191	72.23642	-2534.67717	60.25153	997.72295	2
204	C	73.57671	71.29555	70.07843	574.26774	-389.43119	-377.02542	2
205	C	72.92520	70.02605	70.06035	688.82679	-287.33580	-257.96133	2
206	H	72.33997	69.68072	70.93204	331.14182	1470.38163	2269.80013	2
207	C	74.32350	71.74215	68.94674	-383.52382	-675.04808	144.24917	2
208	H	74.82072	72.73196	68.95853	4.09847	1517.59662	2262.86397	2
209	C	73.04968	69.22923	68.92185	-134.76730	428.45285	-649.50303	2
210	H	72.55085	68.24437	68.90849	-903.23433	1600.49020	2011.53387	2
211	C	74.41993	70.90702	67.83045	-335.53281	-615.00040	-364.39058	2
212	H	75.00593	71.25893	66.96363	1596.45398	-1369.33862	1732.02659	2
213	C	73.79719	69.62582	67.77513	585.48547	-340.24194	-406.23938	2
214	O	73.89398	68.76695	66.64875	-419.15649	-173.04408	-511.94141	2
215	H	74.47320	69.31622	66.06991	-1071.84350	1559.71507	-1960.13012	2
216	C	73.12299	74.92834	73.66258	291.41878	-183.13091	710.72246	1
217	O	73.42332	73.98951	74.35957	379.87695	523.47396	-222.23622	1
218	N	70.06111	76.76292	72.17417	564.30591	373.09380	277.24371	1
219	H	70.13522	77.41632	71.40177	-120.59931	-2436.07824	-1214.35098	1
220	C	70.32406	77.28453	73.26567	404.07514	-299.37480	608.84009	1
221	H	72.86333	77.34948	74.18956	-1071.07882	-841.69025	2359.66467	1
222	C	70.72128	78.75831	73.40208	-683.12807	68.71770	-390.13096	1
223	H	70.28261	79.39033	72.60262	2068.88918	1596.58590	770.89603	1
224	H	70.44939	79.18255	74.38802	1379.86429	2342.49779	-179.85638	1
225	C	72.40583	80.88593	73.79076	-176.39967	537.49466	550.97268	1
226	H	72.13329	80.76388	74.86219	-396.28051	1942.22168	1869.33314	1
227	H	73.49043	81.11907	73.73002	-94.44700	586.00678	-2659.20016	1
228	C	71.53921	81.97596	73.09636	-291.69381	-718.18079	-150.72929	1
229	H	71.80965	82.21977	72.03398	-2303.38776	1089.76242	964.62032	1
230	H	70.43316	81.79679	73.19321	884.16729	2568.80533	-207.74283	1
231	N	71.89584	83.03672	73.94329	-594.49522	-252.81478	342.29276	1
232	H	71.94101	82.84417	74.93504	-1735.17426	2084.05705	-263.71605	1
233	C	72.12107	84.23406	73.56673	595.23177	-271.52487	442.22352	1
234	N	72.03228	84.54336	72.20699	585.53813	-424.79750	-105.81303	1
235	H	71.79527	83.93708	71.42268	959.88797	1327.56823	-2177.11905	1
236	H	72.17720	85.46769	71.79953	1578.48647	16.27378	-2220.76233	1
237	N	72.42592	85.04622	74.66688	-452.17763	-390.33541	-421.51853	1
238	H	72.46926	84.81536	75.65864	470.226107	1974.25629	-1817.92087	1
239	H	72.62135	86.04563	74.60355	1856.67307	-1573.97321	-1224.35416	1
240	C	70.29100	76.37286	74.55937	-531.47271	-581.45780	-55.06206	1
241	O	69.83994	75.24643	74.59214	-243.00837	192.73507	609.52485	1
242	N	70.90906	77.02874	75.59150	343.49288	-644.25607	38.09164	1
243	H	71.17122	77.98919	75.33933	-1691.16043	-1535.97525	-1484.73099	1
244	C	70.24492	76.86381	76.87265	542.66492	350.14337	454.42563	1
245	H	69.18490	76.64467	76.61834	1209.57979	-2396.95920	463.86744	1
246	C	70.94700	75.67813	77.64411	-737.14309	145.93010	242.71942	1
247	H	72.05451	75.86458	77.71651	-1050.18303	159.36419	-2509.06125	1
248	C	70.29021	75.64277	79.06815	-706.77696	-252.88343	-245.16230	1
249	H	70.70481	74.81902	79.69423	-1624.64039	-1665.49085	1417.86935	1
250	H	70.46673	76.59779	79.61765	2566.10521	598.51109	693.22305	1
251	H	69.18646	75.49661	79.00812	-1972.69758	107.10018	-1876.34312	1
252	C	70.67286	74.31849	76.91021	412.85148	672.58832	-27.69222	1
253	H	70.93071	73.44443	77.55382	1447.02277	1762.76533	-1490.78944	1
254	H	69.59827	74.21927	76.61957	1320.77379	-145.20455	2378.68491	1
255	H	71.28083	74.23171	75.97475	-1512.10848	1470.52031	1724.75147	1
256	C	70.44558	78.24156	77.70290	-607.11113	499.56689	73.73769	1
257	O	69.47394	78.93752	77.87393	357.97126	460.81534	356.68785	1
258	N	71.70666	78.46432	78.10493	536.55407	-368.62270	332.76306	1
259	H	72.47968	77.77432	77.96629	524.38866	2297.69985	1367.20941	1

260	C	71.80184	79.57998	79.02210	46.50277	-774.29190	-147.97904	1
261	H	70.95563	79.41530	79.72793	1676.51875	1883.29066	1032.55549	1
262	C	73.23152	79.65359	79.68889	-559.41456	-34.19198	-556.30433	1
263	H	73.96795	79.97339	78.91890	-64.66664	395.18769	2695.05373	1
264	H	73.24404	80.45240	80.46386	-2703.44278	-60.40056	333.79418	1
265	C	73.72139	78.29999	80.30866	-519.76435	377.31045	459.42366	1
266	H	73.73863	77.49608	79.52871	-1746.74323	1667.50644	-1261.73691	1
267	C	75.16871	78.65074	80.81530	570.95554	16.46261	-545.27700	1
268	H	75.73648	77.74368	81.13511	2391.58273	28.05277	-1305.07271	1
269	H	75.76244	79.15492	80.01463	175.75588	917.63458	2559.43867	1
270	H	75.14311	79.34668	81.68572	-1063.97851	-2155.34650	1283.00462	1
271	C	72.84748	77.86947	81.53985	193.76014	2.62946	-765.53141	1
272	H	73.25449	76.95277	82.02724	507.39394	-846.55087	2539.60089	1
273	H	72.81127	78.66960	82.31527	1337.57841	1818.19054	1526.01994	1
274	H	71.79705	77.64738	81.24012	1100.88635	-1172.91350	-2199.08909	1
275	C	71.67903	80.97580	78.20883	-549.21115	475.64486	-309.38218	1
276	O	72.13948	81.15773	77.11041	556.06106	-390.37755	-78.24250	1
277	O	71.20984	82.06371	78.97705	-572.27940	-310.19032	-209.75862	1
278	H	70.92027	81.56079	79.79176	-1380.08193	2212.14486	790.85944	1

Listing 34: C00034.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	1.2297	4919
		0.2500	300.00	0.00	0.00	0.00	-1293.8275	0.0000	300.0000
3	H	70.75458	82.90491	85.29892	-2043.14101	-1757.64893	399.89339		1
4	N	71.74711	82.75800	85.47461	426.75047	490.45733	-334.42467		1
5	H	71.93991	81.90077	84.95087	442.25559	-1110.30854	-2448.52907		1
6	C	72.57548	83.82556	85.05684	415.32972	-666.39213	83.73172		1
7	H	71.94553	84.74304	85.02769	879.32219	2491.00447	667.35213		1
8	C	73.79955	83.95179	86.10874	31.35357	477.41777	628.23362		1
9	H	74.36913	82.99042	86.13629	1168.38489	2240.25337	-1019.71136		1
10	H	74.52841	84.72842	85.77534	-360.43770	2534.90498	931.67112		1
11	C	73.24742	84.27501	87.46873	463.18208	512.70242	-382.34388		1
12	H	72.32777	83.66593	87.62375	1725.29117	1863.52247	-987.07854		1
13	C	74.25761	83.90609	88.54899	710.42801	-144.27427	-313.15367		1
14	H	73.86296	84.11904	89.57561	364.20195	-1033.13725	2494.72524		1
15	H	74.52169	82.81776	88.51277	2567.61904	335.80679	847.48802		1
16	H	75.21163	84.48198	88.43370	-2587.99029	680.92867	-512.16411		1
17	C	72.88818	85.75035	87.58683	268.17616	741.64379	-40.42634		1
18	H	72.45327	85.99052	88.59117	1283.54314	-1945.37420	-1411.27812		1
19	H	73.78731	86.40503	87.45126	-1258.57796	1317.15249	-2026.02085		1
20	H	72.13539	86.05844	86.81665	-2502.84526	909.80597	575.92391		1
21	C	73.14422	83.36606	83.62263	619.36578	-458.64843	-172.09273		1
22	O	73.11213	82.20803	83.21919	-81.40433	433.87611	522.34594		1
23	N	73.75218	84.41932	83.02660	175.23996	-622.20190	341.55523		1
24	H	73.61816	85.26133	83.60039	-876.57256	-303.22879	-2561.90213		1
25	C	73.32205	84.61364	81.64148	-571.88214	-534.10783	-106.15033		1
26	H	72.22287	84.45265	81.69284	-2713.20841	-16.25800	-248.80809		1
27	C	73.67756	86.12282	81.30269	166.60354	288.16399	-716.09568		1
28	H	74.79338	86.23543	81.21023	-2097.85574	1636.78449	-586.18044		1
29	O	73.26238	87.09104	82.29476	-317.80580	-363.38227	484.43082		1
30	H	74.11382	87.52003	82.50312	1863.74748	-1451.84923	1357.29467		1
31	C	73.02907	86.28130	79.87826	503.80731	517.99032	318.51606		1
32	H	73.27555	87.26894	79.42395	640.61020	-2157.10410	-1536.29104		1
33	H	73.37825	85.49019	79.17143	1687.88455	465.60692	2087.56452		1
34	H	71.91764	86.21027	79.92948	-1293.07895	-1899.88581	-1463.57452		1
35	C	74.01552	83.54076	80.65009	-153.07550	-733.68902	248.70981		1
36	O	73.36498	83.26086	79.67618	186.15459	-480.78787	-449.34387		1
37	N	75.28430	83.20307	80.92320	-487.53139	543.18517	42.03850		1
38	C	75.92211	82.12199	80.23298	-699.35871	69.34393	360.10701		1
39	H	75.31977	81.90528	79.31851	2.81126	-221.99807	-2715.58072		1

40	C	77.38217	82.72690	79.99636	-507.46439	-592.59194	122.07761	1
41	H	78.13813	81.94229	79.77067	-1975.08116	525.87560	-1801.71556	1
42	H	77.39721	83.44596	79.14810	1588.27743	-1913.22100	1113.83566	1
43	C	77.62370	83.44270	81.35927	-613.62442	-457.55993	-194.14490	1
44	H	77.88672	82.71061	82.15598	1707.54637	-721.27992	1996.92523	1
45	H	78.44830	84.18983	81.32933	758.23357	2100.81767	1560.55011	1
46	C	76.19930	84.09258	81.62954	-352.41524	704.96076	49.21465	1
47	H	75.88959	84.11089	82.70099	1714.76886	-2070.42778	443.35792	1
48	H	76.05356	85.10479	81.18357	1224.15040	1801.50881	1636.97633	1
49	C	76.14715	80.84241	81.20387	566.85117	537.05831	117.62814	1
50	O	76.99099	80.00774	80.90677	-550.26779	-406.08867	4.21666	1
51	N	75.35214	80.85111	82.25950	566.34832	-425.77725	180.18749	1
52	H	74.63261	81.59015	82.38883	644.44502	2646.80550	-52.73430	1
53	C	75.91565	80.20164	83.42170	612.34801	-281.48662	411.56221	1
54	H	77.00532	80.20312	83.18405	1667.23498	-1490.75142	1556.16753	1
55	C	75.52320	81.11762	84.66323	-714.45746	-175.43074	286.98927	1
56	H	74.40170	81.10993	84.74729	-787.09484	1763.03619	-1922.46060	1
57	O	75.90918	82.50724	84.52008	-429.46514	516.51932	-128.40526	1
58	H	75.08775	82.88034	84.13561	1981.82785	436.16847	-1818.18182	1
59	C	76.14087	80.37651	85.90084	630.79189	-468.94448	76.03230	1
60	H	75.86207	80.87995	86.85621	-1775.71861	2062.30353	131.89849	1
61	H	75.79111	79.31799	85.96853	-1855.14608	88.94118	1993.53760	1
62	H	77.25470	80.35886	85.85102	-1504.82350	-780.94249	-2132.90992	1
63	C	75.32641	78.68724	83.44562	288.57638	618.62814	-397.00270	1
64	O	74.57460	78.30637	84.33823	321.70495	-185.26452	574.37218	1
65	N	75.83625	78.03079	82.44091	-447.05792	-446.53431	367.76425	1
66	H	76.44406	78.54493	81.76216	350.31316	1975.63644	-1843.31522	1
67	C	75.59627	76.64110	82.22040	-511.23061	374.03917	-471.51480	1
68	H	76.59283	76.37378	81.80191	2234.79579	-898.70890	-1273.45190	1
69	C	75.29177	75.90783	83.60708	529.53781	-159.34528	563.72604	1
70	H	75.62915	74.83896	83.50656	654.59388	2347.94251	1217.51488	1
71	H	75.95190	76.39642	84.37431	-1526.55661	2103.42026	817.87394	1
72	O	73.92964	75.88307	84.06746	-554.84278	14.12789	399.58769	1
73	H	73.88618	76.84485	84.43997	1297.06236	2061.84854	1220.68812	1
74	C	74.49455	76.47444	81.04896	-662.15484	-412.13544	123.62687	1
75	O	74.47483	77.20496	80.08988	-540.01537	-317.05804	274.91456	1
76	N	73.80188	75.31991	81.21257	-202.76299	-690.00100	-131.49145	1
77	H	73.96953	74.92448	82.14438	-702.62132	-2617.37191	281.70413	1
78	C	72.43684	75.19014	80.66527	-491.73914	576.34187	222.73509	1
79	H	71.99393	74.42723	81.34696	1977.17978	-1823.58850	-434.68928	1
80	C	71.71127	76.51426	80.76923	-649.50797	-328.66843	306.11224	1
81	H	72.27213	77.26453	80.16106	2075.07803	1452.16490	-1004.45904	1
82	C	70.29369	76.43486	80.23240	-615.18735	-489.99689	-70.96352	1
83	H	69.75453	77.41700	80.32995	-1226.32661	-1724.38906	-1716.47170	1
84	H	70.28086	76.14874	79.13895	2381.64273	-969.84735	900.46860	1
85	H	69.68602	75.66466	80.78194	2122.74991	1702.23946	-141.36228	1
86	C	71.67588	77.01721	82.20269	-501.86074	-479.61276	-376.42482	1
87	H	71.14284	78.00312	82.28870	993.79261	-2246.95401	-1177.81305	1
88	H	71.14974	76.29167	82.88174	42.71279	-626.15391	-2651.37258	1
89	H	72.71444	77.15967	82.61620	-2026.39012	-1590.33709	-887.82922	1
90	C	72.55472	74.59623	79.13252	-672.89153	382.57394	-156.34072	1
91	O	71.61266	74.68262	78.37775	410.04627	221.86223	500.35950	1
92	N	73.69672	73.96115	78.92471	-378.11782	-443.79414	-441.10984	1
93	H	74.40320	74.02013	79.65429	2404.15973	-568.14894	1149.30085	1
94	C	73.88386	73.27423	77.68239	-544.54484	466.16019	331.29119	1
95	H	72.90030	72.81428	77.43852	-1409.80988	-170.17955	2325.32679	1
96	C	74.26354	74.40440	76.63583	-184.48284	116.78282	-758.89137	1
97	H	73.45169	75.16485	76.57342	1893.78641	1861.14652	611.04528	1
98	H	75.16936	74.96029	76.96686	-2170.79665	-974.19311	1327.50117	1
99	C	74.49403	73.71836	75.25152	389.51668	672.81878	-138.49152	1
100	H	75.32696	72.98104	75.30348	510.64577	1933.03327	1851.02484	1
101	H	73.58493	73.15498	74.94726	-2302.30869	-1105.72939	-948.89774	1

102	C	74.81586	74.87135	74.20753	-559.93427	-126.34590	542.30857	1
103	O	75.92992	75.10561	73.80526	-670.36003	-111.83166	76.36448	1
104	N	73.67160	75.54458	73.91353	-216.06729	-537.07037	446.51379	1
105	H	72.74135	75.17834	74.14103	-1251.96487	1074.12894	-2168.52500	1
106	H	73.53550	76.09808	73.06293	-2451.83023	-720.73851	944.84612	1
107	C	75.14424	72.25258	77.81528	546.24052	-563.88337	-85.11809	1
108	O	76.14163	72.60558	78.38700	71.70702	-307.40463	606.69673	1
109	N	74.91277	71.10766	77.14958	479.90863	-504.50129	222.86849	1
110	C	75.95521	70.14493	76.98412	75.51268	-600.91904	506.73700	1
111	H	76.66988	70.30754	77.82377	-2033.61562	1795.30103	254.89480	1
112	C	75.12832	68.78642	77.00185	523.79067	517.99274	284.45581	1
113	H	75.68232	67.93781	76.54192	1599.61665	-1127.00911	1895.98173	1
114	H	74.87307	68.47774	78.03991	-1881.83093	1275.82488	-1501.55016	1
115	C	73.85246	69.19394	76.20281	-600.05639	-404.05026	316.64485	1
116	H	74.06281	69.22062	75.10777	-2597.05260	496.36221	657.73249	1
117	H	72.99308	68.50074	76.34691	-1666.24518	1294.38985	-1723.90591	1
118	C	73.58207	70.65396	76.76880	493.57570	-129.95376	-602.56394	1
119	H	73.16556	71.37209	76.02468	-1469.08415	-637.84797	2204.22581	1
120	H	72.96815	70.68993	77.69963	-1038.97840	1068.88701	-2280.71789	1
121	C	76.63916	70.31173	75.50420	188.88100	241.05089	-727.87821	1
122	O	76.00867	70.13188	74.46866	531.88613	-49.19943	427.07960	1
123	N	77.91155	70.60622	75.64165	708.14833	26.93417	-179.73509	1
124	H	78.23247	70.68911	76.60295	-2232.69501	-1179.09831	1023.94816	1
125	C	78.77437	70.87748	74.49475	-738.32412	259.92548	104.42456	1
126	H	78.09145	71.43997	73.81369	2028.89123	1260.02983	1311.33324	1
127	C	79.99775	71.65014	74.96047	-258.65678	-345.52513	661.28459	1
128	H	80.53396	71.01964	75.70489	-1826.06090	-1801.46097	-918.64554	1
129	C	80.94916	71.92679	73.81108	-541.23400	531.92970	-218.41428	1
130	H	81.87257	72.46931	74.15476	1311.73218	-2219.18200	882.19023	1
131	H	81.28612	70.97021	73.31853	-1048.71298	1223.58118	-2196.97971	1
132	H	80.46638	72.55887	73.01559	419.06414	1903.92898	1903.44670	1
133	C	79.61681	72.95034	75.64436	-423.86431	152.66566	-648.55262	1
134	H	80.51910	73.49621	76.03534	105.68386	-2342.50080	1387.51238	1
135	H	79.08433	73.64606	74.93877	-1695.63603	-1484.73621	-1531.02793	1
136	H	78.92620	72.77527	76.51509	-1853.57121	-487.39031	1936.59343	1
137	C	79.18388	69.39624	73.85659	539.71428	-510.58232	267.58633	1
138	O	80.31412	68.98661	73.90476	-15.93758	-278.34085	-624.49402	1
139	N	78.11466	68.84968	73.29990	-676.81886	12.05292	276.17960	1
140	H	77.18405	69.31149	73.41531	-1694.44250	-373.84189	-2100.66098	1
141	C	78.24373	67.51389	72.82680	412.33078	-664.70360	108.35451	1
142	H	79.33018	67.26736	72.91212	1765.77476	1294.44366	1621.76594	1
143	C	77.32265	66.62502	73.76856	-179.66635	-721.95667	-264.73915	1
144	H	77.55717	66.81710	74.83915	-607.34922	2587.87032	-598.10018	1
145	H	76.25395	66.90945	73.64472	-359.69332	-1479.13954	-2259.74260	1
146	C	77.54443	65.12129	73.40746	-240.01076	616.02425	431.85322	1
147	H	77.34886	64.95234	72.32033	-1359.17131	782.54425	2227.99181	1
148	H	78.60380	64.82245	73.57496	-820.36667	85.81767	-2596.78715	1
149	C	76.56539	64.24230	74.28650	-513.07015	236.18570	-551.87280	1
150	H	76.87358	64.24733	75.35726	1816.11944	-1183.11722	-1650.94321	1
151	H	75.53100	64.65564	74.26615	-1800.04429	-1361.53473	1526.34643	1
152	C	76.59177	62.81210	73.69929	726.08972	-253.19732	-179.64713	1
153	H	76.19645	62.73314	72.66677	1224.27271	-456.51798	-2390.90304	1
154	H	77.57333	62.30215	73.76684	1206.40339	-1150.93514	-2154.90344	1
155	N	75.62405	61.92594	74.55383	329.70796	-633.68968	-155.67358	1
156	H	75.51787	60.92247	74.22667	1348.31305	1938.76845	1359.00643	1
157	H	75.87123	61.78578	75.57649	2096.92035	1446.54551	-966.48890	1
158	H	74.60967	62.23312	74.61225	-1197.07217	-2303.53719	827.28733	1
159	C	77.65540	67.38529	71.30494	-378.01186	-556.17301	-413.96481	1
160	O	77.73758	66.33015	70.71393	-409.44433	-307.55053	-453.30833	1
161	N	77.10989	68.51306	70.86873	-429.02477	524.70884	274.08502	1
162	H	77.09729	69.33301	71.47266	1706.34263	-1425.96036	1574.38926	1
163	C	76.36204	68.44723	69.65862	-45.25864	-626.22952	478.93267	1

164	H	76.81439	67.61830	69.06555	1988.63164	570.90773	1772.87287	1
165	C	74.87970	68.11369	70.11171	551.77128	-20.49526	-564.54996	1
166	H	74.81318	67.06116	70.46799	1434.61535	-1753.10253	1513.99471	1
167	H	74.58162	68.74855	70.97946	-714.67738	1819.09770	1898.36494	1
168	C	73.90801	68.36315	68.91395	446.99263	-555.77305	338.97221	1
169	H	73.81579	69.46530	68.75070	1953.68466	1892.25957	-161.67766	1
170	H	74.30201	67.93640	67.96383	-403.03785	2688.07032	-188.43591	1
171	C	72.49633	67.74692	69.27360	567.86262	335.74681	434.04421	1
172	H	72.53754	66.63383	69.30489	-1080.02275	1568.26081	-1948.78900	1
173	H	72.18068	68.07280	70.29264	-919.54108	2111.34692	1456.13463	1
174	C	71.48124	68.24532	68.21780	195.81897	173.33862	-745.11536	1
175	H	71.41091	69.35035	68.13442	1405.67949	-2301.21089	-390.08113	1
176	H	71.59567	67.79574	67.21080	-940.37328	-1118.32446	2299.72133	1
177	N	70.05500	67.82711	68.70336	319.26422	656.36007	-42.02424	1
178	H	69.25415	68.11357	68.06947	1961.03633	619.91968	1787.09422	1
179	H	69.86185	66.79130	68.83201	854.14343	-2156.80752	1429.08711	1
180	H	69.73802	68.23118	69.63175	1237.02905	-1378.50857	-1998.28500	1
181	C	76.41010	69.93771	68.95668	532.53319	-268.57236	517.55729	1
182	O	76.30589	70.95519	69.59574	266.16714	-290.73804	-558.88002	1
183	N	76.51966	69.74956	67.64996	-226.25352	640.49678	-270.32839	1
184	H	76.59371	68.78222	67.33674	2007.69063	-1035.27229	1523.50231	1
185	C	76.33864	70.77099	66.67923	-540.76542	-573.33303	49.50000	1
186	H	76.64900	70.22746	65.75871	-2374.20950	-1036.76023	843.75774	1
187	C	74.79750	71.17757	66.61928	-77.09082	666.87422	-415.84136	1
188	H	74.51629	71.75437	67.54819	-985.81834	617.19825	2463.91927	1
189	O	73.81411	70.13016	66.57064	293.29899	-391.65602	-477.80926	1
190	H	73.21076	70.40924	67.30763	2528.72714	-681.76262	-751.27122	1
191	C	74.83959	72.11524	65.35848	252.47363	-605.14473	440.05134	1
192	H	73.88617	72.67831	65.23557	-2052.65063	1456.49051	-1043.51830	1
193	H	75.66507	72.85984	65.41959	-2152.98800	-1661.97574	-161.70652	1
194	H	75.00003	71.52822	64.42476	-473.12726	-1584.27339	2165.61725	1
195	C	77.33837	72.03110	67.01790	360.36307	488.46713	505.10056	1
196	O	78.52599	71.88022	66.86409	-200.08817	-528.03552	-385.82850	1
197	N	76.69266	73.11780	67.42905	-597.54095	-226.44775	355.20479	1
198	H	75.68224	73.09232	67.55692	2179.23655	-1300.70981	-991.33835	1
199	C	77.34888	74.37145	67.27707	-687.68921	297.39807	-249.45179	1
200	H	78.42967	74.10002	67.32023	-349.16256	-2467.37713	-1101.72831	1
201	C	76.91920	75.05178	65.88642	672.47345	361.54328	-201.62880	1
202	H	75.85765	74.83255	65.63296	1541.41502	582.18425	2169.97026	1
203	H	77.00035	76.16059	65.98569	-2534.67717	60.25153	997.72295	1
204	C	77.87639	74.55272	64.79578	574.26774	-389.43119	-377.02542	1
205	C	79.27563	74.75357	64.99772	688.82679	-287.33580	-257.96133	1
206	H	79.64679	75.24819	65.91343	331.14182	1470.38163	2269.80013	1
207	C	77.40640	73.91693	63.60688	-383.52382	-675.04808	144.24917	1
208	H	76.32530	73.76541	63.43631	4.09847	1517.59662	2262.86397	1
209	C	80.16767	74.30589	64.02561	-134.76730	428.45285	-649.50303	1
210	H	81.24912	74.45106	64.19407	-903.23433	1600.49020	2011.53387	1
211	C	78.33991	73.49499	62.65620	-335.53281	-615.00040	-364.39058	1
212	H	77.96589	73.00928	61.73811	1596.45398	-1369.33862	1732.02659	1
213	C	79.74503	73.66681	62.82406	585.48547	-340.24194	-406.23938	1
214	O	80.70191	73.24315	61.86555	-419.15649	-173.04408	-511.94141	1
215	H	80.09974	72.84887	61.19181	-1071.84350	1559.71507	-1960.13012	1
216	C	76.84422	75.40083	68.41504	291.41878	-183.13091	710.72246	1
217	O	76.56900	76.55460	68.19607	379.87695	523.47396	-222.23622	1
218	N	76.99145	74.82245	69.74587	564.30591	373.09380	277.24371	1
219	H	76.79477	73.84350	69.39866	-120.59931	-2436.07824	-1214.35098	1
220	C	76.05232	75.42759	70.67319	404.07514	-299.37480	608.84009	1
221	H	76.35345	74.84800	71.57416	-1071.07882	-841.69025	2359.66467	1
222	C	76.36121	76.90051	70.83517	-683.12807	68.71770	-390.13096	1
223	H	77.39810	77.13625	70.48881	2068.88918	1596.58590	770.89603	1
224	H	75.68330	77.52879	70.20398	1379.86429	2342.49779	-179.85638	1
225	C	76.18949	77.23291	72.37951	-176.39967	537.49466	550.97268	1

226	H	75.23089	76.80649	72.75851	-396.28051	1942.22168	1869.33314	1
227	H	76.99262	76.72754	72.97195	-94.44700	586.00678	-2659.20016	1
228	C	76.21038	78.80251	72.62837	-291.69381	-718.18079	-150.72929	1
229	H	77.19442	79.31533	72.47346	-2303.38776	1089.76242	964.62032	1
230	H	75.40557	79.39981	72.12720	884.16729	2568.80533	-207.74283	1
231	N	75.93363	78.73304	74.00854	-594.49522	-252.81478	342.29276	1
232	H	75.88716	77.80823	74.41427	-1735.17426	2084.05705	-263.71605	1
233	C	75.74496	79.74059	74.76360	595.23177	-271.52487	442.22352	1
234	N	75.81674	81.00925	74.18306	585.53813	-424.79750	-105.81303	1
235	H	76.00860	81.26130	73.21399	959.88797	1327.56823	-2177.11905	1
236	H	75.68502	81.89194	74.67797	1578.48647	16.27378	-2220.76233	1
237	N	75.49461	79.32921	76.07849	-452.17763	-390.33541	-421.51853	1
238	H	75.43956	78.39763	76.48846	470.26107	1974.25629	-1817.92087	1
239	H	75.30976	79.97336	76.84832	1856.67307	-1573.97321	-1224.35416	1
240	C	74.61390	75.09579	70.30395	-531.47271	-581.45780	-55.06206	1
241	O	74.40617	74.04361	69.74679	-243.00837	192.73507	609.52485	1
242	N	73.64163	75.98476	70.77645	343.49288	-644.25607	38.09164	1
243	H	73.94111	76.88810	71.16589	-1691.16043	-1535.97525	-1484.73099	1
244	C	72.26923	75.90991	70.23927	542.66492	350.14337	454.42563	1
245	H	71.82145	76.86321	70.60449	1209.57979	-2396.95920	463.86744	1
246	C	72.35446	75.85142	68.73283	-737.14309	145.93010	242.71942	1
247	H	72.85286	74.89371	68.44714	-1050.18303	159.36419	-2509.06125	1
248	C	70.97348	75.89457	68.10076	-706.77696	-252.88343	-245.16230	1
249	H	71.02631	75.82119	66.98082	-1624.64039	-1665.49085	1417.86935	1
250	H	70.32346	75.05143	68.46127	2566.10521	598.51109	693.22305	1
251	H	70.43785	76.85167	68.34549	-1972.69758	107.10018	-1876.34312	1
252	C	73.21160	76.97373	68.17041	412.85148	672.58832	-27.69222	1
253	H	73.20662	76.98022	67.04733	1447.02277	1762.76533	-1490.78944	1
254	H	72.84903	77.98103	68.51148	1320.77379	-145.20455	2378.68491	1
255	H	74.28649	76.87670	68.49560	-1512.10848	1470.52031	1724.75147	1
256	C	71.58563	74.61240	71.00091	-607.11113	499.56689	73.73769	1
257	O	71.27652	74.73816	72.16122	357.97126	460.81534	356.68785	1
258	N	71.39030	73.55333	70.21517	536.55407	-368.62270	332.76306	1
259	H	71.76020	73.58282	69.26582	524.38866	2297.69985	1367.20941	1
260	C	71.37873	72.29132	70.88838	46.50277	-774.29190	-147.97904	1
261	H	71.72538	72.50936	71.92411	1676.51875	1883.29066	1032.55549	1
262	C	69.88574	71.67340	70.85178	-559.41456	-34.19198	-556.30433	1
263	H	69.52959	71.63729	69.79488	-64.66664	395.18769	2695.05373	1
264	H	69.90456	70.61483	71.20576	-2703.44278	-60.40056	333.79418	1
265	C	68.94747	72.49325	71.69497	-519.76435	377.31045	459.42366	1
266	H	68.98174	73.54681	71.33516	-1746.74323	1667.50644	-1261.73691	1
267	C	67.52277	71.97015	71.55481	570.95554	16.46261	-545.27700	1
268	H	66.79851	72.57403	72.15992	2391.58273	28.05277	-1305.07271	1
269	H	67.17278	71.99966	70.49093	175.75588	917.63458	2559.43867	1
270	H	67.43806	70.90814	71.90183	-1063.97851	-2155.34650	1283.00462	1
271	C	69.35017	72.47855	73.16326	193.76014	2.62946	-765.53141	1
272	H	68.57649	72.96996	73.80820	507.39394	-846.55087	2539.60089	1
273	H	69.48789	71.43438	73.54643	1337.57841	1818.19054	1526.01994	1
274	H	70.31374	73.03140	73.32839	1100.88635	-1172.91350	-2199.08909	1
275	C	72.29872	71.26400	70.06816	-549.21115	475.64486	-309.38218	1
276	O	72.41778	71.26848	68.86350	556.06106	-390.37755	-78.24250	1
277	O	72.82171	70.19717	70.83317	-572.27940	-310.19032	-209.75862	1
278	H	72.56753	70.52648	71.74292	-1380.08193	2212.14486	790.85944	1

Listing 35: C00035.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.8187	0.0000	300.0000
3	H	72.58912	77.53305	86.68238	-2043.14101	-1757.64893	399.89339		1
4	N	73.04082	77.64417	85.77786	426.75047	490.45733	-334.42467		1
5	H	72.25209	77.87636	85.17693	442.25559	-1110.30854	-2448.52907		1

6	C	74.08827	78.59942	85.73578	415.32972	-666.39213	83.73172	1
7	H	74.47423	78.70371	86.77682	879.32219	2491.00447	667.35213	1
8	C	75.22677	78.03089	84.71661	31.35357	477.41777	628.23362	1
9	H	74.76157	77.83165	83.72336	1168.38489	2240.25337	-1019.71136	1
10	H	76.01081	78.80337	84.54068	-360.43770	2534.90498	931.67112	1
11	C	75.82504	76.77910	85.27840	463.18208	512.70242	-382.34388	1
12	H	74.99372	76.11075	85.60049	1725.29117	1863.52247	-987.07854	1
13	C	76.64842	76.05476	84.21797	710.42801	-144.27427	-313.15367	1
14	H	77.08858	75.10411	84.61455	364.20195	-1033.13725	2494.72524	1
15	H	76.02970	75.78657	83.32372	2567.61904	335.80679	847.48802	1
16	H	77.49927	76.68616	83.85469	-2587.99029	680.92867	-512.16411	1
17	C	76.71593	77.07312	86.47993	268.17616	741.64379	-40.42634	1
18	H	77.18093	76.13871	86.88689	1283.54314	-1945.37420	-1411.27812	1
19	H	77.55202	77.76884	86.21225	-1258.57796	1317.15249	-2026.02085	1
20	H	76.14364	77.54872	87.31650	-2502.84526	909.80597	575.92391	1
21	C	73.49025	79.92748	85.13115	619.36578	-458.64843	-172.09273	1
22	O	72.32934	80.06920	84.49629	-81.40433	433.87611	522.34594	1
23	N	74.33213	80.95395	85.15794	175.23996	-622.20190	341.55523	1
24	H	75.04286	80.61945	85.82668	-876.57256	-303.22879	-2561.90213	1
25	C	73.59920	82.23293	85.02769	-571.88214	-534.10783	-106.15033	1
26	H	73.28848	82.52218	86.05564	-2713.20841	-16.25800	-248.80809	1
27	C	74.64927	83.25333	84.37804	166.60354	288.16399	-716.09568	1
28	H	75.14426	82.72579	83.51579	-2097.85574	1636.78449	-586.18044	1
29	O	75.71791	83.66014	85.24869	-317.80580	-363.38227	484.43082	1
30	H	76.49595	83.30461	84.77248	1863.74748	-1451.84923	1357.29467	1
31	C	73.74740	84.40062	83.79296	503.80731	517.99032	318.51606	1
32	H	74.34503	85.10548	83.16811	640.61020	-2157.10410	-1536.29104	1
33	H	72.93447	83.99464	83.14137	1687.88455	465.60692	2087.56452	1
34	H	73.26555	84.99882	84.59992	-1293.07895	-1899.88581	-1463.57452	1
35	C	72.43434	81.76130	84.08635	-153.07550	-733.68902	248.70981	1
36	O	73.16324	81.81904	82.48953	186.15459	-480.78787	-449.34387	1
37	N	71.34939	82.37389	84.22943	-487.53139	543.18517	42.03850	1
38	C	70.19026	82.05432	83.40295	-699.35871	69.34393	360.10701	1
39	H	70.33565	80.99966	83.08624	2.81126	-221.99807	-2715.58072	1
40	C	68.99407	82.26237	84.40109	-507.46439	-592.59194	122.07761	1
41	H	68.03407	82.47864	83.87930	-1975.08116	525.87560	-1801.71556	1
42	H	68.82160	81.34498	85.00800	1588.27743	-1913.22100	1113.83566	1
43	C	69.47685	83.44293	85.31529	-613.62442	-457.55993	-194.14490	1
44	H	69.31679	84.43678	84.82261	1707.54637	-721.27992	1996.92523	1
45	H	68.93730	83.49357	86.28896	758.23357	2100.81767	1560.55011	1
46	C	71.00441	83.10359	85.48024	-352.41524	704.96076	49.21465	1
47	H	71.67567	83.98725	85.56034	1714.76886	-2070.42778	443.35792	1
48	H	71.22930	82.38722	86.30208	1224.15040	1801.50881	1636.97633	1
49	C	70.05078	83.06402	82.13721	566.85117	537.05831	117.62814	1
50	O	69.62749	82.65066	81.07756	-550.26779	-406.08867	4.21666	1
51	N	70.43350	84.35592	82.40473	566.34832	-425.77725	180.18749	1
52	H	70.60484	84.31628	83.41447	644.44502	2646.80550	-52.73430	1
53	C	69.52131	85.34193	81.84519	612.34801	-281.48662	411.56221	1
54	H	68.51371	84.87208	81.85804	1667.23498	-1490.75142	1556.16753	1
55	C	69.63390	86.62280	82.76836	-714.45746	-175.43074	286.98927	1
56	H	70.70987	86.94114	82.82972	-787.09484	1763.03619	-1922.46060	1
57	O	69.21729	86.42169	84.14845	-429.46514	516.51932	-128.40526	1
58	H	70.00945	86.72950	84.62445	1981.82785	436.16847	-1818.18182	1
59	C	68.82844	87.69100	81.94439	630.79189	-468.94448	76.03230	1
60	H	68.84963	88.69049	82.43804	-1775.71861	2062.30353	131.89849	1
61	H	69.24459	87.82198	80.91573	-1855.14608	88.94118	1993.53760	1
62	H	67.75835	87.39891	81.83069	-1504.82350	-780.94249	-2132.90992	1
63	C	70.02751	85.67452	80.34659	288.57638	618.62814	-397.00270	1
64	O	69.25854	86.03615	79.48743	321.70495	-185.26452	574.37218	1
65	N	71.39207	85.67538	80.29198	-447.05792	-446.53431	367.76425	1
66	H	71.76271	85.29440	81.16809	350.31316	1975.63644	-1843.31522	1
67	C	71.88589	85.02308	79.09412	-511.23061	374.03917	-471.51480	1

68	H	71.02022	84.45948	78.68231	2234.79579	-898.70890	-1273.45190	1
69	C	72.30315	86.23777	78.15712	529.53781	-159.34528	563.72604	1
70	H	72.69449	85.84122	77.18363	654.59388	2347.94251	1217.51488	1
71	H	71.34700	86.77876	77.91674	-1526.55661	2103.42026	817.87394	1
72	O	73.24969	87.20598	78.70272	-554.84278	14.12789	399.58769	1
73	H	72.78997	87.41389	79.53652	1297.06236	2061.84854	1220.68812	1
74	C	73.07500	84.06511	79.63311	-662.15484	-412.13544	123.62687	1
75	O	74.07797	84.46259	80.17323	-540.01537	-317.05804	274.91456	1
76	N	72.68927	82.79202	79.44847	-202.76299	-690.00100	-131.49145	1
77	H	71.81847	82.60534	78.94892	-702.62132	-2617.37191	281.70413	1
78	C	73.68871	81.74731	79.65139	-491.73914	576.34187	222.73509	1
79	H	74.43700	82.21057	80.34135	1977.17978	-1823.58850	-434.68928	1
80	C	72.99002	80.50583	80.21543	-649.50797	-328.66843	306.11224	1
81	H	72.29180	80.10916	79.43907	2075.07803	1452.16490	-1004.45904	1
82	C	74.03272	79.42885	80.51995	-615.18735	-489.99689	-70.96352	1
83	H	73.55203	78.47447	80.86355	-1226.32661	-1724.38906	-1716.47170	1
84	H	74.66179	79.17793	79.62354	2381.64273	-969.84735	900.46860	1
85	H	74.73638	79.75331	81.33154	2122.74991	1702.23946	-141.36228	1
86	C	72.23683	80.80555	81.39100	-501.86074	-479.61276	-376.42482	1
87	H	71.91943	79.89821	81.93389	993.79261	-2246.95401	-1177.81305	1
88	H	73.78260	81.07786	82.71467	42.71279	-626.15391	-2651.37258	1
89	H	71.33942	81.42473	81.18097	-2026.39012	-1590.33709	-887.82922	1
90	C	74.28157	81.41896	78.13340	-672.89153	382.57394	-156.34072	1
91	O	73.58204	81.39941	77.14699	410.04627	221.86223	500.35950	1
92	N	75.53774	81.02197	78.26144	-378.11782	-443.79414	-441.10984	1
93	H	75.94869	81.03809	79.19291	2404.15973	-568.14894	1149.30085	1
94	C	76.18973	80.43868	77.14037	-544.54484	466.16019	331.29119	1
95	H	75.54235	80.69413	76.26940	-1409.80988	-170.17955	2325.32679	1
96	C	77.63181	81.10324	77.16853	-184.48284	116.78282	-758.89137	1
97	H	77.53271	82.20616	77.28800	1893.78641	1861.14652	611.04528	1
98	H	78.19212	80.74882	78.06394	-2170.79665	-974.19311	1327.50117	1
99	C	78.42573	80.76597	75.87089	389.51668	672.81878	-138.49152	1
100	H	78.59252	79.66762	75.80054	510.64577	1933.03327	1851.02484	1
101	H	77.82119	81.01163	74.97026	-2302.30869	-1105.72939	-948.89774	1
102	C	79.80712	81.52355	75.80025	-559.93427	-126.34590	542.30857	1
103	O	80.50769	81.37765	74.83249	-670.36003	-111.83166	76.36448	1
104	N	80.07760	82.30031	76.87127	-216.06729	-537.07037	446.51379	1
105	H	79.53409	82.46023	77.72753	-1251.96487	1074.12894	-2168.52500	1
106	H	80.93751	82.85057	76.97524	-2451.83023	-720.73851	944.84612	1
107	C	76.35552	78.82886	77.40235	546.24052	-563.88337	-85.11809	1
108	O	77.38354	78.46358	77.90997	71.70702	-307.40463	606.69673	1
109	N	75.26262	78.10915	77.08182	479.90863	-504.50129	222.86849	1
110	C	75.32543	76.68641	77.17517	75.51268	-600.91904	506.73700	1
111	H	76.24910	76.49437	77.77002	-2033.61562	1795.30103	254.89480	1
112	C	73.95901	76.33801	77.90262	523.79067	517.99274	284.45581	1
113	H	73.60183	75.31172	77.66267	1599.61665	-1127.00911	1895.98173	1
114	H	74.09056	76.36817	79.00704	-1881.83093	1275.82488	-1501.55016	1
115	C	72.95271	77.44485	77.45116	-600.05639	-404.05026	316.64485	1
116	H	72.38428	77.16336	76.53514	-2597.05260	496.36221	657.73249	1
117	H	72.17786	77.66377	78.22030	-1666.24518	1294.38985	-1723.90591	1
118	C	73.92254	78.67600	77.20512	493.57570	-129.95376	-602.56394	1
119	H	73.70705	79.28272	76.29192	-1469.08415	-637.84797	2204.22581	1
120	H	73.98569	79.35602	78.08266	-1038.97840	1068.88701	-2280.71789	1
121	C	75.39926	75.94342	75.71090	188.88100	241.05089	-727.87821	1
122	O	76.40153	75.30050	75.41689	531.88613	-49.19943	427.07960	1
123	N	74.30199	76.11328	75.01552	708.14833	26.93417	-179.73509	1
124	H	73.63359	76.72384	75.48067	-2232.69501	-1179.09831	1023.94816	1
125	C	74.00287	75.51316	73.73222	-738.32412	259.92548	104.42456	1
126	H	73.02434	75.97586	73.46033	2028.89123	1260.02983	1311.33324	1
127	C	75.12863	75.87675	72.77048	-258.65678	-345.52513	661.28459	1
128	H	76.06645	75.41425	73.15665	-1826.06090	-1801.46097	-918.64554	1
129	C	74.85671	75.35453	71.37292	-541.23400	531.92970	-218.41428	1

130	H	75.64021	75.69643	70.63883	1311.73218	-2219.18200	882.19023	1
131	H	74.84327	74.23174	71.33608	-1048.71298	1223.58118	-2196.97971	1
132	H	73.86239	75.70908	70.98472	419.06414	1903.92898	1903.44670	1
133	C	75.36041	77.37631	72.72832	-423.86431	152.66566	-648.55262	1
134	H	76.23388	77.64582	72.07287	105.68386	-2342.50080	1387.51238	1
135	H	74.46202	77.92349	72.33069	-1695.63603	-1484.73621	-1531.02793	1
136	H	75.57147	77.78554	73.75532	-1853.57121	-487.39031	1936.59343	1
137	C	73.84729	73.85721	73.93634	539.71428	-510.58232	267.58633	1
138	O	72.77968	73.36444	73.69301	-15.93758	-278.34085	-624.49402	1
139	N	74.98397	73.28900	74.28966	-676.81886	12.05292	276.17960	1
140	H	75.80182	73.89712	74.52265	-1694.44250	-373.84189	-2100.66098	1
141	C	75.03591	71.89751	74.58501	412.33078	-664.70360	108.35451	1
142	H	76.07505	71.76086	74.96068	1765.77476	1294.44366	1621.76594	1
143	C	73.95348	71.61593	75.70727	-179.66635	-721.95667	-264.73915	1
144	H	74.03631	72.36639	76.52535	-607.34922	2587.87032	-598.10018	1
145	H	72.92490	71.73757	75.29221	-359.69332	-1479.13954	-2259.74260	1
146	C	74.19236	70.16783	76.24708	-240.01076	616.02425	431.85322	1
147	H	73.99876	69.42824	75.43609	-1359.17131	782.54425	2227.99181	1
148	H	75.25835	70.02643	76.53497	-820.36667	85.81767	-2596.78715	1
149	C	73.25205	69.89093	77.48818	-513.07015	236.18570	-551.87280	1
150	H	73.52937	70.53949	78.35074	1816.11944	-1183.11722	-1650.94321	1
151	H	72.19175	70.13742	77.25065	-1800.04429	-1361.53473	1526.34643	1
152	C	73.40218	68.39354	77.84649	726.08972	-253.19732	-179.64713	1
153	H	72.94210	67.69726	77.11806	1224.27271	-456.51798	-2390.90304	1
154	H	74.43939	68.07326	78.06984	1206.40339	-1150.93514	-2154.90344	1
155	N	72.61641	68.13287	79.17525	329.70796	-633.68968	-155.67358	1
156	H	72.60772	67.12614	79.50982	1348.31305	1938.76845	1359.00643	1
157	H	72.95647	68.63666	80.04541	2096.92035	1446.54551	-966.48890	1
158	H	71.58003	68.36208	79.17868	-1197.07217	-2303.53719	827.28733	1
159	C	74.73711	70.98291	73.26089	-378.01186	-556.17301	-413.96481	1
160	O	74.52191	69.77356	73.34928	-409.44433	-307.55053	-453.30833	1
161	N	74.89920	71.70504	72.17033	-429.02477	524.70884	274.08502	1
162	H	75.05147	72.68137	72.41070	1706.34263	-1425.96036	1574.38926	1
163	C	74.45289	71.26673	70.89399	-45.25864	-626.22952	478.93267	1
164	H	74.47729	70.15452	70.95545	1988.63164	570.90773	1772.87287	1
165	C	72.97426	71.81964	70.75093	551.77128	-20.49526	-564.54996	1
166	H	72.38795	71.61143	71.67498	1434.61535	-1753.10253	1513.99471	1
167	H	72.98020	72.92852	70.65384	-714.67738	1819.09770	1898.36494	1
168	C	72.31383	71.15712	69.49838	446.99263	-555.77305	338.97221	1
169	H	72.93781	71.34546	68.59034	1953.68466	1892.25957	-161.67766	1
170	H	72.26007	70.05100	69.61282	-403.03785	2688.07032	-188.43591	1
171	C	70.86818	71.77355	69.31480	567.86262	335.74681	434.04421	1
172	H	70.21645	71.52928	70.18504	-1080.02275	1568.26081	-1948.78900	1
173	H	70.91401	72.88611	69.27432	-919.54108	2111.34692	1456.13463	1
174	C	70.27985	71.20443	68.00309	195.81897	173.33862	-745.11536	1
175	H	70.83041	71.49714	67.08676	1405.67949	-2301.21089	-390.08113	1
176	H	70.11149	70.10905	68.00867	-940.37328	-1118.32446	2299.72133	1
177	N	68.85390	71.82603	67.81733	319.26422	656.36007	-42.02424	1
178	H	68.33524	71.53084	66.94032	1961.03633	619.91968	1787.09422	1
179	H	68.13232	71.61544	68.56675	854.14343	-2156.80752	1429.08711	1
180	H	68.79419	72.88346	67.74680	1237.02905	-1378.50857	-1998.28500	1
181	C	75.37533	71.91059	69.70722	532.53319	-268.57236	517.55729	1
182	O	75.05057	71.76086	68.55122	266.16714	-290.73804	-558.88002	1
183	N	76.39809	72.62965	70.18911	-226.25352	640.49678	-270.32839	1
184	H	76.51372	72.51489	71.19555	2007.69063	-1035.27229	1523.50231	1
185	C	77.56372	72.80608	69.37900	-540.76542	-573.33303	49.50000	1
186	H	77.20665	73.13312	68.37798	-2374.20950	-1036.76023	843.75774	1
187	C	78.44927	73.87613	70.15879	-77.09082	666.87422	-415.84136	1
188	H	78.69169	73.46453	71.17754	-985.81834	617.19825	2463.91927	1
189	O	77.83001	75.15773	70.41140	293.29899	-391.65602	-477.80926	1
190	H	77.84487	75.18335	71.38830	2528.72714	-681.76262	-751.27122	1
191	C	79.76137	73.92506	69.29437	252.47363	-605.14473	440.05134	1

192	H	80.51971	74.60617	69.74491	-2052.65063	1456.49051	-1043.51830	1
193	H	80.23251	72.91854	69.20430	-2152.98800	-1661.97574	-161.70652	1
194	H	79.55798	74.29311	68.26173	-473.12726	-1584.27339	2165.61725	1
195	C	78.32820	71.35951	69.34174	360.36307	488.46713	505.10056	1
196	O	78.25179	70.58278	70.27188	-200.08817	-528.03552	-385.82850	1
197	N	79.06229	71.30585	68.24807	-597.54095	-226.44775	355.20479	1
198	H	78.94651	72.06194	67.57579	2179.23655	-1300.70981	-991.33835	1
199	C	79.88977	70.19866	67.89046	-687.68921	297.39807	-249.45179	1
200	H	79.43279	69.84092	66.94275	-349.16256	-2467.37713	-1101.72831	1
201	C	81.36769	70.75368	67.67389	672.47345	361.54328	-201.62880	1
202	H	81.74885	71.18835	68.62630	1541.41502	582.18425	2169.97026	1
203	H	82.04025	69.90048	67.42334	-2534.67717	60.25153	997.72295	1
204	C	81.40483	71.80484	66.55222	574.26774	-389.43119	-377.02542	1
205	C	81.16875	71.41083	65.20141	688.82679	-287.33580	-257.96133	1
206	H	80.94802	70.35730	64.95099	331.14182	1470.38163	2269.80013	1
207	C	81.69814	73.16567	66.86608	-383.52382	-675.04808	144.24917	1
208	H	81.89539	73.47327	67.90852	4.09847	1517.59662	2262.86397	1
209	C	81.22991	72.38286	64.20248	-134.76730	428.45285	-649.50303	1
210	H	81.05375	72.07794	63.15617	-903.23433	1600.49020	2011.53387	1
211	C	81.74368	74.10353	65.83149	-335.53281	-615.00040	-364.39058	1
212	H	81.97102	75.15303	66.08784	1596.45398	-1369.33862	1732.02659	1
213	C	81.51485	73.75337	64.46903	585.48547	-340.24194	-406.23938	1
214	O	81.56168	74.69766	63.41023	-419.15649	-173.04408	-511.94141	1
215	H	81.79974	75.50780	63.91942	-1071.84350	1559.71507	-1960.13012	1
216	C	80.00606	69.06530	69.05710	291.41878	-183.13091	710.72246	1
217	O	80.86473	69.12214	69.90852	379.87695	523.47396	-222.23622	1
218	N	79.18059	68.05261	68.76688	564.30591	373.09380	277.24371	1
219	H	78.49791	68.18351	68.02000	-120.59931	-2436.07824	-1214.35098	1
220	C	78.96218	67.08653	69.80278	404.07514	-299.37480	608.84009	1
221	H	79.90738	67.16352	70.39091	-1071.07882	-841.69025	2359.66467	1
222	C	77.71143	67.62035	70.61438	-683.12807	68.71770	-390.13096	1
223	H	77.84223	68.72798	70.80057	2068.88918	1596.58590	770.89603	1
224	H	76.77591	67.53023	70.01646	1379.86429	2342.49779	-179.85638	1
225	C	77.60792	66.82020	71.94904	-176.39967	537.49466	550.97268	1
226	H	77.56589	65.72542	71.75286	-396.28051	1942.22168	1869.33314	1
227	H	78.51273	66.97515	72.57787	-94.44700	586.00678	-2659.20016	1
228	C	76.28921	67.31296	72.70421	-291.69381	-718.18079	-150.72929	1
229	H	76.30432	68.36763	73.08887	-2303.38776	1089.76242	964.62032	1
230	H	75.32953	67.17454	72.14341	884.16729	2568.80533	-207.74283	1
231	N	76.25936	66.44118	73.80288	-594.49522	-252.81478	342.29276	1
232	H	77.01494	65.77907	73.88532	-1735.17426	2084.05705	-263.71605	1
233	C	75.33546	66.41907	74.67860	595.23177	-271.52487	442.22352	1
234	N	74.30328	67.34782	74.54090	585.53813	-424.79750	-105.81303	1
235	H	74.25292	68.13637	73.85131	959.88797	1327.56823	-2177.11905	1
236	H	73.51268	67.41115	75.18957	1578.48647	16.27378	-2220.76233	1
237	N	75.55391	65.42144	75.64244	-452.17763	-390.33541	-421.51853	1
238	H	76.30248	64.73674	75.73376	470.26107	1974.25629	-1817.92087	1
239	H	74.91743	65.24208	76.41949	1856.67307	-1573.97321	-1224.35416	1
240	C	78.79495	65.65582	69.03959	-531.47271	-581.45780	-55.06206	1
241	O	79.73331	65.18338	68.44280	-243.00837	192.73507	609.52485	1
242	N	77.58730	65.11035	69.19843	343.49288	-644.25607	38.09164	1
243	H	76.89088	65.63206	69.72813	-1691.16043	-1535.97525	-1484.73099	1
244	C	77.21215	63.94751	68.38717	542.66492	350.14337	454.42563	1
245	H	77.86743	64.04534	67.48832	1209.57979	-2396.95920	463.86744	1
246	C	77.48454	62.69203	69.19652	-737.14309	145.93010	242.71942	1
247	H	76.99378	62.81950	70.18746	-1050.18303	159.36419	-2509.06125	1
248	C	76.88735	61.46891	68.52676	-706.77696	-252.88343	-245.16230	1
249	H	77.04498	60.53705	69.13739	-1624.64039	-1665.49085	1417.86935	1
250	H	75.77537	61.59574	68.37868	2566.10521	598.51109	693.22305	1
251	H	77.34207	61.28654	67.51339	-1972.69758	107.10018	-1876.34312	1
252	C	78.96949	62.49253	69.43482	412.85148	672.58832	-27.69222	1
253	H	79.17375	61.64115	70.14140	1447.02277	1762.76533	-1490.78944	1

254	H	79.51525	62.27218	68.47577	1320.77379	-145.20455	2378.68491	1
255	H	79.44179	63.42040	69.86837	-1512.10848	1470.52031	1724.75147	1
256	C	75.58829	64.12575	68.08896	-607.11113	499.56689	73.73769	1
257	O	74.76523	63.60333	68.80009	357.97126	460.81534	356.68785	1
258	N	75.40398	64.94638	67.06046	536.55407	-368.62270	332.76306	1
259	H	76.23509	65.27043	66.56639	524.38866	2297.69985	1367.20941	1
260	C	74.12851	64.95217	66.44268	46.50277	-774.29190	-147.97904	1
261	H	73.44556	64.47433	67.18182	1676.51875	1883.29066	1032.55549	1
262	C	73.73969	66.46962	66.05127	-559.41456	-34.19198	-556.30433	1
263	H	74.43220	66.83009	65.25360	-64.66664	395.18769	2695.05373	1
264	H	72.71701	66.50742	65.60569	-2703.44278	-60.40056	333.79418	1
265	C	73.83691	67.35508	67.26502	-519.76435	377.31045	459.42366	1
266	H	74.84016	67.20167	67.72396	-1746.74323	1667.50644	-1261.73691	1
267	C	73.70349	68.82124	66.87277	570.95554	16.46261	-545.27700	1
268	H	73.85989	69.50142	67.74963	2391.58273	28.05277	-1305.07271	1
269	H	74.45440	69.11228	66.09379	175.75588	917.63458	2559.43867	1
270	H	72.68859	69.04643	66.45442	-1063.97851	-2155.34650	1283.00462	1
271	C	72.77433	67.00449	68.29775	193.76014	2.62946	-765.53141	1
272	H	72.82325	67.68302	69.18820	507.39394	-846.55087	2539.60089	1
273	H	71.74103	67.08881	67.87226	1337.57841	1818.19054	1526.01994	1
274	H	72.89614	65.95548	68.67381	1100.88635	-1172.91350	-2199.08909	1
275	C	74.27181	64.13126	65.05731	-549.21115	475.64486	-309.38218	1
276	O	75.31483	63.98725	64.47574	556.06106	-390.37755	-78.24250	1
277	O	73.05756	63.69382	64.47822	-572.27940	-310.19032	-209.75862	1
278	H	72.43158	63.97481	65.20190	-1380.08193	2212.14486	790.85944	1

Listing 36: C00036.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.8737	3495
		0.2500	300.00	0.00	0.00	0.00	-1293.8160	0.0000	300.0000
3	H	74.95760	72.39181	92.82325	-2043.14101	-1757.64893	399.89339		1
4	N	75.71557	72.13772	93.45260	426.75047	490.45733	-334.42467		1
5	H	75.72624	71.12585	93.34543	442.25559	-1110.30854	-2448.52907		1
6	C	76.95423	72.76685	93.15826	415.32972	-666.39213	83.73172		1
7	H	76.61511	73.81502	92.99580	879.32219	2491.00447	667.35213		1
8	C	77.95357	72.63705	94.42693	31.35357	477.41777	628.23362		1
9	H	78.33618	71.59138	94.49355	1168.38489	2240.25337	-1019.71136		1
10	H	78.85176	73.28165	94.27952	-360.43770	2534.90498	931.67112		1
11	C	77.23211	73.00836	95.68940	463.18208	512.70242	-382.34388		1
12	H	76.32567	72.36600	95.77142	1725.29117	1863.52247	-987.07854		1
13	C	78.12077	72.76144	96.90373	710.42801	-144.27427	-313.15367		1
14	H	77.58699	72.99415	97.86066	364.20195	-1033.13725	2494.72524		1
15	H	78.45779	71.69490	96.96172	2567.61904	335.80679	847.48802		1
16	H	79.04146	73.39881	96.87579	-2587.99029	680.92867	-512.16411		1
17	C	76.79024	74.46665	95.68233	268.17616	741.64379	-40.42634		1
18	H	76.28284	74.74841	96.64056	1283.54314	-1945.37420	-1411.27812		1
19	H	77.65868	75.16149	95.54976	-1258.57796	1317.15249	-2026.02085		1
20	H	76.06663	74.67424	94.85306	-2502.84526	909.80597	575.92391		1
21	C	77.47577	72.10164	91.81527	619.36578	-458.64843	-172.09273		1
22	O	76.69949	71.75871	90.85235	-81.40433	433.87611	522.34594		1
23	N	78.77126	71.97010	91.76296	175.23996	-622.20190	341.55523		1
24	H	79.35666	72.31555	92.51935	-876.57256	-303.22879	-2561.90213		1
25	C	79.25519	71.76865	90.42552	-571.88214	-534.10783	-106.15033		1
26	H	79.44631	72.80048	90.06531	-2713.20841	-16.25800	-248.80809		1
27	C	80.57506	70.92166	90.50454	166.60354	288.16399	-716.09568		1
28	H	80.33515	69.91600	90.94650	-2097.85574	1636.78449	-586.18044		1
29	O	81.63503	71.47129	91.32933	-317.80580	-363.38227	484.43082		1
30	H	81.75781	70.76127	91.98445	1863.74748	-1451.84923	1357.29467		1
31	C	80.90886	70.76064	88.97193	503.80731	517.99032	318.51606		1
32	H	81.77329	70.07555	88.81194	640.61020	-2157.10410	-1536.29104		1
33	H	80.04582	70.34487	88.39778	1687.88455	465.60692	2087.56452		1

34	H	81.17403	71.73761	88.50594	-1293.07895	-1899.88581	-1463.57452	1
35	C	78.00295	70.97716	89.59757	-153.07550	-733.68902	248.70981	1
36	O	77.88965	69.74923	89.69655	186.15459	-480.78787	-449.34387	1
37	N	77.85843	71.65667	88.39792	-487.53139	543.18517	42.03850	1
38	C	77.00531	71.16800	87.39056	-699.35871	69.34393	360.10701	1
39	H	76.25537	70.49734	87.87253	2.81126	-221.99807	-2715.58072	1
40	C	76.45250	72.51226	86.71737	-507.46439	-592.59194	122.07761	1
41	H	76.07170	72.35376	85.68390	-1975.08116	525.87560	-1801.71556	1
42	H	75.61669	72.95204	87.30477	1588.27743	-1913.22100	1113.83566	1
43	C	77.72484	73.40161	86.77959	-613.62442	-457.55993	-194.14490	1
44	H	78.46409	73.09727	86.00239	1707.54637	-721.27992	1996.92523	1
45	H	77.52572	74.48616	86.63374	758.23357	2100.81767	1560.55011	1
46	C	78.24838	73.04032	88.24955	-352.41524	704.96076	49.21465	1
47	H	79.35476	73.11723	88.39481	1714.76886	-2070.42778	443.35792	1
48	H	77.73136	73.58692	89.07676	1224.15040	1801.50881	1636.97633	1
49	C	77.90912	70.40431	86.22834	566.85117	537.05831	117.62814	1
50	O	78.93082	70.86931	85.78828	-550.26779	-406.08867	4.21666	1
51	N	77.23352	69.33606	85.83852	566.34832	-425.77725	180.18749	1
52	H	76.35418	69.10438	86.29855	644.44502	2646.80550	-52.73430	1
53	C	77.74257	68.54916	84.77777	612.34801	-281.48662	411.56221	1
54	H	78.67361	69.05211	84.42428	1667.23498	-1490.75142	1556.16753	1
55	C	77.98045	67.08860	85.40887	-714.45746	-175.43074	286.98927	1
56	H	77.02992	66.77983	85.92404	-787.09484	1763.03619	-1922.46060	1
57	O	79.01464	67.00687	86.40313	-429.46514	516.51932	-128.40526	1
58	H	78.48919	66.83350	87.20998	1981.82785	436.16847	-1818.18182	1
59	C	78.19242	66.19079	84.13739	630.79189	-468.94448	76.03230	1
60	H	78.29748	65.11516	84.41034	-1775.71861	2062.30353	131.89849	1
61	H	77.33584	66.26967	83.42959	-1855.14608	88.94118	1993.53760	1
62	H	79.11260	66.48226	83.58008	-1504.82350	-780.94249	-2132.90992	1
63	C	76.53329	68.43241	83.68097	288.57638	618.62814	-397.00270	1
64	O	75.35783	68.26375	84.04640	321.70495	-185.26452	574.37218	1
65	N	77.03106	68.47015	82.47528	-447.05792	-446.53431	367.76425	1
66	H	78.04379	68.58547	82.50613	350.31316	1975.63644	-1843.31522	1
67	C	76.36417	68.20928	81.25235	-511.23061	374.03917	-471.51480	1
68	H	77.22151	68.00895	80.57048	2234.79579	-898.70890	-1273.45190	1
69	C	75.39928	66.93777	81.40547	529.53781	-159.34528	563.72604	1
70	H	75.18548	66.51822	80.38208	654.59388	2347.94251	1217.51488	1
71	H	75.99788	66.15905	81.94663	-1526.55661	2103.42026	817.87394	1
72	O	74.12628	67.15410	82.01921	-554.84278	14.12789	399.58769	1
73	H	74.44601	67.58028	82.90721	1297.06236	2061.84854	1220.68812	1
74	C	75.46381	69.43576	80.70313	-662.15484	-412.13544	123.62687	1
75	O	75.02971	69.37108	79.55921	-540.01537	-317.05804	274.91456	1
76	N	75.35421	70.49260	81.54470	-202.76299	-690.00100	-131.49145	1
77	H	75.74977	70.12487	82.41590	-702.62132	-2617.37191	281.70413	1
78	C	74.10030	71.29743	81.50244	-491.73914	576.34187	222.73509	1
79	H	73.34881	70.53127	81.20120	1977.17978	-1823.58850	-434.68928	1
80	C	73.86391	71.87328	82.87276	-649.50797	-328.66843	306.11224	1
81	H	74.80428	72.37295	83.19846	2075.07803	1452.16490	-1004.45904	1
82	C	72.75001	72.90820	82.88116	-615.18735	-489.99689	-70.96352	1
83	H	72.55914	73.30701	83.91472	-1226.32661	-1724.38906	-1716.47170	1
84	H	72.99890	73.79185	82.22464	2381.64273	-969.84735	900.46860	1
85	H	71.78141	72.47738	82.50711	2122.74991	1702.23946	-141.36228	1
86	C	73.52163	70.80574	83.89869	-501.86074	-479.61276	-376.42482	1
87	H	73.45856	71.23424	84.93649	993.79261	-2246.95401	-1177.81305	1
88	H	72.52668	70.33075	83.67799	42.71279	-626.15391	-2651.37258	1
89	H	74.28751	69.96656	83.92606	-2026.39012	-1590.33709	-887.82922	1
90	C	74.31028	72.43207	80.33858	-672.89153	382.57394	-156.34072	1
91	O	74.38616	73.60575	80.60660	410.04627	221.86223	500.35950	1
92	N	74.28566	71.88077	79.12679	-378.11782	-443.79414	-441.10984	1
93	H	74.31729	70.83546	79.01640	2404.15973	-568.14894	1149.30085	1
94	C	74.78319	72.71995	78.07037	-544.54484	466.16019	331.29119	1
95	H	74.33743	73.71384	78.30542	-1409.80988	-170.17955	2325.32679	1

96	C	76.36169	72.71655	78.20929	-184.48284	116.78282	-758.89137	1
97	H	76.66052	73.09383	79.21412	1893.78641	1861.14652	611.04528	1
98	H	76.75332	71.67563	78.14472	-2170.79665	-974.19311	1327.50117	1
99	C	76.95542	73.60631	77.07313	389.51668	672.81878	-138.49152	1
100	H	76.66014	73.19801	76.07828	510.64577	1933.03327	1851.02484	1
101	H	76.49561	74.61928	77.09719	-2302.30869	-1105.72939	-948.89774	1
102	C	78.52383	73.73977	77.14176	-559.93427	-126.34590	542.30857	1
103	O	79.10163	74.37952	76.30114	-670.36003	-111.83166	76.36448	1
104	N	79.08965	73.10368	78.19016	-216.06729	-537.07037	446.51379	1
105	H	78.65595	72.54688	78.93575	-1251.96487	1074.12894	-2168.52500	1
106	H	80.09801	73.10065	78.37951	-2451.83023	-720.73851	944.84612	1
107	C	74.31858	72.04653	76.66059	546.24052	-563.88337	-85.11809	1
108	O	75.14574	71.48827	75.98926	71.70702	-307.40463	606.69673	1
109	N	73.00745	72.21017	76.41630	479.90863	-504.50129	222.86849	1
110	C	72.34568	71.41793	75.42899	75.51268	-600.91904	506.73700	1
111	H	72.96383	70.50014	75.29213	-2033.61562	1795.30103	254.89480	1
112	C	70.92332	71.19705	76.10620	523.79067	517.99274	284.45581	1
113	H	70.13829	70.90615	75.37275	1599.61665	-1127.00911	1895.98173	1
114	H	70.95830	70.39337	76.87542	-1881.83093	1275.82488	-1501.55016	1
115	C	70.67612	72.59225	76.75814	-600.05639	-404.05026	316.64485	1
116	H	70.35683	73.33961	75.99871	-2597.05260	496.36221	657.73249	1
117	H	69.88822	72.58197	77.54418	-1666.24518	1294.38985	-1723.90591	1
118	C	72.12133	72.92603	77.32683	493.57570	-129.95376	-602.56394	1
119	H	72.40048	74.00555	77.30643	-1469.08415	-637.84797	2204.22581	1
120	H	72.33022	72.51261	78.34164	-1038.97840	1068.88701	-2280.71789	1
121	C	72.09611	72.21551	74.02162	188.88100	241.05089	-727.87821	1
122	O	71.43759	71.68868	73.15633	531.88613	-49.19943	427.07960	1
123	N	72.62391	73.44038	73.99915	708.14833	26.93417	-179.73509	1
124	H	73.17903	73.67768	74.82030	-2232.69501	-1179.09831	1023.94816	1
125	C	72.64210	74.21276	72.76226	-738.32412	259.92548	104.42456	1
126	H	72.27157	73.50575	71.97970	2028.89123	1260.02983	1311.33324	1
127	C	71.75593	75.43585	72.95389	-258.65678	-345.52513	661.28459	1
128	H	72.11007	75.96870	73.86414	-1826.06090	-1801.46097	-918.64554	1
129	C	71.85405	76.39025	71.77905	-541.23400	531.92970	-218.41428	1
130	H	71.23070	77.31394	71.93648	1311.73218	-2219.18200	882.19023	1
131	H	72.91448	76.72743	71.60657	-1048.71298	1223.58118	-2196.97971	1
132	H	71.50250	75.90940	70.82456	419.06414	1903.92898	1903.44670	1
133	C	70.30952	75.03956	73.18474	-423.86431	152.66566	-648.55262	1
134	H	69.65609	75.93330	73.38535	105.68386	-2342.50080	1387.51238	1
135	H	69.88170	74.50400	72.29229	-1695.63603	-1484.73621	-1531.02793	1
136	H	70.21131	74.34263	74.06227	-1853.57121	-487.39031	1936.59343	1
137	C	74.20235	74.74644	72.54958	539.71428	-510.58232	267.58633	1
138	O	74.87254	75.11097	73.48448	-15.93758	-278.34085	-624.49402	1
139	N	74.48207	74.80772	71.25555	-676.81886	12.05292	276.17960	1
140	H	73.77706	74.49322	70.59219	-1694.44250	-373.84189	-2100.66098	1
141	C	75.80335	75.15830	70.87576	412.33078	-664.70360	108.35451	1
142	H	76.34563	75.32065	71.83843	1765.77476	1294.44366	1621.76594	1
143	C	76.37031	73.97382	69.98300	-179.66635	-721.95667	-264.73915	1
144	H	76.19224	72.98745	70.46629	-607.34922	2587.87032	-598.10018	1
145	H	75.84109	73.93220	69.00498	-359.69332	-1479.13954	-2259.74260	1
146	C	77.89794	74.23986	69.78617	-240.01076	616.02425	431.85322	1
147	H	78.07594	75.27652	69.42026	-1359.17131	782.54425	2227.99181	1
148	H	78.44292	74.15906	70.75354	-820.36667	85.81767	-2596.78715	1
149	C	78.44161	73.18746	68.73859	-513.07015	236.18570	-551.87280	1
150	H	78.27566	72.14488	69.09506	1816.11944	-1183.11722	-1650.94321	1
151	H	77.89357	73.26800	67.77168	-1800.04429	-1361.53473	1526.34643	1
152	C	79.95021	73.47883	68.55628	726.08972	-253.19732	-179.64713	1
153	H	80.19716	74.53353	68.30407	1224.27271	-456.51798	-2390.90304	1
154	H	80.59064	73.13898	69.39439	1206.40339	-1150.93514	-2154.90344	1
155	N	80.43279	72.65968	67.31315	329.70796	-633.68968	-155.67358	1
156	H	81.46360	72.76642	67.08738	1348.31305	1938.76845	1359.00643	1
157	H	80.34238	71.60291	67.36590	2096.92035	1446.54551	-966.48890	1

158	H	79.99715	72.87231	66.36840	-1197.07217	-2303.53719	827.28733	1
159	C	75.79341	76.45166	69.85471	-378.01186	-556.17301	-413.96481	1
160	O	75.11871	76.53798	68.82630	-409.44433	-307.55053	-453.30833	1
161	N	76.76253	77.22660	70.26768	-429.02477	524.70884	274.08502	1
162	H	77.23852	76.90475	71.10834	1706.34263	-1425.96036	1574.38926	1
163	C	76.95649	78.56212	69.78966	-45.25864	-626.22952	478.93267	1
164	H	75.92594	78.96524	69.66523	1988.63164	570.90773	1772.87287	1
165	C	77.81613	79.28506	70.90322	551.77128	-20.49526	-564.54996	1
166	H	77.36466	79.13794	71.91013	1434.61535	-1753.10253	1513.99471	1
167	H	78.82417	78.81614	70.96060	-714.67738	1819.09770	1898.36494	1
168	C	77.94838	80.80874	70.57391	446.99263	-555.77305	338.97221	1
169	H	78.27518	80.94815	69.51053	1953.68466	1892.25957	-161.67766	1
170	H	76.97011	81.33125	70.67129	-403.03785	2688.07032	-188.43591	1
171	C	79.02187	81.40833	71.56948	567.86262	335.74681	434.04421	1
172	H	78.67233	81.33576	72.62505	-1080.02275	1568.26081	-1948.78900	1
173	H	79.96906	80.82302	71.52465	-919.54108	2111.34692	1456.13463	1
174	C	79.28067	82.87928	71.17030	195.81897	173.33862	-745.11536	1
175	H	79.71171	83.01183	70.15778	1405.67949	-2301.21089	-390.08113	1
176	H	78.41297	83.55542	71.30417	-940.37328	-1118.32446	2299.72133	1
177	N	80.37827	83.44213	72.13612	319.26422	656.36007	-42.02424	1
178	H	80.67062	84.44663	71.96133	1961.03633	619.91968	1787.09422	1
179	H	80.14626	83.46947	73.17146	854.14343	-2156.80752	1429.08711	1
180	H	81.31847	82.94952	72.13461	1237.02905	-1378.50857	-1998.28500	1
181	C	77.75135	78.54370	68.37335	532.53319	-268.57236	517.55729	1
182	O	78.36784	79.51916	68.00464	266.16714	-290.73804	-558.88002	1
183	N	77.61695	77.37369	67.74066	-226.25352	640.49678	-270.32839	1
184	H	76.99207	76.67501	68.15995	2007.69063	-1035.27229	1523.50231	1
185	C	77.85482	77.40561	66.32659	-540.76542	-573.33303	49.50000	1
186	H	78.66500	78.16146	66.19408	-2374.20950	-1036.76023	843.75774	1
187	C	78.29231	75.92805	65.88656	-77.09082	666.87422	-415.84136	1
188	H	77.56262	75.18798	66.31311	-985.81834	617.19825	2463.91927	1
189	O	79.59769	75.53707	66.34656	293.29899	-391.65602	-477.80926	1
190	H	79.39248	74.72267	66.84627	2528.72714	-681.76262	-751.27122	1
191	C	78.12360	75.96393	64.32608	252.47363	-605.14473	440.05134	1
192	H	78.45042	75.00601	63.85777	-2052.65063	1456.49051	-1043.51830	1
193	H	77.05988	76.12452	64.02516	-2152.98800	-1661.97574	-161.70652	1
194	H	78.72744	76.78248	63.86913	-473.12726	-1584.27339	2165.61725	1
195	C	76.49186	77.87899	65.58121	360.36307	488.46713	505.10056	1
196	O	76.61392	78.31702	64.45722	-200.08817	-528.03552	-385.82850	1
197	N	75.37004	77.67826	66.26842	-597.54095	-226.44775	355.20479	1
198	H	75.33569	77.28919	67.24146	2179.23655	-1300.70981	-991.33835	1
199	C	74.17805	77.83323	65.49344	-687.68921	297.39807	-249.45179	1
200	H	74.57354	78.23382	64.52324	-349.16256	-2467.37713	-1101.72831	1
201	C	73.49736	76.38915	65.32779	672.47345	361.54328	-201.62880	1
202	H	73.31622	75.92375	66.32384	1541.41502	582.18425	2169.97026	1
203	H	72.51127	76.49082	64.81700	-2534.67717	60.25153	997.72295	1
204	C	74.42552	75.51079	64.47851	574.26774	-389.43119	-377.02542	1
205	C	74.47605	75.72696	63.06816	688.82679	-287.33580	-257.96133	1
206	H	73.85412	76.50715	62.59333	331.14182	1470.38163	2269.80013	1
207	C	75.23774	74.50859	65.08997	-383.52382	-675.04808	144.24917	1
208	H	75.20835	74.35046	66.18324	4.09847	1517.59662	2262.86397	1
209	C	75.33209	74.93619	62.30357	-134.76730	428.45285	-649.50303	1
210	H	75.37384	75.10421	61.21311	-903.23433	1600.49020	2011.53387	1
211	C	76.07361	73.73706	64.27883	-335.53281	-615.00040	-364.39058	1
212	H	76.69843	72.96400	64.75879	1596.45398	-1369.33862	1732.02659	1
213	C	76.15523	73.91820	62.86708	585.48547	-340.24194	-406.23938	1
214	O	77.01353	73.15066	62.03718	-419.15649	-173.04408	-511.94141	1
215	H	77.38707	72.53388	62.70989	-1071.84350	1559.71507	-1960.13012	1
216	C	73.21528	78.90396	66.24279	291.41878	-183.13091	710.72246	1
217	O	73.62978	80.03706	66.47925	379.87695	523.47396	-222.23622	1
218	N	72.01488	78.40596	66.43050	564.30591	373.09380	277.24371	1
219	H	71.86492	77.43981	66.13985	-120.59931	-2436.07824	-1214.35098	1

220	C	71.06155	79.00438	67.30870	404.07514	-299.37480	608.84009	1
221	H	70.33752	78.18128	67.50511	-1071.07882	-841.69025	2359.66467	1
222	C	71.86527	79.45677	68.60460	-683.12807	68.71770	-390.13096	1
223	H	72.53658	78.63694	68.94742	2068.88918	1596.58590	770.89603	1
224	H	72.54075	80.31334	68.37007	1379.86429	2342.49779	-179.85638	1
225	C	70.84831	79.84895	69.71683	-176.39967	537.49466	550.97268	1
226	H	70.19885	80.69130	69.38814	-396.28051	1942.22168	1869.33314	1
227	H	70.15862	79.00771	69.95121	-94.44700	586.00678	-2659.20016	1
228	C	71.73073	80.24980	70.98852	-291.69381	-718.18079	-150.72929	1
229	H	72.34765	79.42634	71.43047	-2303.38776	1089.76242	964.62032	1
230	H	72.39813	81.13852	70.85133	884.16729	2568.80533	-207.74283	1
231	N	70.74071	80.59690	71.91918	-594.49522	-252.81478	342.29276	1
232	H	69.78460	80.54319	71.60325	-1735.17426	2084.05705	-263.71605	1
233	C	70.96768	80.97456	73.11192	595.23177	-271.52487	442.22352	1
234	N	72.30061	81.04491	73.53013	585.53813	-424.79750	-105.81303	1
235	H	73.15273	80.82965	73.01386	959.88797	1327.56823	-2177.11905	1
236	H	72.60652	81.33160	74.46057	1578.48647	16.27378	-2220.76233	1
237	N	69.76799	81.25290	73.78154	-452.17763	-390.33541	-421.51853	1
238	H	68.80044	81.21020	73.46493	470.26107	1974.25629	-1817.92087	1
239	H	69.73026	81.58248	74.74674	1856.67307	-1573.97321	-1224.35416	1
240	C	70.34211	80.26274	66.57440	-531.47271	-581.45780	-55.06206	1
241	O	69.13326	80.26510	66.46292	-243.00837	192.73507	609.52485	1
242	N	71.19927	81.20819	66.22129	343.49288	-644.25607	38.09164	1
243	H	72.22974	81.04746	66.34757	-1691.16043	-1535.97525	-1484.73099	1
244	C	70.68672	82.41118	65.54832	542.66492	350.14337	454.42563	1
245	H	69.75357	82.60652	66.12841	1209.57979	-2396.95920	463.86744	1
246	C	71.72741	83.51257	65.61301	-737.14309	145.93010	242.71942	1
247	H	72.65109	83.13667	65.11706	-1050.18303	159.36419	-2509.06125	1
248	C	71.26686	84.75242	64.86772	-706.77696	-252.88343	-245.16230	1
249	H	72.04355	85.56585	64.89017	-1624.64039	-1665.49085	1417.86935	1
250	H	71.05275	84.52384	63.78514	2566.10521	598.51109	693.22305	1
251	H	70.32454	85.17777	65.31131	-1972.69758	107.10018	-1876.34312	1
252	C	72.08595	83.87460	67.04268	412.85148	672.58832	-27.69222	1
253	H	72.88550	84.66479	67.08374	1447.02277	1762.76533	-1490.78944	1
254	H	71.19525	84.27228	67.60296	1320.77379	-145.20455	2378.68491	1
255	H	72.46511	82.98201	67.61264	-1512.10848	1470.52031	1724.75147	1
256	C	70.34380	81.98989	63.98191	-607.11113	499.56689	73.73769	1
257	O	71.04679	82.35192	63.07190	357.97126	460.81534	356.68785	1
258	N	69.23817	81.26653	63.93841	536.55407	-368.62270	332.76306	1
259	H	68.76450	80.95801	64.81165	524.38866	2297.69985	1367.20941	1
260	C	68.78046	80.88181	62.64767	46.50277	-774.29190	-147.97904	1
261	H	69.16504	81.67469	61.96635	1676.51875	1883.29066	1032.55549	1
262	C	69.40895	79.43620	62.27985	-559.41456	-34.19198	-556.30433	1
263	H	69.21214	78.72616	63.11754	-64.66664	395.18769	2695.05373	1
264	H	68.90148	79.00510	61.38447	-2703.44278	-60.40056	333.79418	1
265	C	70.88496	79.57135	62.03502	-519.76435	377.31045	459.42366	1
266	H	71.34273	80.09143	62.91092	-1746.74323	1667.50644	-1261.73691	1
267	C	71.52770	78.19782	61.88397	570.95554	16.46261	-545.27700	1
268	H	72.63098	78.27655	61.70583	2391.58273	28.05277	-1305.07271	1
269	H	71.38209	77.56854	62.79931	175.75588	917.63458	2559.43867	1
270	H	71.09238	77.63303	61.01953	-1063.97851	-2155.34650	1283.00462	1
271	C	71.17130	80.40522	60.79289	193.76014	2.62946	-765.53141	1
272	H	72.25549	80.36925	60.51215	507.39394	-846.55087	2539.60089	1
273	H	70.58505	80.05026	59.90606	1337.57841	1818.19054	1526.01994	1
274	H	70.91448	81.48523	60.96056	1100.88635	-1172.91350	-2199.08909	1
275	C	67.17852	80.75210	62.69294	-549.21115	475.64486	-309.38218	1
276	O	66.52181	80.90927	63.68848	556.06106	-390.37755	-78.24250	1
277	O	66.55295	80.42032	61.46422	-572.27940	-310.19032	-209.75862	1
278	H	67.35966	80.40298	60.88147	-1380.08193	2212.14486	790.85944	1

Listing 37: C00037.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	1.8545	7418
		0.2500	300.00	0.00	0.00	0.00	-1293.8088	0.0000	300.0000
3	H	69.44136	77.30548	71.89115	-2043.14101	-1757.64893	399.89339		1
4	N	69.29526	78.30699	71.75896	426.75047	490.45733	-334.42467		1
5	H	68.83847	78.55911	72.63808	442.25559	-1110.30854	-2448.52907		1
6	C	70.50450	79.02763	71.57384	415.32972	-666.39213	83.73172		1
7	H	71.31273	78.32704	71.87470	879.32219	2491.00447	667.35213		1
8	C	70.63020	79.46530	70.02785	31.35357	477.41777	628.23362		1
9	H	69.77767	80.13400	69.76085	1168.38489	2240.25337	-1019.71136		1
10	H	71.55907	80.06157	69.86180	-360.43770	2534.90498	931.67112		1
11	C	70.62396	78.23140	69.16351	463.18208	512.70242	-382.34388		1
12	H	69.78803	77.57673	69.49936	1725.29117	1863.52247	-987.07854		1
13	C	70.38555	78.60479	67.70572	710.42801	-144.27427	-313.15367		1
14	H	70.35091	77.69919	67.04679	364.20195	-1033.13725	2494.72524		1
15	H	69.41568	79.14990	67.57155	2567.61904	335.80679	847.48802		1
16	H	71.19677	79.27008	67.31246	-2587.99029	680.92867	-512.16411		1
17	C	71.93088	77.46030	69.28797	268.17616	741.64379	-40.42634		1
18	H	71.92214	76.52892	68.66484	1283.54314	-1945.37420	-1411.27812		1
19	H	72.80585	78.07501	68.95338	-1258.57796	1317.15249	-2026.02085		1
20	H	72.13477	77.14873	70.34526	-2502.84526	909.80597	575.92391		1
21	C	70.35967	80.33389	72.55998	619.36578	-458.64843	-172.09273		1
22	O	69.95450	80.12056	73.87222	-81.40433	433.87611	522.34594		1
23	N	71.66909	80.99314	72.43702	175.23996	-622.20190	341.55523		1
24	H	71.84368	81.37762	71.50605	-876.57256	-303.22879	-2561.90213		1
25	C	71.81801	81.96868	73.48467	-571.88214	-534.10783	-106.15033		1
26	H	71.70029	81.38287	74.42468	-2713.20841	-16.25800	-248.80809		1
27	C	73.27172	82.60073	73.31152	166.60354	288.16399	-716.09568		1
28	H	73.27558	83.24523	72.39026	-2097.85574	1636.78449	-586.18044		1
29	O	74.35295	81.66248	73.15294	-317.80580	-363.38227	484.43082		1
30	H	74.69254	81.90931	72.26978	1863.74748	-1451.84923	1357.29467		1
31	C	73.33337	83.51807	74.58850	503.80731	517.99032	318.51606		1
32	H	74.26302	84.13301	74.60190	640.61020	-2157.10410	-1536.29104		1
33	H	72.46825	84.22295	74.63292	1687.88455	465.60692	2087.56452		1
34	H	73.32314	82.91228	75.52478	-1293.07895	-1899.88581	-1463.57452		1
35	C	70.67457	83.10310	73.29023	-153.07550	-733.68902	248.70981		1
36	O	71.01396	84.17720	72.86976	186.15459	-480.78787	-449.34387		1
37	N	69.40352	82.68141	73.59615	-487.53139	543.18517	42.03850		1
38	C	68.24024	83.37059	73.06318	-699.35871	69.34393	360.10701		1
39	H	68.52410	83.78762	72.07117	2.81126	-221.99807	-2715.58072		1
40	C	67.18672	82.19848	73.05083	-507.46439	-592.59194	122.07761		1
41	H	66.13551	82.55530	72.96862	-1975.08116	525.87560	-1801.71556		1
42	H	67.35832	81.48653	72.21297	1588.27743	-1913.22100	1113.83566		1
43	C	67.53252	81.55697	74.44125	-613.62442	-457.55993	-194.14490		1
44	H	67.16484	82.18628	75.28879	1707.54637	-721.27992	1996.92523		1
45	H	67.09608	80.54065	74.58133	758.23357	2100.81767	1560.55011		1
46	C	69.09762	81.55818	74.36121	-352.41524	704.96076	49.21465		1
47	H	69.69690	81.53852	75.30624	1714.76886	-2070.42778	443.35792		1
48	H	69.69829	81.10678	72.07371	1224.15040	1801.50881	1636.97633		1
49	C	67.64535	84.48556	74.09345	566.85117	537.05831	117.62814		1
50	O	66.51425	84.93961	73.88520	-550.26779	-406.08867	4.21666		1
51	N	68.49465	84.81136	75.04339	566.34832	-425.77725	180.18749		1
52	H	69.36962	84.30751	74.89808	644.44502	2646.80550	-52.73430		1
53	C	68.11028	85.15707	76.38280	612.34801	-281.48662	411.56221		1
54	H	68.80758	85.98423	76.63545	1667.23498	-1490.75142	1556.16753		1
55	C	66.57964	85.55657	76.48041	-714.45746	-175.43074	286.98927		1
56	H	65.98190	84.68411	76.08671	-787.09484	1763.03619	-1922.46060		1
57	O	66.19172	86.68106	75.69049	-429.46514	516.51932	-128.40526		1
58	H	66.03475	86.19457	74.79015	1981.82785	436.16847	-1818.18182		1
59	C	66.35996	85.68246	78.03370	630.79189	-468.94448	76.03230		1
60	H	65.29023	85.88056	78.27836	-1775.71861	2062.30353	131.89849		1

61	H	66.65891	84.74969	78.57387	-1855.14608	88.94118	1993.53760	1
62	H	66.95511	86.52071	78.46469	-1504.82350	-780.94249	-2132.90992	1
63	C	68.43112	83.81012	77.25531	288.57638	618.62814	-397.00270	1
64	O	67.55680	82.98110	77.43429	321.70495	-185.26452	574.37218	1
65	N	69.72639	83.76438	77.53463	-447.05792	-446.53431	367.76425	1
66	H	70.24185	84.56217	77.15508	350.31316	1975.63644	-1843.31522	1
67	C	70.26915	83.17485	78.71129	-511.23061	374.03917	-471.51480	1
68	H	71.35301	83.33323	78.51221	2234.79579	-898.70890	-1273.45190	1
69	C	69.84629	84.01751	80.01346	529.53781	-159.34528	563.72604	1
70	H	70.47949	83.62448	80.85424	654.59388	2347.94251	1217.51488	1
71	H	70.15450	85.08451	79.83865	-1526.55661	2103.42026	817.87394	1
72	O	68.44652	84.01833	80.38322	-554.84278	14.12789	399.58769	1
73	H	68.39640	83.15020	80.83213	1297.06236	2061.84854	1220.68812	1
74	C	69.92212	81.60990	78.90713	-662.15484	-412.13544	123.62687	1
75	O	70.05228	81.08601	79.98720	-540.01537	-317.05804	274.91456	1
76	N	69.75524	80.94694	77.70316	-202.76299	-690.00100	-131.49145	1
77	H	69.37268	81.69707	77.11824	-702.62132	-2617.37191	281.70413	1
78	C	69.26282	79.55601	77.77210	-491.73914	576.34187	222.73509	1
79	H	68.96143	79.43448	78.84068	1977.17978	-1823.58850	-434.68928	1
80	C	68.14124	79.38520	76.77256	-649.50797	-328.66843	306.11224	1
81	H	68.46046	79.87186	75.82455	2075.07803	1452.16490	-1004.45904	1
82	C	67.86769	77.92486	76.45599	-615.18735	-489.99689	-70.96352	1
83	H	67.03766	77.81130	75.70574	-1226.32661	-1724.38906	-1716.47170	1
84	H	68.77792	77.42204	76.02620	2381.64273	-969.84735	900.46860	1
85	H	67.57190	77.34975	77.37554	2122.74991	1702.23946	-141.36228	1
86	C	66.86710	80.05260	77.25083	-501.86074	-479.61276	-376.42482	1
87	H	66.03297	79.94855	76.50414	993.79261	-2246.95401	-1177.81305	1
88	H	66.50384	79.60934	78.21822	42.71279	-626.15391	-2651.37258	1
89	H	67.03404	81.17928	77.42728	-2026.39012	-1590.33709	-887.82922	1
90	C	70.53239	78.58274	77.36918	-672.89153	382.57394	-156.34072	1
91	O	70.76718	77.61340	78.05929	410.04627	221.86223	500.35950	1
92	N	71.10284	78.92841	76.23204	-378.11782	-443.79414	-441.10984	1
93	H	70.76979	79.74415	75.71097	2404.15973	-568.14894	1149.30085	1
94	C	72.28548	78.20591	75.86483	-544.54484	466.16019	331.29119	1
95	H	72.02917	77.15168	76.11036	-1409.80988	-170.17955	2325.32679	1
96	C	72.57170	78.51068	74.33912	-184.48284	116.78282	-758.89137	1
97	H	71.62218	78.56431	73.75707	1893.78641	1861.14652	611.04528	1
98	H	73.06036	79.50610	74.21823	-2170.79665	-974.19311	1327.50117	1
99	C	73.49993	77.35183	73.85597	389.51668	672.81878	-138.49152	1
100	H	74.33947	77.22305	74.57325	510.64577	1933.03327	1851.02484	1
101	H	72.95690	76.38241	73.90311	-2302.30869	-1105.72939	-948.89774	1
102	C	74.08935	77.55193	72.41018	-559.93427	-126.34590	542.30857	1
103	O	74.77298	76.68541	71.92826	-670.36003	-111.83166	76.36448	1
104	N	73.77764	78.73584	71.84014	-216.06729	-537.07037	446.51379	1
105	H	73.26179	79.53543	72.22923	-1251.96487	1074.12894	-2168.52500	1
106	H	74.13647	79.04516	70.93155	-2451.83023	-720.73851	944.84612	1
107	C	73.55916	78.78306	76.71975	546.24052	-563.88337	-85.11809	1
108	O	73.88914	79.93490	76.61851	71.70702	-307.40463	606.69673	1
109	N	74.15124	77.78363	77.39469	479.90863	-504.50129	222.86849	1
110	C	75.27333	78.04067	78.24053	75.51268	-600.91904	506.73700	1
111	H	75.15916	79.08935	78.59915	-2033.61562	1795.30103	254.89480	1
112	C	75.12741	76.91850	79.35227	523.79067	517.99274	284.45581	1
113	H	76.09330	76.67821	79.85072	1599.61665	-1127.00911	1895.98173	1
114	H	74.42524	77.23619	80.15533	-1881.83093	1275.82488	-1501.55016	1
115	C	74.53893	75.72313	78.53826	-600.05639	-404.05026	316.64485	1
116	H	75.33333	75.20102	77.95939	-2597.05260	496.36221	657.73249	1
117	H	74.04757	74.95041	79.17149	-1666.24518	1294.38985	-1723.90591	1
118	C	73.52517	76.47988	77.57967	493.57570	-129.95376	-602.56394	1
119	H	73.38542	76.00717	76.57859	-1469.08415	-637.84797	2204.22581	1
120	H	72.51117	76.71423	78.02969	-1038.97840	1068.88701	-2280.71789	1
121	C	76.68980	77.83310	77.43391	188.88100	241.05089	-727.87821	1
122	O	77.69718	78.29914	77.91106	531.88613	-49.19943	427.07960	1

123	N	76.56391	77.03286	76.37048	708.14833	26.93417	-179.73509	1
124	H	75.59202	76.78431	76.18878	-2232.69501	-1179.09831	1023.94816	1
125	C	77.50685	77.12428	75.30073	-738.32412	259.92548	104.42456	1
126	H	77.01249	76.56874	74.47312	2028.89123	1260.02983	1311.33324	1
127	C	77.69546	78.66107	74.94685	-258.65678	-345.52513	661.28459	1
128	H	78.04496	79.21708	75.84715	-1826.06090	-1801.46097	-918.64554	1
129	C	78.70491	78.81417	73.75886	-541.23400	531.92970	-218.41428	1
130	H	78.81961	79.87994	73.44928	1311.73218	-2219.18200	882.19023	1
131	H	79.72298	78.43363	74.03670	-1048.71298	1223.58118	-2196.97971	1
132	H	78.37118	78.24058	72.86188	419.06414	1903.92898	1903.44670	1
133	C	76.32636	79.23326	74.43935	-423.86431	152.66566	-648.55262	1
134	H	76.40589	80.30475	74.13762	105.68386	-2342.50080	1387.51238	1
135	H	75.95013	78.67093	73.55179	-1695.63603	-1484.73621	-1531.02793	1
136	H	75.53869	79.17523	75.23013	-1853.57121	-487.39031	1936.59343	1
137	C	78.89703	76.41802	75.76794	539.71428	-510.58232	267.58633	1
138	O	79.94782	76.70259	75.23700	-15.93758	-278.34085	-624.49402	1
139	N	78.65938	75.39381	76.60347	-676.81886	12.05292	276.17960	1
140	H	77.70290	75.38592	76.95471	-1694.44250	-373.84189	-2100.66098	1
141	C	79.76877	74.92914	77.39691	412.33078	-664.70360	108.35451	1
142	H	80.39706	75.83674	77.53921	1765.77476	1294.44366	1621.76594	1
143	C	79.17873	74.34806	78.73748	-179.66635	-721.95667	-264.73915	1
144	H	78.47247	75.06788	79.20978	-607.34922	2587.87032	-598.10018	1
145	H	78.57844	73.43507	78.52439	-359.69332	-1479.13954	-2259.74260	1
146	C	80.36454	74.01239	79.70586	-240.01076	616.02425	431.85322	1
147	H	81.17533	73.47262	79.14542	-1359.17131	782.54425	2227.99181	1
148	H	80.83316	74.94200	80.10065	-820.36667	85.81767	-2596.78715	1
149	C	79.83066	73.10263	80.88296	-513.07015	236.18570	-551.87280	1
150	H	79.13196	73.66817	81.54128	1816.11944	-1183.11722	-1650.94321	1
151	H	79.24514	72.24222	80.48495	-1800.04429	-1361.53473	1526.34643	1
152	C	81.06107	72.59713	81.67277	726.08972	-253.19732	-179.64713	1
153	H	81.74795	71.95034	81.09067	1224.27271	-456.51798	-2390.90304	1
154	H	81.63677	73.39112	82.18883	1206.40339	-1150.93514	-2154.90344	1
155	N	80.54702	71.66825	82.82364	329.70796	-633.68968	-155.67358	1
156	H	81.30165	71.26216	83.44871	1348.31305	1938.76845	1359.00643	1
157	H	79.89079	72.09611	83.54004	2096.92035	1446.54551	-966.48890	1
158	H	80.02449	70.78967	82.53715	-1197.07217	-2303.53719	827.28733	1
159	C	80.58144	73.76186	76.61094	-378.01186	-556.17301	-413.96481	1
160	O	81.46753	73.14826	77.18139	-409.44433	-307.55053	-453.30833	1
161	N	80.06801	73.48280	75.38819	-429.02477	524.70884	274.08502	1
162	H	79.40282	74.24484	75.22848	1706.34263	-1425.96036	1574.38926	1
163	C	80.98645	73.12850	74.31900	-45.25864	-626.22952	478.93267	1
164	H	81.34007	74.11781	73.95591	1988.63164	570.90773	1772.87287	1
165	C	82.13737	72.23082	74.89634	551.77128	-20.49526	-564.54996	1
166	H	82.83738	72.85285	75.50568	1434.61535	-1753.10253	1513.99471	1
167	H	81.69613	71.50130	75.61584	-714.67738	1819.09770	1898.36494	1
168	C	82.96166	71.48861	73.78645	446.99263	-555.77305	338.97221	1
169	H	82.28837	70.89583	73.11482	1953.68466	1892.25957	-161.67766	1
170	H	83.50166	72.20939	73.13194	-403.03785	2688.07032	-188.43591	1
171	C	83.96665	70.53523	74.54750	567.86262	335.74681	434.04421	1
172	H	84.65983	71.12363	75.19169	-1080.02275	1568.26081	-1948.78900	1
173	H	83.41537	69.85663	75.23860	-919.54108	2111.34692	1456.13463	1
174	C	84.75403	69.71279	73.50108	195.81897	173.33862	-745.11536	1
175	H	84.13192	69.03451	72.88350	1405.67949	-2301.21089	-390.08113	1
176	H	85.42467	70.30971	72.85135	-940.37328	-1118.32446	2299.72133	1
177	N	85.71021	68.75640	74.29140	319.26422	656.36007	-42.02424	1
178	H	86.32270	68.12533	73.69842	1961.03633	619.91968	1787.09422	1
179	H	86.42976	69.20825	74.92769	854.14343	-2156.80752	1429.08711	1
180	H	85.25355	68.05174	74.94075	1237.02905	-1378.50857	-1998.28500	1
181	C	80.05332	72.38367	73.22650	532.53319	-268.57236	517.55729	1
182	O	80.27424	71.22431	72.89013	266.16714	-290.73804	-558.88002	1
183	N	79.08605	73.18705	72.81391	-226.25352	640.49678	-270.32839	1
184	H	79.08621	74.13217	73.19559	2007.69063	-1035.27229	1523.50231	1

185	C	78.23591	72.83770	71.73327	-540.76542	-573.33303	49.50000	1
186	H	77.62388	73.75577	71.58715	-2374.20950	-1036.76023	843.75774	1
187	C	79.15683	72.50099	70.47251	-77.09082	666.87422	-415.84136	1
188	H	79.72593	71.55665	70.70012	-985.81834	617.19825	2463.91927	1
189	O	80.13955	73.49993	70.13523	293.29899	-391.65602	-477.80926	1
190	H	80.96836	73.01245	70.31105	2528.72714	-681.76262	-751.27122	1
191	C	78.09104	72.21991	69.35114	252.47363	-605.14473	440.05134	1
192	H	78.57792	71.91878	68.39452	-2052.65063	1456.49051	-1043.51830	1
193	H	77.38821	71.39556	69.64294	-2152.98800	-1661.97574	-161.70652	1
194	H	77.47714	73.12570	69.13673	-473.12726	-1584.27339	2165.61725	1
195	C	77.34970	71.54361	72.22130	360.36307	488.46713	505.10056	1
196	O	77.19565	70.55920	71.52743	-200.08817	-528.03552	-385.82850	1
197	N	76.81849	71.83293	73.39948	-597.54095	-226.44775	355.20479	1
198	H	77.08665	72.74644	73.76750	2179.23655	-1300.70981	-991.33835	1
199	C	76.14006	70.89451	74.21285	-687.68921	297.39807	-249.45179	1
200	H	75.61213	71.51736	74.96727	-349.16256	-2467.37713	-1101.72831	1
201	C	75.15468	69.97965	73.34192	672.47345	361.54328	-201.62880	1
202	H	75.73499	69.44640	72.54535	1541.41502	582.18425	2169.97026	1
203	H	74.69730	69.20138	73.99576	-2534.67717	60.25153	997.72295	1
204	C	74.07048	70.86521	72.71200	574.26774	-389.43119	-377.02542	1
205	C	72.94266	71.28039	73.48149	688.82679	-287.33580	-257.96133	1
206	H	72.82653	70.95769	74.53201	331.14182	1470.38163	2269.80013	1
207	C	74.20945	71.28535	71.35471	-383.52382	-675.04808	144.24917	1
208	H	75.08592	70.96759	70.75785	4.09847	1517.59662	2262.86397	1
209	C	71.99126	72.10378	72.87916	-134.76730	428.45285	-649.50303	1
210	H	71.11793	72.42242	73.47403	-903.23433	1600.49020	2011.53387	1
211	C	73.23109	72.11054	70.79620	-335.53281	-615.00040	-364.39058	1
212	H	73.35445	72.42925	69.74628	1596.45398	-1369.33862	1732.02659	1
213	C	72.09198	72.55325	71.53036	585.48547	-340.24194	-406.23938	1
214	O	71.09577	73.39699	70.97296	-419.15649	-173.04408	-511.94141	1
215	H	71.45808	73.49956	70.06069	-1071.84350	1559.71507	-1960.13012	1
216	C	77.19144	69.86958	74.91769	291.41878	-183.13091	710.72246	1
217	O	76.76877	69.07658	75.72945	379.87695	523.47396	-222.23622	1
218	N	78.43512	70.03946	74.49125	564.30591	373.09380	277.24371	1
219	H	78.65510	70.76846	73.79444	-120.59931	-2436.07824	-1214.35098	1
220	C	79.50432	69.19524	74.89893	404.07514	-299.37480	608.84009	1
221	H	80.40671	69.81758	74.68863	-1071.07882	-841.69025	2359.66467	1
222	C	79.28917	68.83875	76.42809	-683.12807	68.71770	-390.13096	1
223	H	78.95203	69.74150	76.98666	2068.88918	1596.58590	770.89603	1
224	H	78.46298	68.09042	76.53533	1379.86429	2342.49779	-179.85638	1
225	C	80.61502	68.27637	77.03035	-176.39967	537.49466	550.97268	1
226	H	80.92848	67.34339	76.50754	-396.28051	1942.22168	1869.33314	1
227	H	81.45782	68.99333	76.90733	-94.44700	586.00678	-2659.20016	1
228	C	80.28932	68.01707	78.57397	-291.69381	-718.18079	-150.72929	1
229	H	79.98098	68.91677	79.16465	-2303.38776	1089.76242	964.62032	1
230	H	79.53107	67.21134	78.75044	884.16729	2568.80533	-207.74283	1
231	N	81.50634	67.56061	79.09485	-594.49522	-252.81478	342.29276	1
232	H	82.18468	67.22850	78.42709	-1735.17426	2084.05705	-263.71605	1
233	C	81.79331	67.51370	80.33227	595.23177	-271.52487	442.22352	1
234	N	80.83543	67.95998	81.24964	585.53813	-424.79750	-105.81303	1
235	H	79.89082	68.30466	81.08382	959.88797	1327.56823	-2177.11905	1
236	H	80.94925	67.94602	82.26366	1578.48647	16.27378	-2220.76233	1
237	N	83.07881	66.99183	80.53293	-452.17763	-390.33541	-421.51853	1
238	H	83.77577	66.65390	79.87095	470.26107	1974.25629	-1817.92087	1
239	H	83.48742	66.86028	81.45915	1856.67307	-1573.97321	-1224.35416	1
240	C	79.52018	67.81056	74.02276	-531.47271	-581.45780	-55.06206	1
241	O	80.50906	67.11223	74.05231	-243.00837	192.73507	609.52485	1
242	N	78.39653	67.64482	73.33238	343.49288	-644.25607	38.09164	1
243	H	77.72297	68.39379	73.50188	-1691.16043	-1535.97525	-1484.73099	1
244	C	77.98545	66.40384	72.69013	542.66492	350.14337	454.42563	1
245	H	77.12594	66.70546	72.04396	1209.57979	-2396.95920	463.86744	1
246	C	79.16730	65.88494	71.88967	-737.14309	145.93010	242.71942	1

247	H	80.03014	65.76681	72.59973	-1050.18303	159.36419	-2509.06125	1
248	C	78.90403	64.54794	71.22870	-706.77696	-252.88343	-245.16230	1
249	H	79.79473	64.19908	70.63644	-1624.64039	-1665.49085	1417.86935	1
250	H	78.67151	63.72808	71.99111	2566.10521	598.51109	693.22305	1
251	H	78.03512	64.60111	70.51600	-1972.69758	107.10018	-1876.34312	1
252	C	79.57910	66.89498	70.83138	412.85148	672.58832	-27.69222	1
253	H	80.50843	66.57567	70.28537	1447.02277	1762.76533	-1490.78944	1
254	H	78.77213	67.04032	70.06204	1320.77379	-145.20455	2378.68491	1
255	H	79.78443	67.90216	71.28938	-1512.10848	1470.52031	1724.75147	1
256	C	77.47708	65.37382	73.89447	-607.11113	499.56689	73.73769	1
257	O	77.72227	65.53290	75.06534	357.97126	460.81534	356.68785	1
258	N	76.74693	64.41600	73.33746	536.55407	-368.62270	332.76306	1
259	H	76.68005	64.41193	72.32260	524.38866	2297.69985	1367.20941	1
260	C	76.39341	63.30637	74.15434	46.50277	-774.29190	-147.97904	1
261	H	76.30530	63.74177	75.17598	1676.51875	1883.29066	1032.55549	1
262	C	75.04864	62.62843	73.57481	-559.41456	-34.19198	-556.30433	1
263	H	75.26609	62.18378	72.57424	-64.66664	395.18769	2695.05373	1
264	H	74.73328	61.77548	74.22222	-2703.44278	-60.40056	333.79418	1
265	C	73.94941	63.65138	73.46026	-519.76435	377.31045	459.42366	1
266	H	74.33793	64.52101	72.88374	-1746.74323	1667.50644	-1261.73691	1
267	C	72.75898	63.06575	72.71081	570.95554	16.46261	-545.27700	1
268	H	71.93423	63.81487	72.59209	2391.58273	28.05277	-1305.07271	1
269	H	73.04422	62.71974	71.68388	175.75588	917.63458	2559.43867	1
270	H	72.32821	62.18247	73.24903	-1063.97851	-2155.34650	1283.00462	1
271	C	73.50203	64.14285	74.83011	193.76014	2.62946	-765.53141	1
272	H	72.65884	64.87677	74.75046	507.39394	-846.55087	2539.60089	1
273	H	73.14713	63.29862	75.47592	1337.57841	1818.19054	1526.01994	1
274	H	74.33551	64.65464	75.37742	1100.88635	-1172.91350	-2199.08909	1
275	C	77.56351	62.20484	74.06143	-549.21115	475.64486	-309.38218	1
276	O	78.40818	62.18984	73.19683	556.06106	-390.37755	-78.24250	1
277	O	77.47658	61.15008	74.99505	-572.27940	-310.19032	-209.75862	1
278	H	76.71355	61.49463	75.54249	-1380.08193	2212.14486	790.85944	1

Listing 38: C00038.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	1.1302	4521
		0.2500	300.00	0.00	0.00	0.00	-1293.8079	0.0000	300.0000
3	H	65.35693	62.33953	70.99840	-2043.14101	-1757.64893	399.89339		1
4	N	65.64673	62.81309	70.14344	426.75047	490.45733	-334.42467		1
5	H	64.91415	63.52074	70.01103	442.25559	-1110.30854	-2448.52907		1
6	C	66.91889	63.42016	70.22570	415.32972	-666.39213	83.73172		1
7	H	67.49704	62.90581	71.02404	879.32219	2491.00447	667.35213		1
8	C	67.61703	63.31349	68.77442	31.35357	477.41777	628.23362		1
9	H	66.90322	63.67297	67.99536	1168.38489	2240.25337	-1019.71136		1
10	H	68.51056	63.98082	68.71393	-360.43770	2534.90498	931.67112		1
11	C	67.99771	61.87748	68.52782	463.18208	512.70242	-382.34388		1
12	H	67.14927	61.23302	68.85209	1725.29117	1863.52247	-987.07854		1
13	C	68.24430	61.63595	67.04382	710.42801	-144.27427	-313.15367		1
14	H	68.51435	60.56804	66.83773	364.20195	-1033.13725	2494.72524		1
15	H	67.33778	61.87383	66.42942	2567.61904	335.80679	847.48802		1
16	H	69.08323	62.27033	66.65726	-2587.99029	680.92867	-512.16411		1
17	C	69.24149	61.49305	69.31789	268.17616	741.64379	-40.42634		1
18	H	69.52852	60.42414	69.14224	1283.54314	-1945.37420	-1411.27812		1
19	H	70.12222	62.12332	69.02971	-1258.57796	1317.15249	-2026.02085		1
20	H	69.09116	61.61908	70.42071	-2502.84526	909.80597	575.92391		1
21	C	66.57111	64.97729	70.54359	619.36578	-458.64843	-172.09273		1
22	O	65.47171	65.45378	70.33706	-81.40433	433.87611	522.34594		1
23	N	67.66656	65.57378	71.00159	175.23996	-622.20190	341.55523		1
24	H	68.53486	65.04203	71.05762	-876.57256	-303.22879	-2561.90213		1
25	C	67.63083	66.96839	71.25404	-571.88214	-534.10783	-106.15033		1
26	H	66.55366	67.25509	71.23837	-2713.20841	-16.25800	-248.80809		1

27	C	68.38918	67.19545	72.65224	166.60354	288.16399	-716.09568	1
28	H	69.44996	66.84229	72.53115	-2097.85574	1636.78449	-586.18044	1
29	O	67.85726	66.48306	73.78057	-317.80580	-363.38227	484.43082	1
30	H	68.61379	65.90736	74.01419	1863.74748	-1451.84923	1357.29467	1
31	C	68.37844	68.76208	72.77462	503.80731	517.99032	318.51606	1
32	H	68.98959	69.11309	73.63822	640.61020	-2157.10410	-1536.29104	1
33	H	68.79264	69.25266	71.86082	1687.88455	465.60692	2087.56452	1
34	H	67.34595	69.15379	72.92671	-1293.07895	-1899.88581	-1463.57452	1
35	C	68.55555	67.64964	70.08631	-153.07550	-733.68902	248.70981	1
36	O	69.64053	67.17684	69.87773	186.15459	-480.78787	-449.34387	1
37	N	67.99174	68.74693	69.56524	-487.53139	543.18517	42.03850	1
38	C	68.58193	69.38419	68.42379	-699.35871	69.34393	360.10701	1
39	H	68.88432	68.55124	67.74941	2.81126	-221.99807	-2715.58072	1
40	C	67.41043	70.29534	67.87292	-507.46439	-592.59194	122.07761	1
41	H	67.78489	71.21589	67.37073	-1975.08116	525.87560	-1801.71556	1
42	H	66.80405	69.75266	67.11340	1588.27743	-1913.22100	1113.83566	1
43	C	66.56053	70.59857	69.14765	-613.62442	-457.55993	-194.14490	1
44	H	67.01023	71.42044	69.74822	1707.54637	-721.27992	1996.92523	1
45	H	65.51447	70.90717	68.92402	758.23357	2100.81767	1560.55011	1
46	C	66.65087	69.20349	69.90319	-352.41524	704.96076	49.21465	1
47	H	66.55173	69.25915	71.01160	1714.76886	-2070.42778	443.35792	1
48	H	65.95839	68.42034	69.51093	1224.15040	1801.50881	1636.97633	1
49	C	69.90319	70.26523	68.84131	566.85117	537.05831	117.62814	1
50	O	70.83791	70.24771	68.08296	-550.26779	-406.08867	4.21666	1
51	N	69.72488	70.96647	69.94722	566.34832	-425.77725	180.18749	1
52	H	68.88438	70.86757	70.53983	644.44502	2646.80550	-52.73430	1
53	C	70.73792	71.83473	70.44360	612.34801	-281.48662	411.56221	1
54	H	71.73309	71.44403	70.13241	1667.23498	-1490.75142	1556.16753	1
55	C	70.42994	73.29521	69.84572	-714.45746	-175.43074	286.98927	1
56	H	69.34739	73.52304	70.04876	-787.09484	1763.03619	-1922.46060	1
57	O	70.60499	73.45805	68.42957	-429.46514	516.51932	-128.40526	1
58	H	69.68217	73.60242	68.13789	1981.82785	436.16847	-1818.18182	1
59	C	71.33660	74.22529	70.72899	630.79189	-468.94448	76.03230	1
60	H	71.19104	75.29990	70.47241	-1775.71861	2062.30353	131.89849	1
61	H	71.11267	74.11003	71.81589	-1855.14608	88.94118	1993.53760	1
62	H	72.41840	73.99742	70.58723	-1504.82350	-780.94249	-2132.90992	1
63	C	70.37088	71.78202	72.02615	288.57638	618.62814	-397.00270	1
64	O	69.23395	71.44682	72.32222	321.70495	-185.26452	574.37218	1
65	N	71.37706	72.13158	72.82487	-447.05792	-446.53431	367.76425	1
66	H	72.24453	72.44478	72.39008	350.31316	1975.63644	-1843.31522	1
67	C	71.03284	72.65972	74.10270	-511.23061	374.03917	-471.51480	1
68	H	69.91918	72.62427	74.13577	2234.79579	-898.70890	-1273.45190	1
69	C	71.69917	71.69836	75.19613	529.53781	-159.34528	563.72604	1
70	H	71.12401	71.84481	76.15264	654.59388	2347.94251	1217.51488	1
71	H	71.51483	70.64663	74.85295	-1526.55661	2103.42026	817.87394	1
72	O	73.09097	71.91898	75.52836	-554.84278	14.12789	399.58769	1
73	H	73.51423	71.36284	74.84159	1297.06236	2061.84854	1220.68812	1
74	C	71.67160	74.15819	74.21613	-662.15484	-412.13544	123.62687	1
75	O	72.58474	74.53603	73.51075	-540.01537	-317.05804	274.91456	1
76	N	71.04956	74.79680	75.19367	-202.76299	-690.00100	-131.49145	1
77	H	70.27344	74.32023	75.64900	-702.62132	-2617.37191	281.70413	1
78	C	71.31876	76.16488	75.48009	-491.73914	576.34187	222.73509	1
79	H	72.41223	76.31162	75.32470	1977.17978	-1823.58850	-434.68928	1
80	C	70.45490	77.07784	74.50497	-649.50797	-328.66843	306.11224	1
81	H	69.38306	76.78647	74.54633	2075.07803	1452.16490	-1004.45904	1
82	C	70.66318	78.55751	74.97641	-615.18735	-489.99689	-70.96352	1
83	H	70.16470	79.28483	74.29375	-1226.32661	-1724.38906	-1716.47170	1
84	H	70.24615	78.71932	75.99909	2381.64273	-969.84735	900.46860	1
85	H	71.74478	78.82201	75.01842	2122.74991	1702.23946	-141.36228	1
86	C	71.00345	76.96300	73.04220	-501.86074	-479.61276	-376.42482	1
87	H	70.42044	77.59105	72.32837	993.79261	-2246.95401	-1177.81305	1
88	H	72.06988	77.27968	72.97546	42.71279	-626.15391	-2651.37258	1

89	H	70.95590	75.90871	72.68119	-2026.39012	-1590.33709	-887.82922	1
90	C	70.76327	76.43135	76.99508	-672.89153	382.57394	-156.34072	1
91	O	69.57871	76.50728	77.21142	410.04627	221.86223	500.35950	1
92	N	71.78232	76.58136	77.84325	-378.11782	-443.79414	-441.10984	1
93	H	72.77246	76.37094	77.54971	2404.15973	-568.14894	1149.30085	1
94	C	71.41322	76.84070	79.20124	-544.54484	466.16019	331.29119	1
95	H	70.40840	77.31630	79.10347	-1409.80988	-170.17955	2325.32679	1
96	C	71.30636	75.43236	79.93453	-184.48284	116.78282	-758.89137	1
97	H	70.57736	74.76892	79.41629	1893.78641	1861.14652	611.04528	1
98	H	72.28223	74.88920	79.90142	-2170.79665	-974.19311	1327.50117	1
99	C	70.87460	75.71417	81.40540	389.51668	672.81878	-138.49152	1
100	H	71.51741	76.51313	81.84417	510.64577	1933.03327	1851.02484	1
101	H	69.85352	76.15567	81.42818	-2302.30869	-1105.72939	-948.89774	1
102	C	70.92416	74.43818	82.32816	-559.93427	-126.34590	542.30857	1
103	O	70.65752	74.54349	83.49733	-670.36003	-111.83166	76.36448	1
104	N	71.27650	73.30270	81.68780	-216.06729	-537.07037	446.51379	1
105	H	71.49602	73.14851	80.69679	-1251.96487	1074.12894	-2168.52500	1
106	H	71.34321	72.38606	82.14396	-2451.83023	-720.73851	944.84612	1
107	C	72.47793	77.76610	80.02142	546.24052	-563.88337	-85.11809	1
108	O	71.96445	78.50929	80.82287	71.70702	-307.40463	606.69673	1
109	N	73.79354	77.52795	79.85608	479.90863	-504.50129	222.86849	1
110	C	74.72030	78.28351	80.63544	75.51268	-600.91904	506.73700	1
111	H	74.12649	78.92035	81.33362	-2033.61562	1795.30103	254.89480	1
112	C	75.53337	77.07879	81.28824	523.79067	517.99274	284.45581	1
113	H	76.50241	77.40060	81.72958	1599.61665	-1127.00911	1895.98173	1
114	H	74.95180	76.60016	82.10697	-1881.83093	1275.82488	-1501.55016	1
115	C	75.70449	76.10822	80.07945	-600.05639	-404.05026	316.64485	1
116	H	76.60504	76.37120	79.47399	-2597.05260	496.36221	657.73249	1
117	H	75.84050	75.04748	80.38882	-1666.24518	1294.38985	-1723.90591	1
118	C	74.37344	76.34190	79.24340	493.57570	-129.95376	-602.56394	1
119	H	74.56331	76.61086	78.17389	-1469.08415	-637.84797	2204.22581	1
120	H	73.62158	75.51749	79.30478	-1038.97840	1068.88701	-2280.71789	1
121	C	75.73843	79.10531	79.64119	188.88100	241.05089	-727.87821	1
122	O	76.59348	78.51018	79.02911	531.88613	-49.19943	427.07960	1
123	N	75.57019	80.43013	79.77891	708.14833	26.93417	-179.73509	1
124	H	74.74241	80.60327	80.35502	-2232.69501	-1179.09831	1023.94816	1
125	C	75.85602	81.38108	78.68996	-738.32412	259.92548	104.42456	1
126	H	76.01787	82.34178	79.23246	2028.89123	1260.02983	1311.33324	1
127	C	77.07669	80.94302	77.91648	-258.65678	-345.52513	661.28459	1
128	H	76.86201	79.93420	77.47041	-1826.06090	-1801.46097	-918.64554	1
129	C	77.43782	81.87627	76.77521	-541.23400	531.92970	-218.41428	1
130	H	78.40412	81.57276	76.28699	1311.73218	-2219.18200	882.19023	1
131	H	76.64769	81.87674	75.96000	-1048.71298	1223.58118	-2196.97971	1
132	H	77.56499	82.93669	77.12701	419.06414	1903.92898	1903.44670	1
133	C	78.28648	80.80509	78.82771	-423.86431	152.66566	-648.55262	1
134	H	79.16703	80.36735	78.28549	105.68386	-2342.50080	1387.51238	1
135	H	78.60858	81.79688	79.24718	-1695.63603	-1484.73621	-1531.02793	1
136	H	78.06133	80.12941	79.69933	-1853.57121	-487.39031	1936.59343	1
137	C	74.48284	81.46928	77.77556	539.71428	-510.58232	267.58633	1
138	O	73.58884	80.66028	77.82655	-15.93758	-278.34085	-624.49402	1
139	N	74.52519	82.59224	77.05184	-676.81886	12.05292	276.17960	1
140	H	75.39784	83.11021	77.12579	-1694.44250	-373.84189	-2100.66098	1
141	C	73.75195	82.59737	75.84438	412.33078	-664.70360	108.35451	1
142	H	72.75257	82.21154	76.14571	1765.77476	1294.44366	1621.76594	1
143	C	73.78524	84.07609	75.30594	-179.66635	-721.95667	-264.73915	1
144	H	73.40638	84.78616	76.07542	-607.34922	2587.87032	-598.10018	1
145	H	74.83600	84.38508	75.10472	-359.69332	-1479.13954	-2259.74260	1
146	C	72.92964	84.16369	73.99609	-240.01076	616.02425	431.85322	1
147	H	73.26525	83.40386	73.25505	-1359.17131	782.54425	2227.99181	1
148	H	71.85852	83.94396	74.20218	-820.36667	85.81767	-2596.78715	1
149	C	73.11114	85.62534	73.42033	-513.07015	236.18570	-551.87280	1
150	H	72.82202	86.38813	74.17932	1816.11944	-1183.11722	-1650.94321	1

151	H	74.18194	85.82514	73.18480	-1800.04429	-1361.53473	1526.34643	1
152	C	72.23964	85.76337	72.15064	726.08972	-253.19732	-179.64713	1
153	H	72.54173	85.10871	71.30901	1224.27271	-456.51798	-2390.90304	1
154	H	71.14926	85.67432	72.32737	1206.40339	-1150.93514	-2154.90344	1
155	N	72.43165	87.21968	71.60585	329.70796	-633.68968	-155.67358	1
156	H	71.87496	87.46094	70.73578	1348.31305	1938.76845	1359.00643	1
157	H	72.16261	88.01736	72.25235	2096.92035	1446.54551	-966.48890	1
158	H	73.41188	87.49871	71.30934	-1197.07217	-2303.53719	827.28733	1
159	C	74.51734	81.60932	74.77084	-378.01186	-556.17301	-413.96481	1
160	O	75.54334	81.94969	74.21993	-409.44433	-307.55053	-453.30833	1
161	N	73.78163	80.52600	74.60046	-429.02477	524.70884	274.08502	1
162	H	72.94742	80.46443	75.18343	1706.34263	-1425.96036	1574.38926	1
163	C	74.26445	79.35641	73.95006	-45.25864	-626.22952	478.93267	1
164	H	73.34617	78.80488	73.65269	1988.63164	570.90773	1772.87287	1
165	C	75.17659	79.80954	72.74172	551.77128	-20.49526	-564.54996	1
166	H	74.72105	80.67459	72.20862	1434.61535	-1753.10253	1513.99471	1
167	H	76.16745	80.17335	73.11002	-714.67738	1819.09770	1898.36494	1
168	C	75.34663	78.57490	71.79345	446.99263	-555.77305	338.97221	1
169	H	75.87738	77.72742	72.32803	1953.68466	1892.25957	-161.67766	1
170	H	74.35517	78.17712	71.47932	-403.03785	2688.07032	-188.43591	1
171	C	76.18247	79.05175	70.54008	567.86262	335.74681	434.04421	1
172	H	75.69706	79.92411	70.04492	-1080.02275	1568.26081	-1948.78900	1
173	H	77.19445	79.40187	70.84932	-919.54108	2111.34692	1456.13463	1
174	C	76.28855	77.85522	69.56561	195.81897	173.33862	-745.11536	1
175	H	76.87029	76.99503	69.95348	1405.67949	-2301.21089	-390.08113	1
176	H	75.31908	77.50443	69.15864	-940.37328	-1118.32446	2299.72133	1
177	N	77.08701	78.34420	68.31068	319.26422	656.36007	-42.02424	1
178	H	77.21232	77.62816	67.53819	1961.03633	619.91968	1787.09422	1
179	H	76.68678	79.16572	67.77038	854.14343	-2156.80752	1429.08711	1
180	H	78.08934	78.65404	68.47178	1237.02905	-1378.50857	-1998.28500	1
181	C	75.19890	78.49016	74.99212	532.53319	-268.57236	517.55729	1
182	O	76.07795	78.96634	75.67139	266.16714	-290.73804	-558.88002	1
183	N	74.83170	77.21806	74.88880	-226.25352	640.49678	-270.32839	1
184	H	74.12774	76.97567	74.19379	2007.69063	-1035.27229	1523.50231	1
185	C	75.70753	76.22436	75.45118	-540.76542	-573.33303	49.50000	1
186	H	76.09597	76.68088	76.39323	-2374.20950	-1036.76023	843.75774	1
187	C	74.84891	74.93932	75.64994	-77.09082	666.87422	-415.84136	1
188	H	74.21190	74.73877	74.74718	-985.81834	617.19825	2463.91927	1
189	O	73.70798	75.18091	76.76571	293.29899	-391.65602	-477.80926	1
190	H	72.99513	74.76525	76.28943	2528.72714	-681.76262	-751.27122	1
191	C	75.73887	73.72046	75.97732	252.47363	-605.14473	440.05134	1
192	H	75.11794	72.79139	76.06956	-2052.65063	1456.49051	-1043.51830	1
193	H	76.49904	73.53501	75.17850	-2152.98800	-1661.97574	-161.70652	1
194	H	76.28644	73.85886	76.94203	-473.12726	-1584.27339	2165.61725	1
195	C	76.92759	75.97205	74.36009	360.36307	488.46713	505.10056	1
196	O	76.85725	76.30022	73.18962	-200.08817	-528.03552	-385.82850	1
197	N	77.90085	75.37356	75.01772	-597.54095	-226.44775	355.20479	1
198	H	77.68401	75.24226	76.00461	2179.23655	-1300.70981	-991.33835	1
199	C	78.89513	74.56203	74.40496	-687.68921	297.39807	-249.45179	1
200	H	78.94076	73.70117	75.10725	-349.16256	-2467.37713	-1101.72831	1
201	C	78.52781	74.15692	72.90922	672.47345	361.54328	-201.62880	1
202	H	78.28293	75.06738	72.30192	1541.41502	582.18425	2169.97026	1
203	H	79.41471	73.67849	72.43135	-2534.67717	60.25153	997.72295	1
204	C	77.34453	73.17193	72.94131	574.26774	-389.43119	-377.02542	1
205	C	77.52313	71.87012	73.49553	688.82679	-287.33580	-257.96133	1
206	H	78.50399	71.55929	73.89843	331.14182	1470.38163	2269.80013	1
207	C	76.06788	73.56333	72.44053	-383.52382	-675.04808	144.24917	1
208	H	75.91530	74.57629	72.02238	4.09847	1517.59662	2262.86397	1
209	C	76.43329	70.99632	73.52125	-134.76730	428.45285	-649.50303	1
210	H	76.57697	69.98975	73.95103	-903.23433	1600.49020	2011.53387	1
211	C	75.00650	72.65296	72.49369	-335.53281	-615.00040	-364.39058	1
212	H	74.02831	72.98463	72.10670	1596.45398	-1369.33862	1732.02659	1

213	C	75.14316	71.33810	73.02329	585.48547	-340.24194	-406.23938	1
214	O	74.07790	70.38862	73.07337	-419.15649	-173.04408	-511.94141	1
215	H	73.33439	70.95500	72.76568	-1071.84350	1559.71507	-1960.13012	1
216	C	80.30675	75.38750	74.42825	291.41878	-183.13091	710.72246	1
217	O	80.86201	75.78420	73.43002	379.87695	523.47396	-222.23622	1
218	N	80.74163	75.42519	75.68734	564.30591	373.09380	277.24371	1
219	H	80.13478	75.08095	76.43066	-120.59931	-2436.07824	-1214.35098	1
220	C	81.86808	76.25128	75.97036	404.07514	-299.37480	608.84009	1
221	H	82.43562	76.32317	75.01188	-1071.07882	-841.69025	2359.66467	1
222	C	81.25431	77.63461	76.45578	-683.12807	68.71770	-390.13096	1
223	H	80.51678	78.01254	75.71189	2068.88918	1596.58590	770.89603	1
224	H	80.67933	77.48797	77.39772	1379.86429	2342.49779	-179.85638	1
225	C	82.40815	78.65980	76.66602	-176.39967	537.49466	550.97268	1
226	H	83.17949	78.26726	77.36849	-396.28051	1942.22168	1869.33314	1
227	H	82.94441	78.86964	75.71369	-94.44700	586.00678	-2659.20016	1
228	C	81.70853	79.97619	77.24644	-291.69381	-718.18079	-150.72929	1
229	H	80.92229	80.44321	76.60070	-2303.38776	1089.76242	964.62032	1
230	H	81.29093	79.85455	78.27845	884.16729	2568.80533	-207.74283	1
231	N	82.78931	80.86312	77.33353	-594.49522	-252.81478	342.29276	1
232	H	83.70964	80.45003	77.32173	-1735.17426	2084.05705	-263.71605	1
233	C	82.68782	82.12518	77.45245	595.23177	-271.52487	442.22352	1
234	N	81.40479	82.68030	77.49237	585.53813	-424.79750	-105.81303	1
235	H	80.49563	82.22063	77.46053	959.88797	1327.56823	-2177.11905	1
236	H	81.20385	83.67528	77.59812	1578.48647	16.27378	-2220.76233	1
237	N	83.95534	82.71830	77.52454	-452.17763	-390.33541	-421.51853	1
238	H	84.88602	82.30317	77.51153	470.26107	1974.25629	-1817.92087	1
239	H	84.10050	83.72257	77.63490	1856.67307	-1573.97321	-1224.35416	1
240	C	82.62904	75.55389	77.23259	-531.47271	-581.45780	-55.06206	1
241	O	82.11419	75.47217	78.33888	-243.00837	192.73507	609.52485	1
242	N	83.88632	75.18018	76.89511	343.49288	-644.25607	38.09164	1
243	H	83.93052	75.39523	75.89479	-1691.16043	-1535.97525	-1484.73099	1
244	C	84.36846	73.85860	77.39345	542.66492	350.14337	454.42563	1
245	H	83.41939	73.32493	77.62930	1209.57979	-2396.95920	463.86744	1
246	C	85.18691	73.19745	76.31661	-737.14309	145.93010	242.71942	1
247	H	86.00804	73.89549	76.03606	-1050.18303	159.36419	-2509.06125	1
248	C	85.81424	71.89868	76.79518	-706.77696	-252.88343	-245.16230	1
249	H	86.42238	71.40732	75.98707	-1624.64039	-1665.49085	1417.86935	1
250	H	86.50157	72.07280	77.67316	2566.10521	598.51109	693.22305	1
251	H	85.03513	71.15705	77.12271	-1972.69758	107.10018	-1876.34312	1
252	C	84.36695	72.91347	75.06808	412.85148	672.58832	-27.69222	1
253	H	84.99522	72.46232	74.25248	1447.02277	1762.76533	-1490.78944	1
254	H	83.53129	72.19239	75.28086	1320.77379	-145.20455	2378.68491	1
255	H	83.89781	73.84505	74.65020	-1512.10848	1470.52031	1724.75147	1
256	C	85.22997	74.22281	78.74252	-607.11113	499.56689	73.73769	1
257	O	86.38070	73.88624	78.86408	357.97126	460.81534	356.68785	1
258	N	84.42838	74.81423	79.62033	536.55407	-368.62270	332.76306	1
259	H	83.42414	74.98064	79.35993	524.38866	2297.69985	1367.20941	1
260	C	85.00364	75.65569	80.61655	46.50277	-774.29190	-147.97904	1
261	H	84.11454	75.94445	81.21923	1676.51875	1883.29066	1032.55549	1
262	C	86.10954	74.84731	81.46593	-559.41456	-34.19198	-556.30433	1
263	H	87.00569	74.66384	80.81944	-64.66664	395.18769	2695.05373	1
264	H	86.47078	75.45905	82.32745	-2703.44278	-60.40056	333.79418	1
265	C	85.51788	73.54067	81.92286	-519.76435	377.31045	459.42366	1
266	H	85.05444	73.05352	81.03431	-1746.74323	1667.50644	-1261.73691	1
267	C	86.59934	72.61454	82.46475	570.95554	16.46261	-545.27700	1
268	H	86.17908	71.61940	82.76258	2391.58273	28.05277	-1305.07271	1
269	H	87.39773	72.42325	81.70191	175.75588	917.63458	2559.43867	1
270	H	87.09949	73.04724	83.36893	-1063.97851	-2155.34650	1283.00462	1
271	C	84.44167	73.74862	82.97978	193.76014	2.62946	-765.53141	1
272	H	83.98535	72.77680	83.30032	507.39394	-846.55087	2539.60089	1
273	H	84.85344	74.24077	83.89804	1337.57841	1818.19054	1526.01994	1
274	H	83.60890	74.39479	82.60061	1100.88635	-1172.91350	-2199.08909	1

275	C	85.65495	76.93046	79.88873	-549.21115	475.64486	-309.38218	1
276	O	86.53875	77.56439	80.40568	556.06106	-390.37755	-78.24250	1
277	O	85.03380	77.40368	78.70586	-572.27940	-310.19032	-209.75862	1
278	H	84.46709	76.60986	78.49902	-1380.08193	2212.14486	790.85944	1

Listing 39: C00039.xmolout

1	276							
2	150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
	0.2500	300.00	0.00	0.00	0.00	-1293.8012	0.0000	300.0000
3	H	79.56307	71.49838	77.05859	-2043.14101	-1757.64893	399.89339	1
4	N	79.42056	72.50538	77.13012	426.75047	490.45733	-334.42467	1
5	H	79.31074	72.62630	78.13889	442.25559	-1110.30854	-2448.52907	1
6	C	80.54121	73.22787	76.67060	415.32972	-666.39213	83.73172	1
7	H	81.35306	72.49281	76.49126	879.32219	2491.00447	667.35213	1
8	C	80.14231	74.11334	75.39398	31.35357	477.41777	628.23362	1
9	H	79.35720	74.83785	75.73299	1168.38489	2240.25337	-1019.71136	1
10	H	81.01567	74.73540	75.07777	-360.43770	2534.90498	931.67112	1
11	C	79.63760	73.28301	74.23444	463.18208	512.70242	-382.34388	1
12	H	78.84190	72.59610	74.60084	1725.29117	1863.52247	-987.07854	1
13	C	79.04204	74.19702	73.17170	710.42801	-144.27427	-313.15367	1
14	H	78.71742	73.60828	72.27340	364.20195	-1033.13725	2494.72524	1
15	H	78.14851	74.75514	73.55622	2567.61904	335.80679	847.48802	1
16	H	79.78361	74.95894	72.81610	-2587.99029	680.92867	-512.16411	1
17	C	80.74998	72.45250	73.61308	268.17616	741.64379	-40.42634	1
18	H	80.36854	71.85317	72.74151	1283.54314	-1945.37420	-1411.27812	1
19	H	81.58440	73.09898	73.23377	-1258.57796	1317.15249	-2026.02085	1
20	H	81.19428	71.73208	74.34810	-2502.84526	909.80597	575.92391	1
21	C	80.87729	74.39358	77.80527	619.36578	-458.64843	-172.09273	1
22	O	80.28667	75.45563	77.74003	-81.40433	433.87611	522.34594	1
23	N	82.34460	74.33609	77.71105	175.23996	-622.20190	341.55523	1
24	H	82.75050	74.84560	76.92398	-876.57256	-303.22879	-2561.90213	1
25	C	82.92889	74.79363	78.96619	-571.88214	-534.10783	-106.15033	1
26	H	83.96544	74.38786	79.00755	-2713.20841	-16.25800	-248.80809	1
27	C	82.93255	76.40015	78.79698	166.60354	288.16399	-716.09568	1
28	H	81.86503	76.74667	78.70313	-2097.85574	1636.78449	-586.18044	1
29	O	83.61388	76.84253	77.61208	-317.80580	-363.38227	484.43082	1
30	H	82.88234	77.29324	77.14028	1863.74748	-1451.84923	1357.29467	1
31	C	83.51280	76.91461	80.15996	503.80731	517.99032	318.51606	1
32	H	83.50802	78.02909	80.20473	640.61020	-2157.10410	-1536.29104	1
33	H	82.91452	76.54563	81.03611	1687.88455	465.60692	2087.56452	1
34	H	84.56885	76.58765	80.30509	-1293.07895	-1899.88581	-1463.57452	1
35	C	81.94789	74.19291	80.03764	-153.07550	-733.68902	248.70981	1
36	O	80.81093	73.79611	79.58802	186.15459	-480.78787	-449.34387	1
37	N	82.37833	74.18919	81.26330	-487.53139	543.18517	42.03850	1
38	C	81.45590	74.21514	82.38487	-699.35871	69.34393	360.10701	1
39	H	80.64620	73.48718	82.15429	2.81126	-221.99807	-2715.58072	1
40	C	82.40942	73.82838	83.58841	-507.46439	-592.59194	122.07761	1
41	H	82.02762	74.18315	84.57202	-1975.08116	525.87560	-1801.71556	1
42	H	82.53740	72.72637	83.67423	1588.27743	-1913.22100	1113.83566	1
43	C	83.74013	74.52361	83.15930	-613.62442	-457.55993	-194.14490	1
44	H	83.65823	75.63111	83.26974	1707.54637	-721.27992	1996.92523	1
45	H	84.63052	74.19729	83.74293	758.23357	2100.81767	1560.55011	1
46	C	83.79330	74.09772	81.63422	-352.41524	704.96076	49.21465	1
47	H	84.39711	74.75731	80.97256	1714.76886	-2070.42778	443.35792	1
48	H	84.08498	73.03602	81.45873	1224.15040	1801.50881	1636.97633	1
49	C	80.91665	75.72989	82.57307	566.85117	537.05831	117.62814	1
50	O	81.69631	76.66899	82.73226	-550.26779	-406.08867	4.21666	1
51	N	79.61280	75.73133	82.56504	566.34832	-425.77725	180.18749	1
52	H	79.05294	74.87397	82.41024	644.44502	2646.80550	-52.73430	1
53	C	78.86544	76.87521	83.02297	612.34801	-281.48662	411.56221	1
54	H	79.36822	77.27459	83.93543	1667.23498	-1490.75142	1556.16753	1

55	C	78.90726	77.95247	81.83463	-714.45746	-175.43074	286.98927	1
56	H	78.70250	77.42924	80.85483	-787.09484	1763.03619	-1922.46060	1
57	O	80.18867	78.55207	81.57008	-429.46514	516.51932	-128.40526	1
58	H	80.80048	77.87041	82.02345	1981.82785	436.16847	-1818.18182	1
59	C	77.73360	78.93101	82.16057	630.79189	-468.94448	76.03230	1
60	H	77.59882	79.68734	81.35099	-1775.71861	2062.30353	131.89849	1
61	H	76.76071	78.38942	82.26069	-1855.14608	88.94118	1993.53760	1
62	H	77.90920	79.48660	83.11223	-1504.82350	-780.94249	-2132.90992	1
63	C	77.46298	76.15713	83.28360	288.57638	618.62814	-397.00270	1
64	O	77.27185	75.01477	82.90900	321.70495	-185.26452	574.37218	1
65	N	76.56688	76.93195	83.94321	-447.05792	-446.53431	367.76425	1
66	H	76.63731	77.91488	84.27846	350.31316	1975.63644	-1843.31522	1
67	C	75.37541	76.53250	84.28752	-511.23061	374.03917	-471.51480	1
68	H	75.14600	75.48490	84.01456	2234.79579	-898.70890	-1273.45190	1
69	C	74.44116	77.47000	84.96845	529.53781	-159.34528	563.72604	1
70	H	73.44323	77.00656	85.11118	654.59388	2347.94251	1217.51488	1
71	H	74.82184	77.84959	85.97169	-1526.55661	2103.42026	817.87394	1
72	O	74.51405	79.12031	84.56610	-554.84278	14.12789	399.58769	1
73	H	73.78064	79.39346	85.09207	1297.06236	2061.84854	1220.68812	1
74	C	74.57068	78.95406	81.18421	-662.15484	-412.13544	123.62687	2
75	O	75.43792	78.71841	80.42570	-540.01537	-317.05804	274.91456	2
76	N	73.64532	79.20747	81.99485	-202.76299	-690.00100	-131.49145	2
77	H	73.81324	79.11580	83.04767	-702.62132	-2617.37191	281.70413	2
78	C	72.49187	79.89371	81.52474	-491.73914	576.34187	222.73509	2
79	H	71.92306	80.06053	82.46726	1977.17978	-1823.58850	-434.68928	2
80	C	72.98975	81.25787	80.87220	-649.50797	-328.66843	306.11224	2
81	H	73.59408	81.05958	79.96131	2075.07803	1452.16490	-1004.45904	2
82	C	71.76959	82.18577	80.55195	-615.18735	-489.99689	-70.96352	2
83	H	72.09641	83.13593	80.06755	-1226.32661	-1724.38906	-1716.47170	2
84	H	71.04026	81.69669	79.86455	2381.64273	-969.84735	900.46860	2
85	H	71.21335	82.46098	81.47834	2122.74991	1702.23946	-141.36228	2
86	C	73.85797	82.01788	81.93250	-501.86074	-479.61276	-376.42482	2
87	H	74.26307	82.97458	81.52729	993.79261	-2246.95401	-1177.81305	2
88	H	73.26575	82.26520	82.84446	42.71279	-626.15391	-2651.37258	2
89	H	74.72662	81.39981	82.26222	-2026.39012	-1590.33709	-887.82922	2
90	C	71.69050	78.86928	80.51136	-672.89153	382.57394	-156.34072	2
91	O	71.23353	77.84090	80.95655	410.04627	221.86223	500.35950	2
92	N	71.60373	79.32547	79.27233	-378.11782	-443.79414	-441.10984	2
93	H	72.02511	80.22402	79.05165	2404.15973	-568.14894	1149.30085	2
94	C	71.00830	78.49034	78.27764	-544.54484	466.16019	331.29119	2
95	H	70.28458	77.88935	78.87699	-1409.80988	-170.17955	2325.32679	2
96	C	70.34504	79.46849	77.21846	-184.48284	116.78282	-758.89137	2
97	H	69.67284	80.19057	77.73369	1893.78641	1861.14652	611.04528	2
98	H	71.12157	80.08947	76.71843	-2170.79665	-974.19311	1327.50117	2
99	C	69.56128	78.63069	76.16078	389.51668	672.81878	-138.49152	2
100	H	70.23541	77.87931	75.68778	510.64577	1933.03327	1851.02484	2
101	H	68.78441	78.01256	76.66325	-2302.30869	-1105.72939	-948.89774	2
102	C	68.89343	79.51297	75.03650	-559.93427	-126.34590	542.30857	2
103	O	68.44320	78.98754	74.05099	-670.36003	-111.83166	76.36448	2
104	N	68.86725	80.83385	75.31714	-216.06729	-537.07037	446.51379	2
105	H	69.19772	81.33205	76.15129	-1251.96487	1074.12894	-2168.52500	2
106	H	68.41784	81.53802	74.72151	-2451.83023	-720.73851	944.84612	2
107	C	72.04732	77.49861	77.50110	546.24052	-563.88337	-85.11809	2
108	O	71.53817	76.52821	76.99073	71.70702	-307.40463	606.69673	2
109	N	73.33169	77.87580	77.42267	479.90863	-504.50129	222.86849	2
110	C	74.28329	77.06199	76.72758	75.51268	-600.91904	506.73700	2
111	H	73.70851	76.51164	75.94716	-2033.61562	1795.30103	254.89480	2
112	C	75.32370	78.14357	76.20025	523.79067	517.99274	284.45581	2
113	H	76.31223	77.69761	75.94823	1599.61665	-1127.00911	1895.98173	2
114	H	74.95570	78.65926	75.28546	-1881.83093	1275.82488	-1501.55016	2
115	C	75.38233	79.11556	77.41848	-600.05639	-404.05026	316.64485	2
116	H	76.03530	78.70136	78.22214	-2597.05260	496.36221	657.73249	2

117	H	75.78783	80.12233	77.16997	-1666.24518	1294.38985	-1723.90591	2
118	C	73.86257	79.15096	77.88225	493.57570	-129.95376	-602.56394	2
119	H	73.71932	79.17404	78.98837	-1469.08415	-637.84797	2204.22581	2
120	H	73.23922	79.94326	77.40506	-1038.97840	1068.88701	-2280.71789	2
121	C	75.06719	76.06128	77.75619	188.88100	241.05089	-727.87821	2
122	O	76.24074	75.78209	77.52014	531.88613	-49.19943	427.07960	2
123	N	74.29604	75.60830	78.71587	708.14833	26.93417	-179.73509	2
124	H	73.33111	75.93205	78.70495	-2232.69501	-1179.09831	1023.94816	2
125	C	74.87331	74.79665	79.74129	-738.32412	259.92548	104.42456	2
126	H	75.85550	75.29030	79.91816	2028.89123	1260.02983	1311.33324	2
127	C	73.90314	74.73078	80.99001	-258.65678	-345.52513	661.28459	2
128	H	72.91351	74.32217	80.68896	-1826.06090	-1801.46097	-918.64554	2
129	C	74.56290	73.83741	82.09717	-541.23400	531.92970	-218.41428	2
130	H	73.93352	73.79175	83.01716	1311.73218	-2219.18200	882.19023	2
131	H	74.70502	72.78703	81.74435	-1048.71298	1223.58118	-2196.97971	2
132	H	75.58350	74.23445	82.39896	419.06414	1903.92898	1903.44670	2
133	C	73.74520	76.16451	81.60417	-423.86431	152.66566	-648.55262	2
134	H	73.08224	76.16353	82.50158	105.68386	-2342.50080	1387.51238	2
135	H	74.72941	76.58871	81.91605	-1695.63603	-1484.73621	-1531.02793	2
136	H	73.30003	76.87592	80.86732	-1853.57121	-487.39031	1936.59343	2
137	C	75.05871	73.27494	79.15108	539.71428	-510.58232	267.58633	2
138	O	74.33273	72.38863	79.52468	-15.93758	-278.34085	-624.49402	2
139	N	76.07734	73.25816	78.30645	-676.81886	12.05292	276.17960	2
140	H	76.55887	74.15947	78.06066	-1694.44250	-373.84189	-2100.66098	2
141	C	76.63222	72.03882	77.84300	412.33078	-664.70360	108.35451	2
142	H	77.56077	72.39344	77.33839	1765.77476	1294.44366	1621.76594	2
143	C	76.86866	71.07820	79.08056	-179.66635	-721.95667	-264.73915	2
144	H	77.44456	71.59165	79.88335	-607.34922	2587.87032	-598.10018	2
145	H	75.88644	70.80582	79.53686	-359.69332	-1479.13954	-2259.74260	2
146	C	77.61380	69.79942	78.57467	-240.01076	616.02425	431.85322	2
147	H	77.08139	69.36916	77.69542	-1359.17131	782.54425	2227.99181	2
148	H	78.64057	70.04287	78.22330	-820.36667	85.81767	-2596.78715	2
149	C	77.65434	68.74053	79.74872	-513.07015	236.18570	-551.87280	2
150	H	78.32375	69.07671	80.57366	1816.11944	-1183.11722	-1650.94321	2
151	H	76.64581	68.61298	80.20565	-1800.04429	-1361.53473	1526.34643	2
152	C	78.14211	67.41081	79.12738	726.08972	-253.19732	-179.64713	2
153	H	77.44463	66.96798	78.38828	1224.27271	-456.51798	-2390.90304	2
154	H	79.16657	67.44559	78.70630	1206.40339	-1150.93514	-2154.90344	2
155	N	78.21977	66.34610	80.27236	329.70796	-633.68968	-155.67358	2
156	H	78.52107	65.37468	79.97082	1348.31305	1938.76845	1359.00643	2
157	H	78.89578	66.53626	81.06828	2096.92035	1446.54551	-966.48890	2
158	H	77.31951	66.13188	80.79232	-1197.07217	-2303.53719	827.28733	2
159	C	75.61840	71.26327	76.80658	-378.01186	-556.17301	-413.96481	2
160	O	75.04699	70.24795	77.13559	-409.44433	-307.55053	-453.30833	2
161	N	75.63116	71.84419	75.61063	-429.02477	524.70884	274.08502	2
162	H	76.14570	72.71740	75.50954	1706.34263	-1425.96036	1574.38926	2
163	C	74.81394	71.21930	74.61719	-45.25864	-626.22952	478.93267	2
164	H	74.79431	70.14865	74.93104	1988.63164	570.90773	1772.87287	2
165	C	73.37534	71.87460	74.71985	551.77128	-20.49526	-564.54996	2
166	H	73.03817	71.94328	75.77851	1434.61535	-1753.10253	1513.99471	2
167	H	73.38254	72.91873	74.33480	-714.67738	1819.09770	1898.36494	2
168	C	72.42545	70.96039	73.86660	446.99263	-555.77305	338.97221	2
169	H	72.85019	70.79786	72.84771	1953.68466	1892.25957	-161.67766	2
170	H	72.32891	69.95004	74.32646	-403.03785	2688.07032	-188.43591	2
171	C	71.03794	71.67184	73.76871	567.86262	335.74681	434.04421	2
172	H	70.57753	71.80690	74.77213	-1080.02275	1568.26081	-1948.78900	2
173	H	71.15844	72.69486	73.35472	-919.54108	2111.34692	1456.13463	2
174	C	70.10743	70.78465	72.81689	195.81897	173.33862	-745.11536	2
175	H	70.44359	70.76494	71.75040	1405.67949	-2301.21089	-390.08113	2
176	H	69.97559	69.73549	73.18175	-940.37328	-1118.32446	2299.72133	2
177	N	68.80180	71.38310	72.82173	319.26422	656.36007	-42.02424	2
178	H	68.18427	71.04005	72.09093	1961.03633	619.91968	1787.09422	2

179	H	68.25233	71.17413	73.65117	854.14343	-2156.80752	1429.08711	2
180	H	68.65822	74.90668	72.56344	1237.02905	-1378.50857	-1998.28500	2
181	C	75.30428	71.45510	73.06913	532.53319	-268.57236	517.55729	2
182	O	75.04827	70.55645	72.27229	266.16714	-290.73804	-558.88002	2
183	N	75.78564	72.65457	72.84361	-226.25352	640.49678	-270.32839	2
184	H	75.85494	73.22552	73.68461	2007.69063	-1035.27229	1523.50231	2
185	C	76.33414	73.09781	71.60985	-540.76542	-573.33303	49.50000	2
186	H	76.90014	74.01144	71.89338	-2374.20950	-1036.76023	843.75774	2
187	C	77.26137	71.93853	71.00978	-77.09082	666.87422	-415.84136	2
188	H	76.60845	71.04841	70.78034	-985.81834	617.19825	2463.91927	2
189	O	78.30488	71.43815	71.87316	293.29899	-391.65602	-477.80926	2
190	H	77.96320	70.54082	72.06103	2528.72714	-681.76262	-751.27122	2
191	C	77.74942	72.58646	69.66466	252.47363	-605.14473	440.05134	2
192	H	78.33125	71.86047	69.05037	-2052.65063	1456.49051	-1043.51830	2
193	H	76.89427	72.94441	69.04085	-2152.98800	-1661.97574	-161.70652	2
194	H	78.41075	73.46425	69.85150	-473.12726	-1584.27339	2165.61725	2
195	C	75.15866	73.47426	70.54317	360.36307	488.46713	505.10056	2
196	O	75.34844	74.43768	69.81335	-200.08817	-528.03552	-385.82850	2
197	N	74.18027	72.60494	70.56408	-597.54095	-226.44775	355.20479	2
198	H	74.27880	71.78706	71.19847	2179.23655	-1300.70981	-991.33835	2
199	C	72.90983	72.85189	69.98322	-687.68921	297.39807	-249.45179	2
200	H	72.25582	72.10208	70.48141	-349.16256	-2467.37713	-1101.72831	2
201	C	72.45151	74.35371	70.21987	672.47345	361.54328	-201.62880	2
202	H	73.32627	75.04467	70.22340	1541.41502	582.18425	2169.97026	2
203	H	71.79258	74.67638	69.38291	-2534.67717	60.25153	997.72295	2
204	C	71.66422	74.44506	71.56783	574.26774	-389.43119	-377.02542	2
205	C	70.33967	74.06674	71.53902	688.82679	-287.33580	-257.96133	2
206	H	69.89025	73.67591	70.61843	331.14182	1470.38163	2269.80013	2
207	C	72.31353	74.93860	72.75076	-383.52382	-675.04808	144.24917	2
208	H	73.38051	75.20943	72.71983	4.09847	1517.59662	2262.86397	2
209	C	69.52104	74.23213	72.79739	-134.76730	428.45285	-649.50303	2
210	H	69.03887	73.24131	73.01976	-903.23433	1600.49020	2011.53387	2
211	C	71.59021	75.07622	73.93431	-335.53281	-615.00040	-364.39058	2
212	H	72.12540	75.46410	74.82183	1596.45398	-1369.33862	1732.02659	2
213	C	70.23655	74.76064	74.08495	585.48547	-340.24194	-406.23938	2
214	O	69.48043	74.85316	75.20468	-419.15649	-173.04408	-511.94141	2
215	H	70.17107	75.30143	75.82916	-1071.84350	1559.71507	-1960.13012	2
216	C	72.94043	72.61958	68.35515	291.41878	-183.13091	710.72246	2
217	O	72.11911	71.87911	67.87617	379.87695	523.47396	-222.23622	2
218	N	73.79196	73.45126	67.76898	564.30591	373.09380	277.24371	2
219	H	74.39675	74.02658	68.40591	-120.59931	-2436.07824	-1214.35098	2
220	C	74.37024	73.10459	66.49400	404.07514	-299.37480	608.84009	2
221	H	75.40986	72.78869	66.73056	-1071.07882	-841.69025	2359.66467	2
222	C	73.53720	72.01075	65.72833	-683.12807	68.71770	-390.13096	2
223	H	73.52672	71.04737	66.29114	2068.88918	1596.58590	770.89603	2
224	H	72.46923	72.32758	65.66233	1379.86429	2342.49779	-179.85638	2
225	C	74.14929	71.81326	64.30272	-176.39967	537.49466	550.97268	2
226	H	74.30102	72.79414	63.79638	-396.28051	1942.22168	1869.33314	2
227	H	75.15864	71.34954	64.36093	-94.44700	586.00678	-2659.20016	2
228	C	73.13458	70.90235	63.47316	-291.69381	-718.18079	-150.72929	2
229	H	72.92762	69.88761	63.89883	-2303.38776	1089.76242	964.62032	2
230	H	72.15028	71.38006	63.23248	884.16729	2568.80533	-207.74283	2
231	N	73.83290	70.72833	62.26860	-594.49522	-252.81478	342.29276	2
232	H	74.69502	71.24073	62.16422	-1735.17426	2084.05705	-263.71605	2
233	C	73.45430	69.98018	61.31328	595.23177	-271.52487	442.22352	2
234	N	72.25203	69.28125	61.46776	585.53813	-424.79750	-105.81303	2
235	H	71.60081	69.28097	62.25178	959.88797	1327.56823	-2177.11905	2
236	H	71.84676	68.65451	60.77182	1578.48647	16.27378	-2220.76233	2
237	N	74.36858	70.01536	60.25067	-452.17763	-390.33541	-421.51853	2
238	H	75.24772	70.51878	60.14197	470.26107	1974.25629	-1817.92087	2
239	H	74.24915	69.47467	59.39323	1856.67307	-1573.97321	-1224.35416	2
240	C	74.35546	74.45487	65.58384	-531.47271	-581.45780	-55.06206	2

241	O	75.20127	74.66778	64.74852	-243.00837	192.73507	609.52485	2
242	N	73.14585	75.11208	65.70918	343.49288	-644.25607	38.09164	2
243	H	72.83128	74.74659	66.61748	-1691.16043	-1535.97525	-1484.73099	2
244	C	73.12189	76.56092	65.40590	542.66492	350.14337	454.42563	2
245	H	74.18277	76.89044	65.48379	1209.57979	-2396.95920	463.86744	2
246	C	72.53899	76.74376	64.02286	-737.14309	145.93010	242.71942	2
247	H	71.58025	76.17429	63.98160	-1050.18303	159.36419	-2509.06125	2
248	C	72.21368	78.19875	63.73267	-706.77696	-252.88343	-245.16230	2
249	H	71.82838	78.33750	62.68525	-1624.64039	-1665.49085	1417.86935	2
250	H	71.41679	78.58299	64.43203	2566.10521	598.51109	693.22305	2
251	H	73.11402	78.86144	63.85257	-1972.69758	107.10018	-1876.34312	2
252	C	73.45428	76.20070	62.94038	412.85148	672.58832	-27.69222	2
253	H	73.00226	76.30498	61.91593	1447.02277	1762.76533	-1490.78944	2
254	H	74.44237	76.73811	62.92781	1320.77379	-145.20455	2378.68491	2
255	H	73.67778	75.10904	63.10201	-1512.10848	1470.52031	1724.75147	2
256	C	72.12902	77.27540	66.51028	-607.11113	499.56689	73.73769	2
257	O	72.35131	78.41491	66.84413	357.97126	460.81534	356.68785	2
258	N	71.15205	76.45656	66.92281	536.55407	-368.62270	332.76306	2
259	H	71.16889	75.56565	66.42545	524.38866	2297.69985	1367.20941	2
260	C	69.86720	77.02185	67.21797	46.50277	-774.29190	-147.97904	2
261	H	69.29543	76.14898	67.60103	1676.51875	1883.29066	1032.55549	2
262	C	70.01347	78.19672	68.30825	-559.41456	-34.19198	-556.30433	2
263	H	70.58810	79.04745	67.85603	-64.66664	395.18769	2695.05373	2
264	H	69.01842	78.61378	68.59619	-2703.44278	-60.40056	333.79418	2
265	C	70.74104	77.66366	69.51515	-519.76435	377.31045	459.42366	2
266	H	71.59740	77.04820	69.15641	-1746.74323	1667.50644	-1261.73691	2
267	C	71.29510	78.80744	70.35553	570.95554	16.46261	-545.27700	2
268	H	71.87063	78.42879	71.23946	2391.58273	28.05277	-1305.07271	2
269	H	71.98714	79.45794	69.75992	175.75588	917.63458	2559.43867	2
270	H	70.47621	79.46310	70.75008	-1063.97851	-2155.34650	1283.00462	2
271	C	69.82952	76.80011	70.37614	193.76014	2.62946	-765.53141	2
272	H	70.35766	76.43687	71.29556	507.39394	-846.55087	2539.60089	2
273	H	68.92620	77.36681	70.72086	1337.57841	1818.19054	1526.01994	2
274	H	69.46624	75.89714	69.82128	1100.88635	-1172.91350	-2199.08909	2
275	C	69.25075	77.55949	65.84539	-549.21115	475.64486	-309.38218	2
276	O	69.63049	77.18532	64.76380	556.06106	-390.37755	-78.24250	2
277	O	68.13245	78.42752	65.94162	-572.27940	-310.19032	-209.75862	2
278	H	68.04316	78.45714	66.92967	-1380.08193	2212.14486	790.85944	2

Listing 40: C00040.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.3537	9415
		0.2500	300.00	0.00	0.00	0.00	-1293.7932	0.0000	300.0000
3	H	85.65516	69.35480	80.41490	-2043.14101	-1757.64893	399.89339		1
4	N	85.74069	69.77449	79.48950	426.75047	490.45733	-334.42467		1
5	H	84.80943	70.17133	79.30544	442.25559	-1110.30854	-2448.52907		1
6	C	86.83618	70.65016	79.33944	415.32972	-666.39213	83.73172		1
7	H	87.69461	70.14115	79.82907	879.32219	2491.00447	667.35213		1
8	C	87.06199	70.90420	77.76049	31.35357	477.41777	628.23362		1
9	H	86.14217	71.36999	77.33309	1168.38489	2240.25337	-1019.71136		1
10	H	87.88732	71.63600	77.59267	-360.43770	2534.90498	931.67112		1
11	C	87.36030	69.59576	77.07836	463.18208	512.70242	-382.34388		1
12	H	86.57895	68.86219	77.38146	1725.29117	1863.52247	-987.07854		1
13	C	87.30969	69.76557	75.56480	710.42801	-144.27427	-313.15367		1
14	H	87.49684	68.79671	75.03372	364.20195	-1033.13725	2494.72524		1
15	H	86.31214	70.14508	75.22371	2567.61904	335.80679	847.48802		1
16	H	88.08219	70.49384	75.20634	-2587.99029	680.92867	-512.16411		1
17	C	88.72341	69.04858	77.47975	268.17616	741.64379	-40.42634		1
18	H	88.95101	68.08434	76.95579	1283.54314	-1945.37420	-1411.27812		1
19	H	89.54714	69.76486	77.22677	-1258.57796	1317.15249	-2026.02085		1
20	H	88.78380	68.84778	78.58018	-2502.84526	909.80597	575.92391		1

21	C	86.45564	72.05891	80.04207	619.36578	-458.64843	-172.09273	1
22	O	85.31809	72.36712	80.39858	-81.40433	433.87611	522.34594	1
23	N	87.55285	72.78116	80.03384	175.23996	-622.20190	341.55523	1
24	H	88.40750	72.31771	79.73088	-876.57256	-303.22879	-2561.90213	1
25	C	87.60448	74.07037	80.65539	-571.88214	-534.10783	-106.15033	1
26	H	87.19912	73.87777	81.67399	-2713.20841	-16.25800	-248.80809	1
27	C	89.14648	74.48479	80.65712	166.60354	288.16399	-716.09568	1
28	H	89.49046	74.63076	79.59678	-2097.85574	1636.78449	-586.18044	1
29	O	90.03274	73.49916	81.22487	-317.80580	-363.38227	484.43082	1
30	H	90.64734	73.34738	80.48034	1863.74748	-1451.84923	1357.29467	1
31	C	89.13894	75.88294	81.37629	503.80731	517.99032	318.51606	1
32	H	90.16976	76.29678	81.47036	640.61020	-2157.10410	-1536.29104	1
33	H	88.53277	76.63815	80.82079	1687.88455	465.60692	2087.56452	1
34	H	88.71598	75.81015	82.40535	-1293.07895	-1899.88581	-1463.57452	1
35	C	86.66167	75.15244	79.88649	-153.07550	-733.68902	248.70981	1
36	O	86.34737	76.10353	80.55348	186.15459	-480.78787	-449.34387	1
37	N	86.49699	74.97081	78.57120	-487.53139	543.18517	42.03850	1
38	C	85.33788	75.48795	77.90022	-699.35871	69.34393	360.10701	1
39	H	85.21079	76.50769	78.32831	2.81126	-221.99807	-2715.58072	1
40	C	85.74378	75.44635	76.37494	-507.46439	-592.59194	122.07761	1
41	H	84.87323	75.25705	75.70628	-1975.08116	525.87560	-1801.71556	1
42	H	86.16505	76.42460	76.05213	1588.27743	-1913.22100	1113.83566	1
43	C	86.83448	74.32704	76.30554	-613.62442	-457.55993	-194.14490	1
44	H	86.38433	73.31198	76.24795	1707.54637	-721.27992	1996.92523	1
45	H	87.50917	74.41897	75.42520	758.23357	2100.81767	1560.55011	1
46	C	87.57963	74.55052	77.68920	-352.41524	704.96076	49.21465	1
47	H	88.05711	73.64443	78.12498	1714.76886	-2070.42778	443.35792	1
48	H	88.31495	75.38965	77.69142	1224.15040	1801.50881	1636.97633	1
49	C	84.04944	74.55147	78.30928	566.85117	537.05831	117.62814	1
50	O	83.46278	74.82283	79.33192	-550.26779	-406.08867	4.21666	1
51	N	83.87784	73.54304	77.46711	566.34832	-425.77725	180.18749	1
52	H	84.54446	73.48231	76.70044	644.44502	2646.80550	-52.73430	1
53	C	82.61969	72.88433	77.31963	612.34801	-281.48662	411.56221	1
54	H	82.77892	72.09231	76.55285	1667.23498	-1490.75142	1556.16753	1
55	C	82.31356	72.26101	78.75668	-714.45746	-175.43074	286.98927	1
56	H	82.41498	73.08736	79.52782	-787.09484	1763.03619	-1922.46060	1
57	O	83.25595	71.24394	79.16958	-429.46514	516.51932	-128.40526	1
58	H	83.88476	71.81053	79.74786	1981.82785	436.16847	-1818.18182	1
59	C	80.81586	71.82539	78.67645	630.79189	-468.94448	76.03230	1
60	H	80.45098	71.44376	79.65938	-1775.71861	2062.30353	131.89849	1
61	H	80.15345	72.67426	78.38463	-1855.14608	88.94118	1993.53760	1
62	H	80.66531	71.01114	77.92915	-1504.82350	-780.94249	-2132.90992	1
63	C	81.57340	74.01251	76.79256	288.57638	618.62814	-397.00270	1
64	O	81.71551	75.22707	77.03963	321.70495	-185.26452	574.37218	1
65	N	80.61985	73.42328	76.12985	-447.05792	-446.53431	367.76425	1
66	H	80.73166	72.41204	76.07643	350.31316	1975.63644	-1843.31522	1
67	C	79.47421	74.06575	75.58777	-511.23061	374.03917	-471.51480	1
68	H	78.83559	73.19483	75.31916	2234.79579	-898.70890	-1273.45190	1
69	C	78.84086	74.94889	76.75498	529.53781	-159.34528	563.72604	1
70	H	77.72953	75.01301	76.60363	654.59388	2347.94251	1217.51488	1
71	H	79.00248	74.36821	77.70195	-1526.55661	2103.42026	817.87394	1
72	O	79.32274	76.29555	76.93437	-554.84278	14.12789	399.58769	1
73	H	80.31055	76.09207	77.08396	1297.06236	2061.84854	1220.68812	1
74	C	79.86855	74.91675	74.25219	-662.15484	-412.13544	123.62687	1
75	O	79.24174	74.66156	73.23359	-540.01537	-317.05804	274.91456	1
76	N	80.79431	75.81869	74.47398	-202.76299	-690.00100	-131.49145	1
77	H	81.15769	75.88872	75.44552	-702.62132	-2617.37191	281.70413	1
78	C	81.62691	76.32624	73.43778	-491.73914	576.34187	222.73509	1
79	H	82.45012	76.81449	74.00494	1977.17978	-1823.58850	-434.68928	1
80	C	82.13315	75.09908	72.56263	-649.50797	-328.66843	306.11224	1
81	H	81.27687	74.47043	72.23165	2075.07803	1452.16490	-1004.45904	1
82	C	82.92555	75.65638	71.33172	-615.18735	-489.99689	-70.96352	1

83	H	83.34410	74.83478	70.70433	-1226.32661	-1724.38906	-1716.47170	1
84	H	82.27085	76.27692	70.67469	2381.64273	-969.84735	900.46860	1
85	H	83.77796	76.30106	71.65068	2122.74991	1702.23946	-141.36228	1
86	C	83.12195	74.26399	73.44697	-501.86074	-479.61276	-376.42482	1
87	H	83.48328	73.35343	72.91450	993.79261	-2246.95401	-1177.81305	1
88	H	84.01959	74.86120	73.73086	42.71279	-626.15391	-2651.37258	1
89	H	82.63372	73.92810	74.39261	-2026.39012	-1590.33709	-887.82922	1
90	C	80.85795	77.41261	72.48073	-672.89153	382.57394	-156.34072	1
91	O	81.36910	78.49453	72.33018	410.04627	221.86223	500.35950	1
92	N	79.76209	76.92914	71.91201	-378.11782	-443.79414	-441.10984	1
93	H	79.41712	75.95805	72.12195	2404.15973	-568.14894	1149.30085	1
94	C	78.92841	77.87421	71.21886	-544.54484	466.16019	331.29119	1
95	H	79.24110	78.85675	71.64585	-1409.80988	-170.17955	2325.32679	1
96	C	79.32725	77.76184	69.68050	-184.48284	116.78282	-758.89137	1
97	H	80.43300	77.83005	69.57155	1893.78641	1861.14652	611.04528	1
98	H	79.04110	76.76787	69.26927	-2170.79665	-974.19311	1327.50117	1
99	C	78.61993	78.91039	68.90148	389.51668	672.81878	-138.49152	1
100	H	77.51377	78.79760	68.98305	510.64577	1933.03327	1851.02484	1
101	H	78.83179	79.88700	69.39037	-2302.30869	-1105.72939	-948.89774	1
102	C	79.02261	78.99658	67.38008	-559.93427	-126.34590	542.30857	1
103	O	78.46587	79.79564	66.67266	-670.36003	-111.83166	76.36448	1
104	N	80.00404	78.14703	67.00957	-216.06729	-537.07037	446.51379	1
105	H	80.52089	77.45686	67.56673	-1251.96487	1074.12894	-2168.52500	1
106	H	80.39267	78.10050	66.06086	-2451.83023	-720.73851	944.84612	1
107	C	77.38666	77.49283	71.48699	546.24052	-563.88337	-85.11809	1
108	O	76.59306	77.50597	70.55320	71.70702	-307.40463	606.69673	1
109	N	77.12206	77.29263	72.77329	479.90863	-504.50129	222.86849	1
110	C	75.92022	76.61012	73.18111	75.51268	-600.91904	506.73700	1
111	H	75.75498	75.80415	72.42811	-2033.61562	1795.30103	254.89480	1
112	C	76.31550	76.14313	74.64797	523.79067	517.99274	284.45581	1
113	H	75.43364	75.86744	75.26989	1599.61665	-1127.00911	1895.98173	1
114	H	76.99294	75.26007	74.62359	-1881.83093	1275.82488	-1501.55016	1
115	C	77.05627	77.42266	75.14382	-600.05639	-404.05026	316.64485	1
116	H	76.33063	78.24408	75.35201	-2597.05260	496.36221	657.73249	1
117	H	77.65250	77.26707	76.07593	-1666.24518	1294.38985	-1723.90591	1
118	C	77.96139	77.74090	73.87700	493.57570	-129.95376	-602.56394	1
119	H	78.21652	78.81488	73.71900	-1469.08415	-637.84797	2204.22581	1
120	H	78.89333	77.13050	73.82575	-1038.97840	1068.88701	-2280.71789	1
121	C	74.72605	77.71374	73.20604	188.88100	241.05089	-727.87821	1
122	O	74.34468	78.22506	74.21975	531.88613	-49.19943	427.07960	1
123	N	74.24068	77.84996	71.94309	708.14833	26.93417	-179.73509	1
124	H	74.86740	77.51815	71.17622	-2232.69501	-1179.09831	1023.94816	1
125	C	73.24736	78.92953	71.71382	-738.32412	259.92548	104.42456	1
126	H	73.67505	79.77490	72.30157	2028.89123	1260.02983	1311.33324	1
127	C	73.17543	79.23345	70.23794	-258.65678	-345.52513	661.28459	1
128	H	72.83749	78.30950	69.71640	-1826.06090	-1801.46097	-918.64554	1
129	C	72.19136	80.34850	69.92260	-541.23400	531.92970	-218.41428	1
130	H	72.18424	80.59996	68.82721	1311.73218	-2219.18200	882.19023	1
131	H	71.13699	80.07377	70.20810	-1048.71298	1223.58118	-2196.97971	1
132	H	72.44747	81.29160	70.47831	419.06414	1903.92898	1903.44670	1
133	C	74.52794	79.62023	69.66440	-423.86431	152.66566	-648.55262	1
134	H	74.48743	79.75398	68.54890	105.68386	-2342.50080	1387.51238	1
135	H	74.90071	80.58663	70.10128	-1695.63603	-1484.73621	-1531.02793	1
136	H	75.31340	78.82525	69.88712	-1853.57121	-487.39031	1936.59343	1
137	C	71.79133	78.48334	72.32999	539.71428	-510.58232	267.58633	1
138	O	70.84824	79.23131	72.20898	-15.93758	-278.34085	-624.49402	1
139	N	71.75058	77.25399	72.94250	-676.81886	12.05292	276.17960	1
140	H	72.71578	76.93738	72.77297	-1694.44250	-373.84189	-2100.66098	1
141	C	71.37271	77.34502	74.35453	412.33078	-664.70360	108.35451	1
142	H	72.14265	78.01700	74.79702	1765.77476	1294.44366	1621.76594	1
143	C	69.94266	77.99211	74.32139	-179.66635	-721.95667	-264.73915	1
144	H	70.03611	79.10325	74.34102	-607.34922	2587.87032	-598.10018	1

145	H	69.50382	77.76058	73.32467	-359.69332	-1479.13954	-2259.74260	1
146	C	68.93092	77.55407	75.43420	-240.01076	616.02425	431.85322	1
147	H	68.97944	76.45923	75.63709	-1359.17131	782.54425	2227.99181	1
148	H	69.10712	78.08133	76.39765	-820.36667	85.81767	-2596.78715	1
149	C	67.55990	77.95293	74.75208	-513.07015	236.18570	-551.87280	1
150	H	67.63653	78.97894	74.32449	1816.11944	-1183.11722	-1650.94321	1
151	H	67.39473	77.26941	73.88620	-1800.04429	-1361.53473	1526.34643	1
152	C	66.32645	77.88370	75.67730	726.08972	-253.19732	-179.64713	1
153	H	66.02316	76.86085	75.97618	1224.27271	-456.51798	-2390.90304	1
154	H	66.34819	78.56287	76.55341	1206.40339	-1150.93514	-2154.90344	1
155	N	65.11893	78.39476	74.80900	329.70796	-633.68968	-155.67358	1
156	H	64.15662	78.31005	75.24740	1348.31305	1938.76845	1359.00643	1
157	H	65.13297	79.41853	74.53307	2096.92035	1446.54551	-966.48890	1
158	H	64.96805	77.92423	73.87024	-1197.07217	-2303.53719	827.28733	1
159	C	71.47195	75.85910	74.98020	-378.01186	-556.17301	-413.96481	1
160	O	72.30536	75.65163	75.85489	-409.44433	-307.55053	-453.30833	1
161	N	70.57044	75.05354	74.47067	-429.02477	524.70884	274.08502	1
162	H	69.87421	75.42993	73.78702	1706.34263	-1425.96036	1574.38926	1
163	C	70.60708	73.63974	74.58648	-45.25864	-626.22952	478.93267	1
164	H	69.89276	73.32730	73.79133	1988.63164	570.90773	1772.87287	1
165	C	72.08690	73.11976	74.36600	551.77128	-20.49526	-564.54996	1
166	H	72.49518	73.46223	73.38543	1434.61535	-1753.10253	1513.99471	1
167	H	72.77361	73.53129	75.14333	-714.67738	1819.09770	1898.36494	1
168	C	71.99187	71.55949	74.43603	446.99263	-555.77305	338.97221	1
169	H	71.61850	71.23650	75.43541	1953.68466	1892.25957	-161.67766	1
170	H	71.24791	71.18186	73.69921	-403.03785	2688.07032	-188.43591	1
171	C	73.41748	70.94730	74.13386	567.86262	335.74681	434.04421	1
172	H	73.75771	71.23975	73.11096	-1080.02275	1568.26081	-1948.78900	1
173	H	74.18302	71.34350	74.84029	-919.54108	2111.34692	1456.13463	1
174	C	73.28816	69.41108	74.26011	195.81897	173.33862	-745.11536	1
175	H	73.01386	69.05302	75.27260	1405.67949	-2301.21089	-390.08113	1
176	H	72.63037	68.94064	73.50223	-940.37328	-1118.32446	2299.72133	1
177	N	74.70105	68.79020	73.99675	319.26422	656.36007	-42.02424	1
178	H	74.75164	67.73151	74.04354	1961.03633	619.91968	1787.09422	1
179	H	75.14224	68.97808	73.04976	854.14343	-2156.80752	1429.08711	1
180	H	75.48153	69.06390	74.66206	1237.02905	-1378.50857	-1998.28500	1
181	C	70.14416	73.07429	76.06227	532.53319	-268.57236	517.55729	1
182	O	69.48157	72.07035	76.12505	266.16714	-290.73804	-558.88002	1
183	N	70.67400	73.79692	77.03694	-226.25352	640.49678	-270.32839	1
184	H	71.35459	74.56072	76.81081	2007.69063	-1035.27229	1523.50231	1
185	C	70.43113	73.37316	78.38328	-540.76542	-573.33303	49.50000	1
186	H	70.58061	72.27004	78.37822	-2374.20950	-1036.76023	843.75774	1
187	C	71.49248	74.17453	79.26223	-77.09082	666.87422	-415.84136	1
188	H	71.32204	75.27463	79.10138	-985.81834	617.19825	2463.91927	1
189	O	72.87003	73.93532	78.89927	293.29899	-391.65602	-477.80926	1
190	H	73.09778	74.78012	78.46340	2528.72714	-681.76262	-751.27122	1
191	C	71.10559	73.80298	80.73945	252.47363	-605.14473	440.05134	1
192	H	71.77639	74.30620	81.47414	-2052.65063	1456.49051	-1043.51830	1
193	H	70.05989	74.10645	80.98758	-2152.98800	-1661.97574	-161.70652	1
194	H	71.18391	72.70484	80.91699	-473.12726	-1584.27339	2165.61725	1
195	C	68.89145	73.73608	78.77686	360.36307	488.46713	505.10056	1
196	O	68.38904	73.19901	79.74053	-200.08817	-528.03552	-385.82850	1
197	N	68.37389	74.69524	78.00889	-597.54095	-226.44775	355.20479	1
198	H	68.94719	75.04081	77.24047	2179.23655	-1300.70981	-991.33835	1
199	C	67.04274	75.08749	78.28340	-687.68921	297.39807	-249.45179	1
200	H	66.78332	74.59177	79.25018	-349.16256	-2467.37713	-1101.72831	1
201	C	66.98611	76.69198	78.30787	672.47345	361.54328	-201.62880	1
202	H	67.38268	77.09206	77.34599	1541.41502	582.18425	2169.97026	1
203	H	65.92293	77.01589	78.38756	-2534.67717	60.25153	997.72295	1
204	C	67.79310	77.25450	79.48266	574.26774	-389.43119	-377.02542	1
205	C	67.17604	77.34864	80.76725	688.82679	-287.33580	-257.96133	1
206	H	66.14812	76.97616	80.92806	331.14182	1470.38163	2269.80013	1

207	C	69.13283	77.71199	79.28926	-383.52382	-675.04808	144.24917	1
208	H	69.62547	77.61452	78.30584	4.09847	1517.59662	2262.86397	1
209	C	67.89170	77.93546	81.80960	-134.76730	428.45285	-649.50303	1
210	H	67.41032	78.01904	82.79974	-903.23433	1600.49020	2011.53387	1
211	C	69.80453	78.29954	80.36349	-335.53281	-615.00040	-364.39058	1
212	H	70.83147	78.66938	80.19742	1596.45398	-1369.33862	1732.02659	1
213	C	69.21505	78.44197	81.65410	585.48547	-340.24194	-406.23938	1
214	O	69.88682	79.04196	82.75057	-419.15649	-173.04408	-511.94141	1
215	H	70.72605	79.30882	82.30646	-1071.84350	1559.71507	-1960.13012	1
216	C	66.02527	74.70155	77.06158	291.41878	-183.13091	710.72246	1
217	O	64.85141	74.58105	77.32976	379.87695	523.47396	-222.23622	1
218	N	66.61573	74.74036	75.88695	564.30591	373.09380	277.24371	1
219	H	67.63679	74.85603	75.77743	-120.59931	-2436.07824	-1214.35098	1
220	C	65.91923	74.39970	74.66494	404.07514	-299.37480	608.84009	1
221	H	65.91325	73.28787	74.71756	-1071.07882	-841.69025	2359.66467	1
222	C	64.45659	74.99275	74.59486	-683.12807	68.71770	-390.13096	1
223	H	63.96193	74.95468	75.60606	2068.88918	1596.58590	770.89603	1
224	H	64.49460	76.06942	74.31776	1379.86429	2342.49779	-179.85638	1
225	C	63.60568	74.18763	73.56137	-176.39967	537.49466	550.97268	1
226	H	64.12451	74.08036	72.58271	-396.28051	1942.22168	1869.33314	1
227	H	63.41462	73.14938	73.91311	-94.44700	586.00678	-2659.20016	1
228	C	62.25035	75.02026	73.41715	-291.69381	-718.18079	-150.72929	1
229	H	61.60920	75.05674	74.33458	-2303.38776	1089.76242	964.62032	1
230	H	62.37315	76.07130	73.05009	884.16729	2568.80533	-207.74283	1
231	N	61.54469	74.31480	72.43344	-594.49522	-252.81478	342.29276	1
232	H	62.00115	73.50862	72.03591	-1735.17426	2084.05705	-263.71605	1
233	C	60.38454	74.62855	72.01936	595.23177	-271.52487	442.22352	1
234	N	59.77489	75.75324	72.58705	585.53813	-424.79750	-105.81303	1
235	H	60.12088	76.38011	73.31241	959.88797	1327.56823	-2177.11905	1
236	H	58.84703	76.10049	72.34280	1578.48647	16.27378	-2220.76233	1
237	N	59.94174	73.73781	71.03165	-452.17763	-390.33541	-421.51853	1
238	H	60.38738	72.91972	70.61887	470.26107	1974.25629	-1817.92087	1
239	H	59.03337	73.82103	70.57340	1856.67307	-1573.97321	-1224.35416	1
240	C	66.97523	74.98852	73.60321	-531.47271	-581.45780	-55.06206	1
241	O	68.14923	75.11472	73.98632	-243.00837	192.73507	609.52485	1
242	N	66.45658	75.32436	72.44140	343.49288	-644.25607	38.09164	1
243	H	65.45462	75.17230	72.32411	-1691.16043	-1535.97525	-1484.73099	1
244	C	67.26776	75.37225	71.26643	542.66492	350.14337	454.42563	1
245	H	66.52291	75.60426	70.47350	1209.57979	-2396.95920	463.86744	1
246	C	68.34594	76.52399	71.43785	-737.14309	145.93010	242.71942	1
247	H	68.93514	76.34130	72.36396	-1050.18303	159.36419	-2509.06125	1
248	C	69.29178	76.70883	70.20196	-706.77696	-252.88343	-245.16230	1
249	H	70.00926	77.54723	70.37203	-1624.64039	-1665.49085	1417.86935	1
250	H	69.90094	75.79876	69.98983	2566.10521	598.51109	693.22305	1
251	H	68.71649	76.94287	69.27600	-1972.69758	107.10018	-1876.34312	1
252	C	67.58208	77.89234	71.51024	412.85148	672.58832	-27.69222	1
253	H	68.27076	78.73350	71.76237	1447.02277	1762.76533	-1490.78944	1
254	H	67.09872	78.14147	70.53708	1320.77379	-145.20455	2378.68491	1
255	H	66.77442	77.87461	72.27808	-1512.10848	1470.52031	1724.75147	1
256	C	67.83230	73.84576	71.10548	-607.11113	499.56689	73.73769	1
257	O	67.02153	72.95695	70.94990	357.97126	460.81534	356.68785	1
258	N	69.14719	73.78453	71.09344	536.55407	-368.62270	332.76306	1
259	H	69.74974	74.60254	71.26779	524.38866	2297.69985	1367.20941	1
260	C	69.81668	72.51615	71.20086	46.50277	-774.29190	-147.97904	1
261	H	69.39286	72.03261	72.10822	1676.51875	1883.29066	1032.55549	1
262	C	69.59654	71.60417	69.88801	-559.41456	-34.19198	-556.30433	1
263	H	69.35725	72.26135	69.01839	-64.66664	395.18769	2695.05373	1
264	H	70.53947	71.06917	69.62172	-2703.44278	-60.40056	333.79418	1
265	C	68.49466	70.61099	70.13047	-519.76435	377.31045	459.42366	1
266	H	67.56994	71.18321	70.44892	-1746.74323	1667.50644	-1261.73691	1
267	C	68.18402	69.84907	68.84790	570.95554	16.46261	-545.27700	1
268	H	67.34258	69.12299	68.99097	2391.58273	28.05277	-1305.07271	1

269	H	67.88877	70.54003	68.01659	175.75588	917.63458	2559.43867	1
270	H	69.07038	69.26260	68.49277	-1063.97851	-2155.34650	1283.00462	1
271	C	68.85953	69.61882	71.22604	193.76014	2.62946	-765.53141	1
272	H	68.06571	68.83828	71.35398	507.39394	-846.55087	2539.60089	1
273	H	69.81684	69.08387	70.99662	1337.57841	1818.19054	1526.01994	1
274	H	68.98914	70.11893	72.21994	1100.88635	-1172.91350	-2199.08909	1
275	C	71.33018	72.98479	71.33800	-549.21115	475.64486	-309.38218	1
276	O	71.61324	74.16397	71.39673	556.06106	-390.37755	-78.24250	1
277	O	72.33748	72.00157	71.42234	-572.27940	-310.19032	-209.75862	1
278	H	71.76226	71.18617	71.34912	-1380.08193	2212.14486	790.85944	1

Listing 41: C00041.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.7837	0.0000	300.0000
3	H	72.71198	65.91386	64.16711	-2043.14101	-1757.64893	399.89339		1
4	N	73.60896	65.85551	64.64405	426.75047	490.45733	-334.42467		1
5	H	73.35058	66.04976	65.60924	442.25559	-1110.30854	-2448.52907		1
6	C	74.62171	66.68077	64.11745	415.32972	-666.39213	83.73172		1
7	H	74.45128	66.65369	63.02074	879.32219	2491.00447	667.35213		1
8	C	74.45543	68.16569	64.71505	31.35357	477.41777	628.23362		1
9	H	74.55820	68.13076	65.82741	1168.38489	2240.25337	-1019.71136		1
10	H	75.29152	68.81099	64.35246	-360.43770	2534.90498	931.67112		1
11	C	73.12189	68.74903	64.32009	463.18208	512.70242	-382.34388		1
12	H	72.31925	68.03524	64.61074	1725.29117	1863.52247	-987.07854		1
13	C	72.87695	70.06301	65.05112	710.42801	-144.27427	-313.15367		1
14	H	71.88321	70.50610	64.78181	364.20195	-1033.13725	2494.72524		1
15	H	72.89165	69.92828	66.16359	2567.61904	335.80679	847.48802		1
16	H	73.65799	70.82569	64.79815	-2587.99029	680.92867	-512.16411		1
17	C	73.04140	68.98472	62.81804	268.17616	741.64379	-40.42634		1
18	H	72.06950	69.46017	62.52565	1283.54314	-1945.37420	-1411.27812		1
19	H	73.86085	69.66220	62.46369	-1258.57796	1317.15249	-2026.02085		1
20	H	73.12816	68.02928	62.23957	-2502.84526	909.80597	575.92391		1
21	C	76.10806	66.15996	64.52750	619.36578	-458.64843	-172.09273		1
22	O	77.06634	66.84759	64.19953	-81.40433	433.87611	522.34594		1
23	N	76.08594	65.01418	65.17989	175.23996	-622.20190	341.55523		1
24	H	75.13578	64.66800	65.31052	-876.57256	-303.22879	-2561.90213		1
25	C	77.18226	64.18303	65.53632	-571.88214	-534.10783	-106.15033		1
26	H	76.72386	63.17120	65.47710	-2713.20841	-16.25800	-248.80809		1
27	C	78.39827	64.34289	64.51446	166.60354	288.16399	-716.09568		1
28	H	78.72831	65.41968	64.47711	-2097.85574	1636.78449	-586.18044		1
29	O	78.10161	64.00119	63.14377	-317.80580	-363.38227	484.43082		1
30	H	78.07087	64.89372	62.74228	1863.74748	-1451.84923	1357.29467		1
31	C	79.50083	63.47496	65.22322	503.80731	517.99032	318.51606		1
32	H	80.48191	63.55359	64.70018	640.61020	-2157.10410	-1536.29104		1
33	H	79.66009	63.78594	66.28241	1687.88455	465.60692	2087.56452		1
34	H	79.21834	62.39660	65.23720	-1293.07895	-1899.88581	-1463.57452		1
35	C	77.50601	64.40311	67.12977	-153.07550	-733.68902	248.70981		1
36	O	77.38427	63.40168	67.78671	186.15459	-480.78787	-449.34387		1
37	N	77.94955	65.60625	67.51674	-487.53139	543.18517	42.03850		1
38	C	77.71907	66.07920	68.85064	-699.35871	69.34393	360.10701		1
39	H	77.73789	65.20469	69.54092	2.81126	-221.99807	-2715.58072		1
40	C	78.89402	67.14049	69.01931	-507.46439	-592.59194	122.07761		1
41	H	78.70480	67.87247	69.83805	-1975.08116	525.87560	-1801.71556		1
42	H	79.86535	66.64790	69.24804	1588.27743	-1913.22100	1113.83566		1
43	C	78.89996	67.78732	67.60095	-613.62442	-457.55993	-194.14490		1
44	H	78.03121	68.47726	67.48154	1707.54637	-721.27992	1996.92523		1
45	H	79.81896	68.37506	67.37680	758.23357	2100.81767	1560.55011		1
46	C	78.73156	66.50442	66.68009	-352.41524	704.96076	49.21465		1
47	H	78.13103	66.67092	65.72710	1714.76886	-2070.42778	443.35792		1
48	H	79.68054	65.96967	66.43793	1224.15040	1801.50881	1636.97633		1

49	C	76.30413	66.89123	68.85240	566.85117	537.05831	117.62814	1
50	O	75.96297	67.60632	67.91338	-550.26779	-406.08867	4.21666	1
51	N	75.70964	66.71307	70.00837	566.34832	-425.77725	180.18749	1
52	H	76.15722	66.10907	70.69323	644.44502	2646.80550	-52.73430	1
53	C	74.40549	67.27199	70.20443	612.34801	-281.48662	411.56221	1
54	H	73.99223	67.22973	69.16973	1667.23498	-1490.75142	1556.16753	1
55	C	73.63440	66.37270	71.27641	-714.45746	-175.43074	286.98927	1
56	H	74.11206	66.52466	72.28192	-787.09484	1763.03619	-1922.46060	1
57	O	73.64621	64.95805	71.01656	-429.46514	516.51932	-128.40526	1
58	H	74.10858	64.62110	71.80918	1981.82785	436.16847	-1818.18182	1
59	C	72.21048	67.04138	71.27020	630.79189	-468.94448	76.03230	1
60	H	71.53658	66.56775	72.02096	-1775.71861	2062.30353	131.89849	1
61	H	72.26132	68.13078	71.50896	-1855.14608	88.94118	1993.53760	1
62	H	71.71801	66.93945	70.27534	-1504.82350	-780.94249	-2132.90992	1
63	C	74.61910	68.80994	70.70443	288.57638	618.62814	-397.00270	1
64	O	74.26750	69.17622	71.81896	321.70495	-185.26452	574.37218	1
65	N	75.08813	69.47978	69.68916	-447.05792	-446.53431	367.76425	1
66	H	75.28090	68.95399	68.80185	350.31316	1975.63644	-1843.31522	1
67	C	75.72353	70.75538	69.80824	-511.23061	374.03917	-471.51480	1
68	H	75.86806	71.04392	68.73990	2234.79579	-898.70890	-1273.45190	1
69	C	74.69930	71.74763	70.56218	529.53781	-159.34528	563.72604	1
70	H	74.90704	72.80053	70.22366	654.59388	2347.94251	1217.51488	1
71	H	73.68610	71.47532	70.16222	-1526.55661	2103.42026	817.87394	1
72	O	74.71248	71.74867	71.98482	-554.84278	14.12789	399.58769	1
73	H	74.48995	70.74895	72.15120	1297.06236	2061.84854	1220.68812	1
74	C	77.11791	70.63974	70.56963	-662.15484	-412.13544	123.62687	1
75	O	77.52160	69.71851	71.38578	-540.01537	-317.05804	274.91456	1
76	N	77.84053	71.67721	70.28542	-202.76299	-690.00100	-131.49145	1
77	H	77.45369	72.32941	69.60992	-702.62132	-2617.37191	281.70413	1
78	C	79.23124	71.48992	70.60734	-491.73914	576.34187	222.73509	1
79	H	79.63310	70.98472	69.70513	1977.17978	-1823.58850	-434.68928	1
80	C	79.85833	72.91287	70.81272	-649.50797	-328.66843	306.11224	1
81	H	79.19181	73.53253	71.45165	2075.07803	1452.16490	-1004.45904	1
82	C	81.27666	72.76155	71.47103	-615.18735	-489.99689	-70.96352	1
83	H	81.75628	73.75274	71.64639	-1226.32661	-1724.38906	-1716.47170	1
84	H	81.20900	72.24345	72.45699	2381.64273	-969.84735	900.46860	1
85	H	81.96645	72.16471	70.83039	2122.74991	1702.23946	-141.36228	1
86	C	80.05493	73.58780	69.40658	-501.86074	-479.61276	-376.42482	1
87	H	80.47471	74.61609	69.49983	993.79261	-2246.95401	-1177.81305	1
88	H	80.75324	73.00135	68.76554	42.71279	-626.15391	-2651.37258	1
89	H	79.09055	73.67204	68.85415	-2026.39012	-1590.33709	-887.82922	1
90	C	79.20977	70.44164	71.91925	-672.89153	382.57394	-156.34072	1
91	O	80.04738	69.57528	72.04134	410.04627	221.86223	500.35950	1
92	N	78.95640	71.37971	73.00339	-378.11782	-443.79414	-441.10984	1
93	H	78.09960	71.92714	72.87456	2404.15973	-568.14894	1149.30085	1
94	C	79.00717	70.76035	74.29972	-544.54484	466.16019	331.29119	1
95	H	79.72680	69.91313	74.24417	-1409.80988	-170.17955	2325.32679	1
96	C	79.38859	71.90494	75.33296	-184.48284	116.78282	-758.89137	1
97	H	80.40065	72.32338	75.13285	1893.78641	1861.14652	611.04528	1
98	H	78.67831	72.75614	75.22839	-2170.79665	-974.19311	1327.50117	1
99	C	79.29146	71.28011	76.75898	389.51668	672.81878	-138.49152	1
100	H	78.43029	70.57813	76.81476	510.64577	1933.03327	1851.02484	1
101	H	80.18213	70.64541	76.96048	-2302.30869	-1105.72939	-948.89774	1
102	C	79.10607	72.35194	77.89996	-559.93427	-126.34590	542.30857	1
103	O	78.63807	72.00996	78.95773	-670.36003	-111.83166	76.36448	1
104	N	79.51720	73.59015	77.55955	-216.06729	-537.07037	446.51379	1
105	H	79.98537	73.88940	76.69581	-1251.96487	1074.12894	-2168.52500	1
106	H	79.55501	74.38444	78.20798	-2451.83023	-720.73851	944.84612	1
107	C	77.49108	70.37738	74.71831	546.24052	-563.88337	-85.11809	1
108	O	76.67560	71.28510	74.78388	71.70702	-307.40463	606.69673	1
109	N	77.37840	69.11261	75.10384	479.90863	-504.50129	222.86849	1
110	C	76.10100	68.47084	75.27699	75.51268	-600.91904	506.73700	1

111	H	75.45859	68.86486	74.45426	-2033.61562	1795.30103	254.89480	1
112	C	76.47959	66.93196	75.18211	523.79067	517.99274	284.45581	1
113	H	75.73095	66.27684	75.68218	1599.61665	-1127.00911	1895.98173	1
114	H	76.55611	66.59099	74.12526	-1881.83093	1275.82488	-1501.55016	1
115	C	77.87292	66.92028	75.88466	-600.05639	-404.05026	316.64485	1
116	H	77.76516	67.01461	76.98864	-2597.05260	496.36221	657.73249	1
117	H	78.46473	65.99605	75.69779	-1666.24518	1294.38985	-1723.90591	1
118	C	78.52509	68.22249	75.25053	493.57570	-129.95376	-602.56394	1
119	H	79.29402	68.72593	75.88231	-1469.08415	-637.84797	2204.22581	1
120	H	78.92653	68.07962	74.21855	-1038.97840	1068.88701	-2280.71789	1
121	C	75.49265	68.77774	76.75258	188.88100	241.05089	-727.87821	1
122	O	74.98589	67.90197	77.39551	531.88613	-49.19943	427.07960	1
123	N	75.67406	70.06984	77.07364	708.14833	26.93417	-179.73509	1
124	H	76.00963	70.69510	76.29993	-2232.69501	-1179.09831	1023.94816	1
125	C	74.87322	70.67973	78.14855	-738.32412	259.92548	104.42456	1
126	H	73.90378	70.13090	78.14099	2028.89123	1260.02983	1311.33324	1
127	C	75.61752	70.57447	79.46135	-258.65678	-345.52513	661.28459	1
128	H	76.68564	70.85196	79.28924	-1826.06090	-1801.46097	-918.64554	1
129	C	75.04789	71.52345	80.49726	-541.23400	531.92970	-218.41428	1
130	H	75.56070	71.40743	81.49144	1311.73218	-2219.18200	882.19023	1
131	H	75.16743	72.62705	80.18237	-1048.71298	1223.58118	-2196.97971	1
132	H	73.95048	71.34251	80.66555	419.06414	1903.92898	1903.44670	1
133	C	75.59909	69.15888	80.01197	-423.86431	152.66566	-648.55262	1
134	H	76.12887	69.08730	81.00154	105.68386	-2342.50080	1387.51238	1
135	H	74.54784	68.78900	80.16656	-1695.63603	-1484.73621	-1531.02793	1
136	H	76.10184	68.43746	79.30853	-1853.57121	-487.39031	1936.59343	1
137	C	74.76332	72.25984	77.65815	539.71428	-510.58232	267.58633	1
138	O	73.69333	72.71855	77.33439	-15.93758	-278.34085	-624.49402	1
139	N	75.95842	72.81910	77.64405	-676.81886	12.05292	276.17960	1
140	H	76.75500	72.24783	77.92842	-1694.44250	-373.84189	-2100.66098	1
141	C	76.13603	74.20901	77.40575	412.33078	-664.70360	108.35451	1
142	H	77.21948	74.29420	77.16142	1765.77476	1294.44366	1621.76594	1
143	C	75.17414	74.56893	76.19549	-179.66635	-721.95667	-264.73915	1
144	H	75.22806	73.75844	75.43138	-607.34922	2587.87032	-598.10018	1
145	H	74.10361	74.60026	76.52651	-359.69332	-1479.13954	-2259.74260	1
146	C	75.59543	75.94428	75.58047	-240.01076	616.02425	431.85322	1
147	H	75.22971	76.78404	76.22047	-1359.17131	782.54425	2227.99181	1
148	H	76.70475	76.03444	75.53691	-820.36667	85.81767	-2596.78715	1
149	C	74.98428	76.06272	74.12873	-513.07015	236.18570	-551.87280	1
150	H	75.33166	75.22930	73.47492	1816.11944	-1183.11722	-1650.94321	1
151	H	73.87252	75.98721	74.15445	-1800.04429	-1361.53473	1526.34643	1
152	C	75.43502	77.43736	73.57295	726.08972	-253.19732	-179.64713	1
153	H	74.99605	78.30980	74.09887	1224.27271	-456.51798	-2390.90304	1
154	H	76.53292	77.56438	73.47971	1206.40339	-1150.93514	-2154.90344	1
155	N	74.89328	77.54230	72.11893	329.70796	-633.68968	-155.67358	1
156	H	75.11308	78.45427	71.61843	1348.31305	1938.76845	1359.00643	1
157	H	75.27067	76.83803	71.41870	2096.92035	1446.54551	-966.48890	1
158	H	73.81519	77.45429	72.02864	-1197.07217	-2303.53719	827.28733	1
159	C	75.76567	75.00816	78.78491	-378.01186	-556.17301	-413.96481	1
160	O	75.38416	74.48274	79.81347	-409.44433	-307.55053	-453.30833	1
161	N	76.07136	76.28255	78.57461	-429.02477	524.70884	274.08502	1
162	H	76.38475	76.50972	77.63415	1706.34263	-1425.96036	1574.38926	1
163	C	75.44137	77.27501	79.38568	-45.25864	-626.22952	478.93267	1
164	H	75.44264	76.86811	80.42221	1988.63164	570.90773	1772.87287	1
165	C	76.29149	78.58451	79.15617	551.77128	-20.49526	-564.54996	1
166	H	77.37930	78.34947	79.17566	1434.61535	-1753.10253	1513.99471	1
167	H	76.09356	78.99735	78.14095	-714.67738	1819.09770	1898.36494	1
168	C	75.93629	79.64407	80.25224	446.99263	-555.77305	338.97221	1
169	H	74.84488	79.88470	80.25162	1953.68466	1892.25957	-161.67766	1
170	H	76.18200	79.26992	81.27167	-403.03785	2688.07032	-188.43591	1
171	C	76.79236	80.91916	79.87779	567.86262	335.74681	434.04421	1
172	H	77.86286	80.64827	79.72743	-1080.02275	1568.26081	-1948.78900	1

173	H	76.44580	81.34409	78.90497	-919.54108	2111.34692	1456.13463	1
174	C	76.65429	81.97217	81.00157	195.81897	173.33862	-745.11536	1
175	H	75.61253	82.29098	81.20425	1405.67949	-2301.21089	-390.08113	1
176	H	77.16793	81.71644	81.95043	-940.37328	-1118.32446	2299.72133	1
177	N	77.38061	83.25083	80.46455	319.26422	656.36007	-42.02424	1
178	H	77.40924	84.10493	81.09344	1961.03633	619.91968	1787.09422	1
179	H	78.40207	83.15315	80.19426	854.14343	-2156.80752	1429.08711	1
180	H	76.95739	83.65167	79.57752	1237.02905	-1378.50857	-1998.28500	1
181	C	73.92836	77.55491	78.80229	532.53319	-268.57236	517.55729	1
182	O	73.63380	77.45199	77.63495	266.16714	-290.73804	-558.88002	1
183	N	73.19331	77.97738	79.82241	-226.25352	640.49678	-270.32839	1
184	H	73.64488	78.04873	80.73210	2007.69063	-1035.27229	1523.50231	1
185	C	71.90686	78.54016	79.57578	-540.76542	-573.33303	49.50000	1
186	H	71.44730	77.92572	78.76903	-2374.20950	-1036.76023	843.75774	1
187	C	71.13412	78.53864	80.97665	-77.09082	666.87422	-415.84136	1
188	H	71.75787	79.11326	81.71548	-985.81834	617.19825	2463.91927	1
189	O	70.91248	77.24588	81.56866	293.29899	-391.65602	-477.80926	1
190	H	71.45453	77.31146	77.37982	2528.72714	-681.76262	-751.27122	1
191	C	69.83781	79.36767	80.65051	252.47363	-605.14473	440.05134	1
192	H	69.23342	79.55964	81.56700	-2052.65063	1456.49051	-1043.51830	1
193	H	70.08068	80.35858	80.20099	-2152.98800	-1661.97574	-161.70652	1
194	H	69.18205	78.82843	79.92866	-473.12726	-1584.27339	2165.61725	1
195	C	72.12683	80.09821	79.14269	360.36307	488.46713	505.10056	1
196	O	72.89300	80.83505	79.76134	-200.08817	-528.03552	-385.82850	1
197	N	71.24234	80.38817	78.21828	-597.54095	-226.44775	355.20479	1
198	H	70.67178	79.61359	77.88479	2179.23655	-1300.70981	-991.33835	1
199	C	71.36195	81.57866	77.43371	-687.68921	297.39807	-249.45179	1
200	H	72.44687	81.64804	77.19607	-349.16256	-2467.37713	-1101.72831	1
201	C	70.36502	81.48492	76.19521	672.47345	361.54328	-201.62880	1
202	H	69.34323	81.22671	76.55663	1541.41502	582.18425	2169.97026	1
203	H	70.28961	82.49212	75.72071	-2534.67717	60.25153	997.72295	1
204	C	70.84709	80.43825	75.17079	574.26774	-389.43119	-377.02542	1
205	C	71.85311	80.79741	74.22898	688.82679	-287.33580	-257.96133	1
206	H	72.31482	81.80046	74.25030	331.14182	1470.38163	2269.80013	1
207	C	70.26965	79.13627	75.15500	-383.52382	-675.04808	144.24917	1
208	H	69.49964	78.85136	75.89323	4.09847	1517.59662	2262.86397	1
209	C	72.23283	79.84933	73.26448	-134.76730	428.45285	-649.50303	1
210	H	73.00707	80.12407	72.52535	-903.23433	1600.49020	2011.53387	1
211	C	70.69000	78.22544	74.16883	-335.53281	-615.00040	-364.39058	1
212	H	70.23587	77.21784	74.15476	1596.45398	-1369.33862	1732.02659	1
213	C	71.66437	78.55414	73.19556	585.48547	-340.24194	-406.23938	1
214	O	72.08853	77.61165	72.14487	-419.15649	-173.04408	-511.94141	1
215	H	71.59526	76.82993	72.45798	-1071.84350	1559.71507	-1960.13012	1
216	C	70.80585	82.87017	78.24304	291.41878	-183.13091	710.72246	1
217	O	69.89406	83.51637	77.78216	379.87695	523.47396	-222.23622	1
218	N	71.53802	83.12056	79.33669	564.30591	373.09380	277.24371	1
219	H	72.28072	82.42973	79.63091	-120.59931	-2436.07824	-1214.35098	1
220	C	70.87664	83.93573	80.32089	404.07514	-299.37480	608.84009	1
221	H	70.27136	84.64338	79.70742	-1071.07882	-841.69025	2359.66467	1
222	C	69.93326	82.97944	81.16506	-683.12807	68.71770	-390.13096	1
223	H	69.30055	82.35737	80.49293	2068.88918	1596.58590	770.89603	1
224	H	70.53512	82.26058	81.76510	1379.86429	2342.49779	-179.85638	1
225	C	69.05393	83.88224	82.08367	-176.39967	537.49466	550.97268	1
226	H	69.70601	84.54044	82.71619	-396.28051	1942.22168	1869.33314	1
227	H	68.42852	84.57418	81.47561	-94.44700	586.00678	-2659.20016	1
228	C	68.13762	82.94638	82.99711	-291.69381	-718.18079	-150.72929	1
229	H	67.32105	82.39061	82.46955	-2303.38776	1089.76242	964.62032	1
230	H	68.68301	82.22326	83.65566	884.16729	2568.80533	-207.74283	1
231	N	67.55484	83.92567	83.81905	-594.49522	-252.81478	342.29276	1
232	H	67.84869	84.87889	83.66903	-1735.17426	2084.05705	-263.71605	1
233	C	66.70069	83.69627	84.73289	595.23177	-271.52487	442.22352	1
234	N	66.30122	82.37130	84.93440	585.53813	-424.79750	-105.81303	1

235	H	66.59786	81.52676	84.44694	959.88797	1327.56823	-2177.11905	1
236	H	65.62613	82.06331	85.63501	1578.48647	16.27378	-2220.76233	1
237	N	66.32582	84.88540	85.37404	-452.17763	-390.33541	-421.51853	1
238	H	66.63173	85.84631	85.22817	470.26107	1974.25629	-1817.92087	1
239	H	65.65799	84.92031	86.14492	1856.67307	-1573.97321	-1224.35416	1
240	C	71.96969	84.66163	81.27189	-531.47271	-581.45780	-55.06206	1
241	O	71.63772	85.14314	82.33705	-243.00837	192.73507	609.52485	1
242	N	73.19737	84.66185	80.73595	343.49288	-644.25607	38.09164	1
243	H	73.26383	84.25455	79.80232	-1691.16043	-1535.97525	-1484.73099	1
244	C	74.02635	85.76759	81.12714	542.66492	350.14337	454.42563	1
245	H	73.34126	86.49143	81.62545	1209.57979	-2396.95920	463.86744	1
246	C	75.11043	85.17004	82.12317	-737.14309	145.93010	242.71942	1
247	H	75.47214	84.19084	81.74812	-1050.18303	159.36419	-2509.06125	1
248	C	76.29558	86.18155	82.28571	-706.77696	-252.88343	-245.16230	1
249	H	77.04838	85.81844	83.02409	-1624.64039	-1665.49085	1417.86935	1
250	H	76.82828	86.34207	81.31892	2566.10521	598.51109	693.22305	1
251	H	75.93773	87.17829	82.63501	-1972.69758	107.10018	-1876.34312	1
252	C	74.42896	85.00152	83.52409	412.85148	672.58832	-27.69222	1
253	H	75.10143	84.49313	84.25435	1447.02277	1762.76533	-1490.78944	1
254	H	74.14398	85.98718	83.96128	1320.77379	-145.20455	2378.68491	1
255	H	73.49256	84.39606	83.44476	-1512.10848	1470.52031	1724.75147	1
256	C	74.74951	86.33057	79.77630	-607.11113	499.56689	73.73769	1
257	O	74.75743	87.51417	79.54537	357.97126	460.81534	356.68785	1
258	N	75.35646	85.33756	79.13276	536.55407	-368.62270	332.76306	1
259	H	75.23233	84.35280	79.42328	524.38866	2297.69985	1367.20941	1
260	C	75.80731	85.55496	77.79222	46.50277	-774.29190	-147.97904	1
261	H	75.12852	86.31156	77.34002	1676.51875	1883.29066	1032.55549	1
262	C	77.35149	86.03308	77.77458	-559.41456	-34.19198	-556.30433	1
263	H	77.97140	85.29421	78.33485	-64.66664	395.18769	2695.05373	1
264	H	77.74265	86.03120	76.72963	-2703.44278	-60.40056	333.79418	1
265	C	77.49289	87.39865	78.38556	-519.76435	377.31045	459.42366	1
266	H	77.03391	87.38113	79.40159	-1746.74323	1667.50644	-1261.73691	1
267	C	78.96501	87.76852	78.52452	570.95554	16.46261	-545.27700	1
268	H	79.09451	88.77838	78.99191	2391.58273	28.05277	-1305.07271	1
269	H	79.51838	87.03325	79.16327	175.75588	917.63458	2559.43867	1
270	H	79.47833	87.79598	77.52933	-1063.97851	-2155.34650	1283.00462	1
271	C	76.77402	88.45735	77.55973	193.76014	2.62946	-765.53141	1
272	H	76.99081	89.49072	77.93432	507.39394	-846.55087	2539.60089	1
273	H	77.07665	88.42226	76.48151	1337.57841	1818.19054	1526.01994	1
274	H	75.66062	88.31997	77.60637	1100.88635	-1172.91350	-2199.08909	1
275	C	75.68600	84.06886	77.22397	-549.21115	475.64486	-309.38218	1
276	O	75.40572	83.15250	77.97202	556.06106	-390.37755	-78.24250	1
277	O	75.96161	83.83529	75.86793	-572.27940	-310.19032	-209.75862	1
278	H	76.15301	84.77823	75.58271	-1380.08193	2212.14486	790.85944	1

Listing 42: C00042.xmolout

1		276								
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100	
		0.2500	300.00	0.00	0.00	0.00	-1293.7837	0.0000	300.0000	
3	H	80.35535	77.07638	75.71892	-2043.14101	-1757.64893	399.89339		1	
4	N	80.21278	78.08263	75.65226	426.75047	490.45733	-334.42467		1	
5	H	79.46964	78.14117	74.95902	442.25559	-1110.30854	-2448.52907		1	
6	C	81.36687	78.84714	75.38252	415.32972	-666.39213	83.73172		1	
7	H	82.11386	78.44032	76.09563	879.32219	2491.00447	667.35213		1	
8	C	81.83344	78.67083	73.85281	31.35357	477.41777	628.23362		1	
9	H	80.99527	78.94382	73.16735	1168.38489	2240.25337	-1019.71136		1	
10	H	82.65371	79.39730	73.63562	-360.43770	2534.90498	931.67112		1	
11	C	82.29608	77.26173	73.58656	463.18208	512.70242	-382.34388		1	
12	H	81.44036	76.57259	73.75876	1725.29117	1863.52247	-987.07854		1	
13	C	82.75561	77.12601	72.13945	710.42801	-144.27427	-313.15367		1	
14	H	83.14485	76.09755	71.92713	364.20195	-1033.13725	2494.72524		1	

15	H	81.92274	77.32658	71.41750	2567.61904	335.80679	847.48802	1
16	H	83.58167	77.84463	71.90088	-2587.99029	680.92867	-512.16411	1
17	C	83.44115	76.85209	74.50303	268.17616	741.64379	-40.42634	1
18	H	83.83198	75.83395	74.24495	1283.54314	-1945.37420	-1411.27812	1
19	H	84.30211	77.56582	74.42880	-1258.57796	1317.15249	-2026.02085	1
20	H	83.12709	76.82024	75.57764	-2502.84526	909.80597	575.92391	1
21	C	81.02553	80.41176	75.64625	619.36578	-458.64843	-172.09273	1
22	O	81.54218	81.28769	74.98627	-81.40433	433.87611	522.34594	1
23	N	80.20577	80.54397	76.68986	175.23996	-622.20190	341.55523	1
24	H	79.90510	79.69330	77.16314	-876.57256	-303.22879	-2561.90213	1
25	C	79.80644	81.85978	77.07061	-571.88214	-534.10783	-106.15033	1
26	H	80.00577	82.49482	76.17464	-2713.20841	-16.25800	-248.80809	1
27	C	78.26054	81.72829	77.49462	166.60354	288.16399	-716.09568	1
28	H	78.18627	80.91037	78.26667	-2097.85574	1636.78449	-586.18044	1
29	O	77.35907	81.33898	76.44599	-317.80580	-363.38227	484.43082	1
30	H	77.07204	80.45815	76.76189	1863.74748	-1451.84923	1357.29467	1
31	C	77.96582	83.11548	78.17155	503.80731	517.99032	318.51606	1
32	H	76.96581	83.12553	78.66354	640.61020	-2157.10410	-1536.29104	1
33	H	78.72292	83.37326	78.95137	1687.88455	465.60692	2087.56452	1
34	H	77.96682	83.94072	77.42277	-1293.07895	-1899.88581	-1463.57452	1
35	C	80.67727	82.26325	78.36814	-153.07550	-733.68902	248.70981	1
36	O	80.64813	81.55036	79.37192	186.15459	-480.78787	-449.34387	1
37	N	81.22491	83.46080	78.22468	-487.53139	543.18517	42.03850	1
38	C	82.06744	83.99564	79.26496	-699.35871	69.34393	360.10701	1
39	H	82.84243	83.23040	79.49022	2.81126	-221.99807	-2715.58072	1
40	C	82.59622	85.34142	78.62473	-507.46439	-592.59194	122.07761	1
41	H	82.90469	86.09112	79.38832	-1975.08116	525.87560	-1801.71556	1
42	H	83.47805	85.17055	77.96759	1588.27743	-1913.22100	1113.83566	1
43	C	81.34213	85.77500	77.80257	-613.62442	-457.55993	-194.14490	1
44	H	80.53513	86.13593	78.48332	1707.54637	-721.27992	1996.92523	1
45	H	81.54157	86.58466	77.06513	758.23357	2100.81767	1560.55011	1
46	C	80.94766	84.38978	77.13437	-352.41524	704.96076	49.21465	1
47	H	79.88069	84.29802	76.82891	1714.76886	-2070.42778	443.35792	1
48	H	81.60895	84.07877	76.29070	1224.15040	1801.50881	1636.97633	1
49	C	81.07811	84.29756	80.54328	566.85117	537.05831	117.62814	1
50	O	80.10728	85.00490	80.42514	-550.26779	-406.08867	4.21666	1
51	N	81.57675	83.68505	81.60615	566.34832	-425.77725	180.18749	1
52	H	82.43766	83.15177	81.48523	644.44502	2646.80550	-52.73430	1
53	C	81.01542	83.82878	82.90241	612.34801	-281.48662	411.56221	1
54	H	81.77867	83.35556	83.56112	1667.23498	-1490.75142	1556.16753	1
55	C	80.87967	85.40219	83.19110	-714.45746	-175.43074	286.98927	1
56	H	80.05601	85.80150	82.53530	-787.09484	1763.03619	-1922.46060	1
57	O	82.05108	86.18714	82.89840	-429.46514	516.51932	-128.40526	1
58	H	81.72982	86.70962	82.13551	1981.82785	436.16847	-1818.18182	1
59	C	80.42153	85.46723	84.69232	630.79189	-468.94448	76.03230	1
60	H	80.17852	86.51222	84.99760	-1775.71861	2062.30353	131.89849	1
61	H	79.50689	84.83791	84.87880	-1855.14608	88.94118	1993.53760	1
62	H	81.22350	85.10472	85.37715	-1504.82350	-780.94249	-2132.90992	1
63	C	79.60851	83.01669	82.93652	288.57638	618.62814	-397.00270	1
64	O	78.79963	83.29019	83.79933	321.70495	-185.26452	574.37218	1
65	N	79.50868	82.07197	82.00504	-447.05792	-446.53431	367.76425	1
66	H	80.25540	81.91974	81.31342	350.31316	1975.63644	-1843.31522	1
67	C	78.48349	81.10205	82.21765	-511.23061	374.03917	-471.51480	1
68	H	77.69769	81.65963	82.78156	2234.79579	-898.70890	-1273.45190	1
69	C	78.02091	80.59484	80.77406	529.53781	-159.34528	563.72604	1
70	H	77.03210	80.06936	80.89609	654.59388	2347.94251	1217.51488	1
71	H	77.82870	81.53591	80.19490	-1526.55661	2103.42026	817.87394	1
72	O	78.87259	79.68662	80.06474	-554.84278	14.12789	399.58769	1
73	H	79.60896	80.33693	79.77916	1297.06236	2061.84854	1220.68812	1
74	C	79.07992	79.85795	83.08352	-662.15484	-412.13544	123.62687	1
75	O	80.24820	79.58579	83.20403	-540.01537	-317.05804	274.91456	1
76	N	78.02588	79.23624	83.67762	-202.76299	-690.00100	-131.49145	1

77	H	77.15457	79.62846	83.31418	-702.62132	-2617.37191	281.70413	1
78	C	78.10244	77.79057	83.91486	-491.73914	576.34187	222.73509	1
79	H	79.17309	77.58034	84.14522	1977.17978	-1823.58850	-434.68928	1
80	C	77.13299	77.46330	85.03172	-649.50797	-328.66843	306.11224	1
81	H	76.13154	77.84558	84.72982	2075.07803	1452.16490	-1004.45904	1
82	C	77.01167	75.96788	85.26266	-615.18735	-489.99689	-70.96352	1
83	H	76.27283	75.73004	86.07637	-1226.32661	-1724.38906	-1716.47170	1
84	H	76.66684	75.43416	84.33295	2381.64273	-969.84735	900.46860	1
85	H	77.99560	75.51260	85.56117	2122.74991	1702.23946	-141.36228	1
86	C	77.51563	78.15634	86.32763	-501.86074	-479.61276	-376.42482	1
87	H	76.75530	77.97888	87.13715	993.79261	-2246.95401	-1177.81305	1
88	H	78.50694	77.79180	86.71366	42.71279	-626.15391	-2651.37258	1
89	H	77.60506	79.26858	86.18409	-2026.39012	-1590.33709	-887.82922	1
90	C	77.54808	77.06093	82.52977	-672.89153	382.57394	-156.34072	1
91	O	76.68033	77.55494	81.85188	410.04627	221.86223	500.35950	1
92	N	78.00325	75.77561	82.47375	-378.11782	-443.79414	-441.10984	1
93	H	78.81171	75.81581	83.10355	2404.15973	-568.14894	1149.30085	1
94	C	78.10933	75.20335	81.14412	-544.54484	466.16019	331.29119	1
95	H	78.94479	75.74287	80.65112	-1409.80988	-170.17955	2325.32679	1
96	C	78.42084	73.68638	81.41715	-184.48284	116.78282	-758.89137	1
97	H	79.35403	73.57705	82.01559	1893.78641	1861.14652	611.04528	1
98	H	77.60830	73.24129	82.03607	-2170.79665	-974.19311	1327.50117	1
99	C	78.54673	72.93555	80.05161	389.51668	672.81878	-138.49152	1
100	H	77.58853	73.00495	79.48755	510.64577	1933.03327	1851.02484	1
101	H	79.28521	73.44328	79.39355	-2302.30869	-1105.72939	-948.89774	1
102	C	78.95457	71.42400	80.23021	-559.93427	-126.34590	542.30857	1
103	O	79.23553	70.76451	79.26246	-670.36003	-111.83166	76.36448	1
104	N	78.94505	70.99330	81.51115	-216.06729	-537.07037	446.51379	1
105	H	78.67209	71.48793	82.36802	-1251.96487	1074.12894	-2168.52500	1
106	H	79.14037	70.02537	81.78959	-2451.83023	-720.73851	944.84612	1
107	C	76.67618	75.37294	80.40254	546.24052	-563.88337	-85.11809	1
108	O	75.73825	74.74531	80.82530	71.70702	-307.40463	606.69673	1
109	N	76.75395	76.14320	79.30205	479.90863	-504.50129	222.86849	1
110	C	75.56683	76.59116	78.64807	75.51268	-600.91904	506.73700	1
111	H	74.77576	76.51419	79.43018	-2033.61562	1795.30103	254.89480	1
112	C	76.00978	78.06640	78.23835	523.79067	517.99274	284.45581	1
113	H	75.34412	78.54208	77.48337	1599.61665	-1127.00911	1895.98173	1
114	H	76.03354	78.74313	79.12138	-1881.83093	1275.82488	-1501.55016	1
115	C	77.44738	77.78306	77.71292	-600.05639	-404.05026	316.64485	1
116	H	77.41709	77.26437	76.70937	-2597.05260	496.36221	657.73249	1
117	H	78.07171	78.69579	77.58542	-1666.24518	1294.38985	-1723.90591	1
118	C	77.96371	76.84282	78.88823	493.57570	-129.95376	-602.56394	1
119	H	78.72687	76.08451	78.59162	-1469.08415	-637.84797	2204.22581	1
120	H	78.31639	77.40439	79.78970	-1038.97840	1068.88701	-2280.71789	1
121	C	75.26190	75.62230	77.35943	188.88100	241.05089	-727.87821	1
122	O	75.44238	74.42951	77.39245	531.88613	-49.19943	427.07960	1
123	N	74.66517	76.33606	76.40745	708.14833	26.93417	-179.73509	1
124	H	74.60565	77.34690	76.52346	-2232.69501	-1179.09831	1023.94816	1
125	C	74.58567	75.75284	75.10468	-738.32412	259.92548	104.42456	1
126	H	74.50274	74.66194	75.32130	2028.89123	1260.02983	1311.33324	1
127	C	73.29654	76.39630	74.43660	-258.65678	-345.52513	661.28459	1
128	H	73.46265	77.48176	74.26824	-1826.06090	-1801.46097	-918.64554	1
129	C	72.86171	75.70606	73.09610	-541.23400	531.92970	-218.41428	1
130	H	71.87300	76.08288	72.74292	1311.73218	-2219.18200	882.19023	1
131	H	73.59415	75.90479	72.27413	-1048.71298	1223.58118	-2196.97971	1
132	H	72.76250	74.60039	73.20430	419.06414	1903.92898	1903.44670	1
133	C	72.09446	76.17437	75.41774	-423.86431	152.66566	-648.55262	1
134	H	71.14779	76.60979	75.02030	105.68386	-2342.50080	1387.51238	1
135	H	71.91249	75.08955	75.60172	-1695.63603	-1484.73621	-1531.02793	1
136	H	72.28895	76.64627	76.40934	-1853.57121	-487.39031	1936.59343	1
137	C	75.98419	76.11957	74.34644	539.71428	-510.58232	267.58633	1
138	O	76.91751	76.69228	74.87426	-15.93758	-278.34085	-624.49402	1

139	N	75.93469	75.58925	73.13155	-676.81886	12.05292	276.17960	1
140	H	75.05726	75.16075	72.84632	-1694.44250	-373.84189	-2100.66098	1
141	C	76.93498	75.99193	72.17856	412.33078	-664.70360	108.35451	1
142	H	76.99742	77.09996	72.26033	1765.77476	1294.44366	1621.76594	1
143	C	78.28294	75.33041	72.67287	-179.66635	-721.95667	-264.73915	1
144	H	78.61441	75.80381	73.62823	-607.34922	2587.87032	-598.10018	1
145	H	78.10129	74.25481	72.92435	-359.69332	-1479.13954	-2259.74260	1
146	C	79.38485	75.43707	71.56818	-240.01076	616.02425	431.85322	1
147	H	78.97372	75.14524	70.57178	-1359.17131	782.54425	2227.99181	1
148	H	79.76094	76.47874	71.45555	-820.36667	85.81767	-2596.78715	1
149	C	80.51996	74.44116	72.04155	-513.07015	236.18570	-551.87280	1
150	H	81.00468	74.81360	72.97190	1816.11944	-1183.11722	-1650.94321	1
151	H	80.08098	73.45329	72.31281	-1800.04429	-1361.53473	1526.34643	1
152	C	81.56517	74.25861	70.91801	726.08972	-253.19732	-179.64713	1
153	H	81.23038	73.62832	70.07037	1224.27271	-456.51798	-2390.90304	1
154	H	82.00731	75.19870	70.53487	1206.40339	-1150.93514	-2154.90344	1
155	N	82.76375	73.47895	71.56097	329.70796	-633.68968	-155.67358	1
156	H	83.59545	73.28019	70.93237	1348.31305	1938.76845	1359.00643	1
157	H	83.23644	73.92418	72.40078	2096.92035	1446.54551	-966.48890	1
158	H	82.54371	72.50945	71.92992	-1197.07217	-2303.53719	827.28733	1
159	C	76.51227	75.47865	70.69756	-378.01186	-556.17301	-413.96481	1
160	O	77.02800	76.00504	69.73670	-409.44433	-307.55053	-453.30833	1
161	N	75.68484	74.43042	70.70137	-429.02477	524.70884	274.08502	1
162	H	75.36610	74.05247	71.59279	1706.34263	-1425.96036	1574.38926	1
163	C	74.91014	74.24269	69.50481	-45.25864	-626.22952	478.93267	1
164	H	74.97657	75.25974	69.05182	1988.63164	570.90773	1772.87287	1
165	C	75.66744	73.17833	68.61868	551.77128	-20.49526	-564.54996	1
166	H	76.75439	73.41720	68.58234	1434.61535	-1753.10253	1513.99471	1
167	H	75.60338	72.16526	69.07537	-714.67738	1819.09770	1898.36494	1
168	C	75.05268	73.19637	67.17800	446.99263	-555.77305	338.97221	1
169	H	73.94986	73.04520	67.20309	1953.68466	1892.25957	-161.67766	1
170	H	75.20866	74.18546	66.69223	-403.03785	2688.07032	-188.43591	1
171	C	75.76521	72.04577	66.36029	567.86262	335.74681	434.04421	1
172	H	76.86375	72.22465	66.30752	-1080.02275	1568.26081	-1948.78900	1
173	H	75.64357	71.06303	66.87119	-919.54108	2111.34692	1456.13463	1
174	C	75.15083	72.00297	64.94196	195.81897	173.33862	-745.11536	1
175	H	74.09217	71.67723	64.90595	1405.67949	-2301.21089	-390.08113	1
176	H	75.28009	72.93345	64.35407	-940.37328	-1118.32446	2299.72133	1
177	N	75.93385	70.91596	64.12969	319.26422	656.36007	-42.02424	1
178	H	75.60921	70.76638	63.13103	1961.03633	619.91968	1787.09422	1
179	H	76.97265	71.08059	63.98603	854.14343	-2156.80752	1429.08711	1
180	H	75.92017	69.92300	64.50459	1237.02905	-1378.50857	-1998.28500	1
181	C	73.40994	73.81884	69.98439	532.53319	-268.57236	517.55729	1
182	O	72.80026	74.55495	70.73621	266.16714	-290.73804	-558.88002	1
183	N	73.00330	72.65779	69.47887	-226.25352	640.49678	-270.32839	1
184	H	73.62513	72.13772	68.86432	2007.69063	-1035.27229	1523.50231	1
185	C	71.61517	72.35919	69.58781	-540.76542	-573.33303	49.50000	1
186	H	71.15771	73.28948	70.00203	-2374.20950	-1036.76023	843.75774	1
187	C	71.06810	71.92146	68.14546	-77.09082	666.87422	-415.84136	1
188	H	71.47406	70.90314	67.89269	-985.81834	617.19825	2463.91927	1
189	O	71.42581	72.76882	67.04337	293.29899	-391.65602	-477.80926	1
190	H	71.86454	72.12738	66.44606	2528.72714	-681.76262	-751.27122	1
191	C	69.53140	71.79848	68.45934	252.47363	-605.14473	440.05134	1
192	H	68.96804	71.37473	67.59504	-2052.65063	1456.49051	-1043.51830	1
193	H	69.33455	71.13288	69.34424	-2152.98800	-1661.97574	-161.70652	1
194	H	69.08127	72.79391	68.68331	-473.12726	-1584.27339	2165.61725	1
195	C	71.42607	71.05629	70.56448	360.36307	488.46713	505.10056	1
196	O	70.50252	71.07963	71.38693	-200.08817	-528.03552	-385.82850	1
197	N	72.24777	70.08929	70.24353	-597.54095	-226.44775	355.20479	1
198	H	72.88269	70.37840	69.49965	2179.23655	-1300.70981	-991.33835	1
199	C	72.44674	68.88859	70.95574	-687.68921	297.39807	-249.45179	1
200	H	73.38940	68.47946	70.53148	-349.16256	-2467.37713	-1101.72831	1

201	C	72.51771	69.20509	72.52274	672.47345	361.54328	-201.62880	1
202	H	71.56916	69.69131	72.85274	1541.41502	582.18425	2169.97026	1
203	H	72.61630	68.25138	73.09050	-2534.67717	60.25153	997.72295	1
204	C	73.71067	70.12872	72.80392	574.26774	-389.43119	-377.02542	1
205	C	75.02633	69.58712	72.91202	688.82679	-287.33580	-257.96133	1
206	H	75.20659	68.50514	72.77748	331.14182	1470.38163	2269.80013	1
207	C	73.47841	71.52794	72.96274	-383.52382	-675.04808	144.24917	1
208	H	72.46164	71.94761	72.85069	4.09847	1517.59662	2262.86397	1
209	C	76.07770	70.45723	73.20337	-134.76730	428.45285	-649.50303	1
210	H	77.09706	70.04370	73.29878	-903.23433	1600.49020	2011.53387	1
211	C	74.56405	72.35268	73.26587	-335.53281	-615.00040	-364.39058	1
212	H	74.37601	73.42850	73.41377	1596.45398	-1369.33862	1732.02659	1
213	C	75.89188	71.85563	73.39434	585.48547	-340.24194	-406.23938	1
214	O	77.00334	72.69748	73.69379	-419.15649	-173.04408	-511.94141	1
215	H	76.53045	73.56303	73.76359	-1071.84350	1559.71507	-1960.13012	1
216	C	71.19215	67.84289	70.80753	291.41878	-183.13091	710.72246	1
217	O	71.40298	66.69563	70.49756	379.87695	523.47396	-222.23622	1
218	N	70.05125	68.41464	71.16547	564.30591	373.09380	277.24371	1
219	H	70.01010	69.43718	71.40234	-120.59931	-2436.07824	-1214.35098	1
220	C	68.86571	67.62702	71.13917	404.07514	-299.37480	608.84009	1
221	H	69.17967	66.60099	70.82833	-1071.07882	-841.69025	2359.66467	1
222	C	68.29971	67.70237	72.62905	-683.12807	68.71770	-390.13096	1
223	H	69.13241	67.54072	73.34914	2068.88918	1596.58590	770.89603	1
224	H	67.90888	68.71918	72.85472	1379.86429	2342.49779	-179.85638	1
225	C	67.19529	66.62493	72.83189	-176.39967	537.49466	550.97268	1
226	H	66.26719	66.89365	72.27924	-396.28051	1942.22168	1869.33314	1
227	H	67.52021	65.64193	72.42360	-94.44700	586.00678	-2659.20016	1
228	C	66.91663	66.51476	74.40291	-291.69381	-718.18079	-150.72929	1
229	H	67.79004	66.21334	75.03534	-2303.38776	1089.76242	964.62032	1
230	H	66.45158	67.42056	74.86866	884.16729	2568.80533	-207.74283	1
231	N	65.97610	65.47429	74.44940	-594.49522	-252.81478	342.29276	1
232	H	65.61819	65.14889	73.56477	-1735.17426	2084.05705	-263.71605	1
233	C	65.54426	64.93022	75.51379	595.23177	-271.52487	442.22352	1
234	N	66.04110	65.39778	76.73514	585.53813	-424.79750	-105.81303	1
235	H	66.71498	66.13941	76.92094	959.88797	1327.56823	-2177.11905	1
236	H	65.76496	65.04159	77.65080	1578.48647	16.27378	-2220.76233	1
237	N	64.61159	63.92464	75.22206	-452.17763	-390.33541	-421.51853	1
238	H	64.24870	63.58431	74.33292	470.26107	1974.25629	-1817.92087	1
239	H	64.14811	63.36927	75.94221	1856.67307	-1573.97321	-1224.35416	1
240	C	67.84373	68.36184	70.11385	-531.47271	-581.45780	-55.06206	1
241	O	68.04353	69.49201	69.66314	-243.00837	192.73507	609.52485	1
242	N	66.80820	67.58793	69.88487	343.49288	-644.25607	38.09164	1
243	H	66.83658	66.68863	70.35529	-1691.16043	-1535.97525	-1484.73099	1
244	C	65.75749	67.98976	68.94576	542.66492	350.14337	454.42563	1
245	H	66.35283	68.28893	68.05113	1209.57979	-2396.95920	463.86744	1
246	C	64.81472	66.82105	68.71645	-737.14309	145.93010	242.71942	1
247	H	64.43084	66.49319	69.70826	-1050.18303	159.36419	-2509.06125	1
248	C	63.62813	67.23914	67.86795	-706.77696	-252.88343	-245.16230	1
249	H	62.90546	66.39144	67.71187	-1624.64039	-1665.49085	1417.86935	1
250	H	63.05936	68.08349	68.35335	2566.10521	598.51109	693.22305	1
251	H	63.95039	67.59561	66.85059	-1972.69758	107.10018	-1876.34312	1
252	C	65.52151	65.63975	68.07806	412.85148	672.58832	-27.69222	1
253	H	64.82912	64.76433	67.93962	1447.02277	1762.76533	-1490.78944	1
254	H	65.93092	65.90384	67.06417	1320.77379	-145.20455	2378.68491	1
255	H	66.38870	65.28714	68.70146	-1512.10848	1470.52031	1724.75147	1
256	C	64.99769	69.30685	69.61994	-607.11113	499.56689	73.73769	1
257	O	63.92622	69.19628	70.15343	357.97126	460.81534	356.68785	1
258	N	65.74629	70.38219	69.44856	536.55407	-368.62270	332.76306	1
259	H	66.70557	70.34348	69.01699	524.38866	2297.69985	1367.20941	1
260	C	65.24698	71.61555	69.92329	46.50277	-774.29190	-147.97904	1
261	H	64.26502	71.39365	70.40274	1676.51875	1883.29066	1032.55549	1
262	C	66.35399	72.26826	70.90784	-559.41456	-34.19198	-556.30433	1

263	H	67.26282	72.53046	70.31587	-64.66664	395.18769	2695.05373	1
264	H	65.97952	73.22855	71.33509	-2703.44278	-60.40056	333.79418	1
265	C	66.70886	71.28823	71.99215	-519.76435	377.31045	459.42366	1
266	H	66.97831	70.31887	71.50577	-1746.74323	1667.50644	-1261.73691	1
267	C	67.90677	71.77654	72.79175	570.95554	16.46261	-545.27700	1
268	H	68.03844	71.19127	73.73808	2391.58273	28.05277	-1305.07271	1
269	H	68.87748	71.66873	72.19704	175.75588	917.63458	2559.43867	1
270	H	67.80232	72.85454	73.08027	-1063.97851	-2155.34650	1283.00462	1
271	C	65.53221	71.05639	72.93117	193.76014	2.62946	-765.53141	1
272	H	65.79884	70.35549	73.76374	507.39394	-846.55087	2539.60089	1
273	H	65.18470	72.01274	73.40077	1337.57841	1818.19054	1526.01994	1
274	H	64.65648	70.61039	72.39202	1100.88635	-1172.91350	-2199.08909	1
275	C	65.17001	72.61117	68.64776	-549.21115	475.64486	-309.38218	1
276	O	65.78220	72.43457	67.62784	556.06106	-390.37755	-78.24250	1
277	O	64.43323	73.80122	68.84951	-572.27940	-310.19032	-209.75862	1
278	H	64.08585	73.61192	69.76591	-1380.08193	2212.14486	790.85944	1

Listing 43: C00043.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.7815	0.0000	300.0000
3	H	65.75450	67.48575	76.09365	-2043.14101	-1757.64893	399.89339		1
4	N	66.51773	67.71593	76.72913	426.75047	490.45733	-334.42467		1
5	H	66.85335	66.79428	77.03788	442.25559	-1110.30854	-2448.52907		1
6	C	67.56031	68.45672	76.12960	415.32972	-666.39213	83.73172		1
7	H	67.15071	68.92167	75.20600	879.32219	2491.00447	667.35213		1
8	C	68.09278	69.55151	77.18911	31.35357	477.41777	628.23362		1
9	H	68.45826	69.02695	78.10394	1168.38489	2240.25337	-1019.71136		1
10	H	68.97143	70.10300	76.77655	-360.43770	2534.90498	931.67112		1
11	C	66.97504	70.49807	77.53673	463.18208	512.70242	-382.34388		1
12	H	66.07995	69.89060	77.80166	1725.29117	1863.52247	-987.07854		1
13	C	67.35588	71.35233	78.73991	710.42801	-144.27427	-313.15367		1
14	H	66.52391	72.04106	79.03825	364.20195	-1033.13725	2494.72524		1
15	H	67.60354	70.72306	79.63334	2567.61904	335.80679	847.48802		1
16	H	68.25177	71.98993	78.52469	-2587.99029	680.92867	-512.16411		1
17	C	66.62197	71.40579	76.36616	268.17616	741.64379	-40.42634		1
18	H	65.79696	72.11685	76.63006	1283.54314	-1945.37420	-1411.27812		1
19	H	67.49970	72.02338	76.04394	-1258.57796	1317.15249	-2026.02085		1
20	H	66.28134	70.82108	75.47357	-2502.84526	909.80597	575.92391		1
21	C	68.70320	67.33425	75.86416	619.36578	-458.64843	-172.09273		1
22	O	68.62910	66.21449	76.32961	-81.40433	433.87611	522.34594		1
23	N	69.69661	67.89257	75.16917	175.23996	-622.20190	341.55523		1
24	H	69.52689	68.83899	74.82719	-876.57256	-303.22879	-2561.90213		1
25	C	70.58003	67.01960	74.43198	-571.88214	-534.10783	-106.15033		1
26	H	69.93104	66.22951	73.99655	-2713.20841	-16.25800	-248.80809		1
27	C	71.26812	67.97966	73.35928	166.60354	288.16399	-716.09568		1
28	H	71.83599	68.78467	73.90229	-2097.85574	1636.78449	-586.18044		1
29	O	70.35920	68.67006	72.47864	-317.80580	-363.38227	484.43082		1
30	H	70.62184	69.60057	72.62540	1863.74748	-1451.84923	1357.29467		1
31	C	72.29755	67.00720	72.67688	503.80731	517.99032	318.51606		1
32	H	72.89321	67.53339	71.89222	640.61020	-2157.10410	-1536.29104		1
33	H	73.01992	66.59785	73.42037	1687.88455	465.60692	2087.56452		1
34	H	71.79081	66.14148	72.18685	-1293.07895	-1899.88581	-1463.57452		1
35	C	71.67790	66.44360	75.46534	-153.07550	-733.68902	248.70981		1
36	O	72.33994	67.23154	76.12072	186.15459	-480.78787	-449.34387		1
37	N	71.82368	65.12426	75.35784	-487.53139	543.18517	42.03850		1
38	C	72.38815	64.34657	76.42577	-699.35871	69.34393	360.10701		1
39	H	71.91221	64.72851	77.35616	2.81126	-221.99807	-2715.58072		1
40	C	72.00614	62.86745	76.02265	-507.46439	-592.59194	122.07761		1
41	H	72.69653	62.10814	76.45526	-1975.08116	525.87560	-1801.71556		1
42	H	70.98099	62.60008	76.36507	1588.27743	-1913.22100	1113.83566		1

43	C	72.07895	62.95042	74.46533	-613.62442	-457.55993	-194.14490	1
44	H	73.13867	62.98657	74.12657	1707.54637	-721.27992	1996.92523	1
45	H	71.59610	62.09449	73.94261	758.23357	2100.81767	1560.55011	1
46	C	71.33454	64.33475	74.23342	-352.41524	704.96076	49.21465	1
47	H	71.57827	64.86198	73.28032	1714.76886	-2070.42778	443.35792	1
48	H	70.22680	64.27969	74.35752	1224.15040	1801.50881	1636.97633	1
49	C	74.02070	64.56556	76.43117	566.85117	537.05831	117.62814	1
50	O	74.72822	64.04240	75.60294	-550.26779	-406.08867	4.21666	1
51	N	74.33373	65.33593	77.45979	566.34832	-425.77725	180.18749	1
52	H	73.56454	65.66020	78.04520	644.44502	2646.80550	-52.73430	1
53	C	75.65768	65.81057	77.69444	612.34801	-281.48662	411.56221	1
54	H	75.55220	66.33830	78.67005	1667.23498	-1490.75142	1556.16753	1
55	C	76.58645	64.50542	77.83143	-714.45746	-175.43074	286.98927	1
56	H	76.66730	64.04495	76.80757	-787.09484	1763.03619	-1922.46060	1
57	O	76.07771	63.48187	78.70607	-429.46514	516.51932	-128.40526	1
58	H	75.85240	62.78676	78.05521	1981.82785	436.16847	-1818.18182	1
59	C	77.98295	65.07603	78.26881	630.79189	-468.94448	76.03230	1
60	H	78.75018	64.26913	78.32885	-1775.71861	2062.30353	131.89849	1
61	H	78.36839	65.85340	77.55360	-1855.14608	88.94118	1993.53760	1
62	H	77.92739	65.54979	79.27675	-1504.82350	-780.94249	-2132.90992	1
63	C	76.09484	66.82577	76.52104	288.57638	618.62814	-397.00270	1
64	O	77.30156	67.03141	76.31768	321.70495	-185.26452	574.37218	1
65	N	75.06179	67.39124	75.96398	-447.05792	-446.53431	367.76425	1
66	H	74.10748	67.11073	76.28555	350.31316	1975.63644	-1843.31522	1
67	C	75.10311	68.35468	74.92414	-511.23061	374.03917	-471.51480	1
68	H	74.05183	68.72132	74.92765	2234.79579	-898.70890	-1273.45190	1
69	C	76.16968	69.49165	75.28034	529.53781	-159.34528	563.72604	1
70	H	75.86672	70.44801	74.77130	654.59388	2347.94251	1217.51488	1
71	H	76.06299	69.66571	76.38374	-1526.55661	2103.42026	817.87394	1
72	O	77.53287	69.23661	74.91562	-554.84278	14.12789	399.58769	1
73	H	77.67402	68.36984	75.44454	1297.06236	2061.84854	1220.68812	1
74	C	75.49039	67.70104	73.47724	-662.15484	-412.13544	123.62687	1
75	O	74.98384	68.16249	72.48649	-540.01537	-317.05804	274.91456	1
76	N	76.41800	66.75097	73.58038	-202.76299	-690.00100	-131.49145	1
77	H	76.71263	66.51363	74.54010	-702.62132	-2617.37191	281.70413	1
78	C	76.78210	65.88731	72.46459	-491.73914	576.34187	222.73509	1
79	H	77.41684	65.10146	72.93905	1977.17978	-1823.58850	-434.68928	1
80	C	75.51251	65.31341	71.85721	-649.50797	-328.66843	306.11224	1
81	H	74.93076	66.16618	71.43414	2075.07803	1452.16490	-1004.45904	1
82	C	75.80624	64.33395	70.73734	-615.18735	-489.99689	-70.96352	1
83	H	74.86386	63.96245	70.24829	-1226.32661	-1724.38906	-1716.47170	1
84	H	76.44444	64.80935	69.93118	2381.64273	-969.84735	900.46860	1
85	H	76.36459	63.43226	71.11206	2122.74991	1702.23946	-141.36228	1
86	C	74.64915	64.63894	72.90879	-501.86074	-479.61276	-376.42482	1
87	H	73.68054	64.26502	72.47767	993.79261	-2246.95401	-1177.81305	1
88	H	75.17323	63.75954	73.37900	42.71279	-626.15391	-2651.37258	1
89	H	74.39902	65.34244	73.75143	-2026.39012	-1590.33709	-887.82922	1
90	C	77.64778	66.79142	71.36080	-672.89153	382.57394	-156.34072	1
91	O	77.81409	66.33429	70.24884	410.04627	221.86223	500.35950	1
92	N	78.09215	67.91401	71.87173	-378.11782	-443.79414	-441.10984	1
93	H	77.80717	68.06323	72.83780	2404.15973	-568.14894	1149.30085	1
94	C	79.09708	68.74754	71.26870	-544.54484	466.16019	331.29119	1
95	H	79.99134	68.60461	71.91070	-1409.80988	-170.17955	2325.32679	1
96	C	79.31248	68.33470	69.76346	-184.48284	116.78282	-758.89137	1
97	H	79.70696	67.29208	69.68733	1893.78641	1861.14652	611.04528	1
98	H	78.32326	68.32388	69.24549	-2170.79665	-974.19311	1327.50117	1
99	C	80.30104	69.33505	69.08002	389.51668	672.81878	-138.49152	1
100	H	79.97650	70.38425	69.25570	510.64577	1933.03327	1851.02484	1
101	H	81.30352	69.27962	69.55810	-2302.30869	-1105.72939	-948.89774	1
102	C	80.43227	69.07327	67.53243	-559.93427	-126.34590	542.30857	1
103	O	81.13695	69.78706	66.86547	-670.36003	-111.83166	76.36448	1
104	N	79.71026	68.02229	67.08549	-216.06729	-537.07037	446.51379	1

105	H	79.09458	67.37856	67.59660	-1251.96487	1074.12894	-2168.52500	1
106	H	79.68785	67.71893	66.10606	-2451.83023	-720.73851	944.84612	1
107	C	78.51171	70.26823	71.34049	546.24052	-563.88337	-85.11809	1
108	O	77.54268	70.56685	70.68963	71.70702	-307.40463	606.69673	1
109	N	79.30219	71.05985	72.07825	479.90863	-504.50129	222.86849	1
110	C	78.83935	72.34190	72.52219	75.51268	-600.91904	506.73700	1
111	H	77.77765	72.21351	72.83286	-2033.61562	1795.30103	254.89480	1
112	C	79.86831	72.67884	73.68275	523.79067	517.99274	284.45581	1
113	H	79.93381	73.76856	73.90047	1599.61665	-1127.00911	1895.98173	1
114	H	79.59170	72.17653	74.63684	-1881.83093	1275.82488	-1501.55016	1
115	C	81.18189	72.08678	73.08602	-600.05639	-404.05026	316.64485	1
116	H	81.56865	72.73238	72.26273	-2597.05260	496.36221	657.73249	1
117	H	82.00448	71.97375	73.82744	-1666.24518	1294.38985	-1723.90591	1
118	C	80.63995	70.70093	72.52533	493.57570	-129.95376	-602.56394	1
119	H	81.20459	70.27815	71.66118	-1469.08415	-637.84797	2204.22581	1
120	H	80.50280	69.91497	73.30597	-1038.97840	1068.88701	-2280.71789	1
121	C	79.01984	73.41046	71.29374	188.88100	241.05089	-727.87821	1
122	O	80.08683	73.65608	70.78693	531.88613	-49.19943	427.07960	1
123	N	77.83740	74.02507	71.09040	708.14833	26.93417	-179.73509	1
124	H	77.06070	73.53534	71.53839	-2232.69501	-1179.09831	1023.94816	1
125	C	77.61782	74.82326	69.88101	-738.32412	259.92548	104.42456	1
126	H	78.55813	75.41837	69.80171	2028.89123	1260.02983	1311.33324	1
127	C	77.46799	73.88162	68.70168	-258.65678	-345.52513	661.28459	1
128	H	76.51906	73.31461	68.83496	-1826.06090	-1801.46097	-918.64554	1
129	C	77.38762	74.63742	67.38827	-541.23400	531.92970	-218.41428	1
130	H	77.18015	73.95104	66.52175	1311.73218	-2219.18200	882.19023	1
131	H	76.56618	75.41513	67.41278	-1048.71298	1223.58118	-2196.97971	1
132	H	78.34811	75.17695	67.16172	419.06414	1903.92898	1903.44670	1
133	C	78.59935	72.87009	68.64658	-423.86431	152.66566	-648.55262	1
134	H	78.50215	72.16586	67.77484	105.68386	-2342.50080	1387.51238	1
135	H	79.60326	73.37732	68.56984	-1695.63603	-1484.73621	-1531.02793	1
136	H	78.63118	72.24902	69.59149	-1853.57121	-487.39031	1936.59343	1
137	C	76.26830	75.76400	70.10735	539.71428	-510.58232	267.58633	1
138	O	75.77050	76.31439	69.14833	-15.93758	-278.34085	-624.49402	1
139	N	75.87514	75.80014	71.36306	-676.81886	12.05292	276.17960	1
140	H	76.47271	75.27834	71.99661	-1694.44250	-373.84189	-2100.66098	1
141	C	74.90784	76.74836	71.84885	412.33078	-664.70360	108.35451	1
142	H	75.39559	77.72844	71.65348	1765.77476	1294.44366	1621.76594	1
143	C	73.58013	76.57552	71.02081	-179.66635	-721.95667	-264.73915	1
144	H	73.78580	76.64938	69.92357	-607.34922	2587.87032	-598.10018	1
145	H	73.15258	75.55989	71.18265	-359.69332	-1479.13954	-2259.74260	1
146	C	72.57872	77.68610	71.49085	-240.01076	616.02425	431.85322	1
147	H	72.45953	77.65770	72.59962	-1359.17131	782.54425	2227.99181	1
148	H	72.96232	78.70243	71.24763	-820.36667	85.81767	-2596.78715	1
149	C	71.19544	77.41081	70.77845	-513.07015	236.18570	-551.87280	1
150	H	71.29350	77.49113	69.67120	1816.11944	-1183.11722	-1650.94321	1
151	H	70.84984	76.37030	70.97791	-1800.04429	-1361.53473	1526.34643	1
152	C	70.17270	78.43580	71.32345	726.08972	-253.19732	-179.64713	1
153	H	69.98352	78.36195	72.41322	1224.27271	-456.51798	-2390.90304	1
154	H	70.37995	79.48853	71.04577	1206.40339	-1150.93514	-2154.90344	1
155	N	68.79178	78.10805	70.66476	329.70796	-633.68968	-155.67358	1
156	H	67.98314	78.73341	70.94829	1348.31305	1938.76845	1359.00643	1
157	H	68.73077	78.14824	69.60543	2096.92035	1446.54551	-966.48890	1
158	H	68.39152	77.14803	70.87250	-1197.07217	-2303.53719	827.28733	1
159	C	74.71147	76.41320	73.43035	-378.01186	-556.17301	-413.96481	1
160	O	73.61078	76.20370	73.89572	-409.44433	-307.55053	-453.30833	1
161	N	75.88062	76.41185	74.06728	-429.02477	524.70884	274.08502	1
162	H	76.72514	76.64851	73.54833	1706.34263	-1425.96036	1574.38926	1
163	C	75.87490	76.14334	75.46291	-45.25864	-626.22952	478.93267	1
164	H	74.84488	75.75049	75.64269	1988.63164	570.90773	1772.87287	1
165	C	77.05102	75.13331	75.78201	551.77128	-20.49526	-564.54996	1
166	H	77.01841	74.24879	75.10665	1434.61535	-1753.10253	1513.99471	1

167	H	78.03772	75.61562	75.60103	-714.67738	1819.09770	1898.36494	1
168	C	76.90614	74.70954	77.28152	446.99263	-555.77305	338.97221	1
169	H	76.86329	75.61446	77.93088	1953.68466	1892.25957	-161.67766	1
170	H	75.95228	74.16261	77.45425	-403.03785	2688.07032	-188.43591	1
171	C	78.15052	73.81802	77.67739	567.86262	335.74681	434.04421	1
172	H	78.12424	72.83299	77.15669	-1080.02275	1568.26081	-1948.78900	1
173	H	79.10312	74.30360	77.36373	-919.54108	2111.34692	1456.13463	1
174	C	78.10838	73.64774	79.21429	195.81897	173.33862	-745.11536	1
175	H	78.22437	74.59172	79.78385	1405.67949	-2301.21089	-390.08113	1
176	H	77.23332	73.08347	79.59372	-940.37328	-1118.32446	2299.72133	1
177	N	79.34926	72.78988	79.63176	319.26422	656.36007	-42.02424	1
178	H	79.45080	72.60864	80.67210	1961.03633	619.91968	1787.09422	1
179	H	79.41295	71.80530	79.24036	854.14343	-2156.80752	1429.08711	1
180	H	80.30662	73.18306	79.39597	1237.02905	-1378.50857	-1998.28500	1
181	C	76.18436	77.54238	76.27886	532.53319	-268.57236	517.55729	1
182	O	77.22030	77.64284	76.94628	266.16714	-290.73804	-558.88002	1
183	N	75.21937	78.39394	76.10852	-226.25352	640.49678	-270.32839	1
184	H	74.50108	78.02749	75.48543	2007.69063	-1035.27229	1523.50231	1
185	C	75.10526	79.70360	76.67813	-540.76542	-573.33303	49.50000	1
186	H	74.45568	79.60223	77.57497	-2374.20950	-1036.76023	843.75774	1
187	C	76.55930	80.21407	77.08236	-77.09082	666.87422	-415.84136	1
188	H	77.26420	79.82453	76.29491	-985.81834	617.19825	2463.91927	1
189	O	77.01887	79.71652	78.33866	293.29899	-391.65602	-477.80926	1
190	H	77.43958	78.82765	78.01640	2528.72714	-681.76262	-751.27122	1
191	C	76.50217	81.77990	76.97487	252.47363	-605.14473	440.05134	1
192	H	77.49813	82.23792	77.19115	-2052.65063	1456.49051	-1043.51830	1
193	H	76.19131	82.12057	75.95606	-2152.98800	-1661.97574	-161.70652	1
194	H	75.78209	82.21283	77.70872	-473.12726	-1584.27339	2165.61725	1
195	C	74.35591	80.55933	75.52048	360.36307	488.46713	505.10056	1
196	O	74.50680	80.30725	74.34472	-200.08817	-528.03552	-385.82850	1
197	N	73.66272	81.56715	76.06100	-597.54095	-226.44775	355.20479	1
198	H	73.63186	81.69987	77.07305	2179.23655	-1300.70981	-991.33835	1
199	C	72.88884	82.35119	75.16562	-687.68921	297.39807	-249.45179	1
200	H	72.74794	81.71193	74.26388	-349.16256	-2467.37713	-1101.72831	1
201	C	71.53459	82.79910	75.89169	672.47345	361.54328	-201.62880	1
202	H	71.75285	83.26683	76.87958	1541.41502	582.18425	2169.97026	1
203	H	71.01235	83.56347	75.27098	-2534.67717	60.25153	997.72295	1
204	C	70.66075	81.54788	76.05445	574.26774	-389.43119	-377.02542	1
205	C	69.98022	81.01465	74.91821	688.82679	-287.33580	-257.96133	1
206	H	70.06872	81.49823	73.92841	331.14182	1470.38163	2269.80013	1
207	C	70.55688	80.91110	77.32759	-383.52382	-675.04808	144.24917	1
208	H	71.09483	81.31479	78.20509	4.09847	1517.59662	2262.86397	1
209	C	69.20289	79.86894	75.08361	-134.76730	428.45285	-649.50303	1
210	H	68.67469	79.45668	74.20616	-903.23433	1600.49020	2011.53387	1
211	C	69.76243	79.76768	77.44218	-335.53281	-615.00040	-364.39058	1
212	H	69.68344	79.28593	78.43240	1596.45398	-1369.33862	1732.02659	1
213	C	69.05833	79.20598	76.33726	585.48547	-340.24194	-406.23938	1
214	O	68.24804	78.04588	76.44774	-419.15649	-173.04408	-511.94141	1
215	H	68.36670	77.85151	77.40760	-1071.84350	1559.71507	-1960.13012	1
216	C	73.68627	83.73301	74.79818	291.41878	-183.13091	710.72246	1
217	O	73.41682	84.32751	73.77883	379.87695	523.47396	-222.23622	1
218	N	74.52225	84.09259	75.76432	564.30591	373.09380	277.24371	1
219	H	74.56799	83.52199	76.60674	-120.59931	-2436.07824	-1214.35098	1
220	C	75.36704	85.22350	75.53580	404.07514	-299.37480	608.84009	1
221	H	75.39266	85.26592	74.42208	-1071.07882	-841.69025	2359.66467	1
222	C	74.59696	86.47176	76.13529	-683.12807	68.71770	-390.13096	1
223	H	73.54439	86.47407	75.77231	2068.88918	1596.58590	770.89603	1
224	H	74.52292	86.40567	77.24383	1379.86429	2342.49779	-179.85638	1
225	C	75.33336	87.77195	75.68594	-176.39967	537.49466	550.97268	1
226	H	76.37951	87.79892	76.06204	-396.28051	1942.22168	1869.33314	1
227	H	75.41321	87.82528	74.57736	-94.44700	586.00678	-2659.20016	1
228	C	74.47347	88.98933	76.26092	-291.69381	-718.18079	-150.72929	1

229	H	73.43668	89.08291	75.84833	-2303.38776	1089.76242	964.62032	1
230	H	74.39865	89.03668	77.37716	884.16729	2568.80533	-207.74283	1
231	N	75.19819	90.11256	75.83777	-594.49522	-252.81478	342.29276	1
232	H	76.05841	89.93894	75.34172	-1735.17426	2084.05705	-263.71605	1
233	C	74.84134	91.31535	76.03945	595.23177	-271.52487	442.22352	1
234	N	73.64418	91.53021	76.73174	585.53813	-424.79750	-105.81303	1
235	H	72.98505	90.85190	77.11175	959.88797	1327.56823	-2177.11905	1
236	H	73.25311	92.44686	76.95125	1578.48647	16.27378	-2220.76233	1
237	N	75.76875	92.21804	75.50062	-452.17763	-390.33541	-421.51853	1
238	H	76.63897	92.06362	74.99338	470.26107	1974.25629	-1817.92087	1
239	H	75.65678	93.23114	75.55875	1856.67307	-1573.97321	-1224.35416	1
240	C	76.81117	84.87001	76.21086	-531.47271	-581.45780	-55.06206	1
241	O	77.48505	83.99103	75.72613	-243.00837	192.73507	609.52485	1
242	N	77.12188	85.64770	77.24765	343.49288	-644.25607	38.09164	1
243	H	76.42782	86.33378	77.53843	-1691.16043	-1535.97525	-1484.73099	1
244	C	78.31742	85.36258	78.04120	542.66492	350.14337	454.42563	1
245	H	79.03277	84.92441	77.30375	1209.57979	-2396.95920	463.86744	1
246	C	78.78634	86.65547	78.69028	-737.14309	145.93010	242.71942	1
247	H	77.93622	87.06798	79.27827	-1050.18303	159.36419	-2509.06125	1
248	C	79.94231	86.41249	79.64200	-706.77696	-252.88343	-245.16230	1
249	H	80.24086	87.35091	80.18619	-1624.64039	-1665.49085	1417.86935	1
250	H	79.68127	85.63717	80.41838	2566.10521	598.51109	693.22305	1
251	H	80.85286	86.03769	79.09778	-1972.69758	107.10018	-1876.34312	1
252	C	79.17341	87.69346	77.65288	412.85148	672.58832	-27.69222	1
253	H	79.45856	88.67292	78.12655	1447.02277	1762.76533	-1490.78944	1
254	H	80.05094	87.35213	77.03728	1320.77379	-145.20455	2378.68491	1
255	H	78.32942	87.89784	76.93872	-1512.10848	1470.52031	1724.75147	1
256	C	77.92481	84.26252	79.22123	-607.11113	499.56689	73.73769	1
257	O	78.81140	83.63039	79.75407	357.97126	460.81534	356.68785	1
258	N	76.63778	84.27902	79.51269	536.55407	-368.62270	332.76306	1
259	H	76.03509	84.87544	78.94944	524.38866	2297.69985	1367.20941	1
260	C	76.12484	83.28963	80.39183	46.50277	-774.29190	-147.97904	1
261	H	76.93324	82.52372	80.44170	1676.51875	1883.29066	1032.55549	1
262	C	75.82155	83.94466	81.83847	-559.41456	-34.19198	-556.30433	1
263	H	74.97247	84.66099	81.73784	-64.66664	395.18769	2695.05373	1
264	H	75.46824	83.15738	82.54588	-2703.44278	-60.40056	333.79418	1
265	C	77.02257	84.65449	82.39894	-519.76435	377.31045	459.42366	1
266	H	77.36898	85.39954	81.64681	-1746.74323	1667.50644	-1261.73691	1
267	C	76.65598	85.39338	83.68148	570.95554	16.46261	-545.27700	1
268	H	77.52888	85.96004	84.09651	2391.58273	28.05277	-1305.07271	1
269	H	75.83029	86.13155	83.51487	175.75588	917.63458	2559.43867	1
270	H	76.31246	84.68690	84.47999	-1063.97851	-2155.34650	1283.00462	1
271	C	78.16935	83.69708	82.68899	193.76014	2.62946	-765.53141	1
272	H	79.00464	84.20713	83.23542	507.39394	-846.55087	2539.60089	1
273	H	77.84158	82.83079	83.31958	1337.57841	1818.19054	1526.01994	1
274	H	78.60532	83.28159	81.72970	1100.88635	-1172.91350	-2199.08909	1
275	C	74.73008	82.79369	79.76078	-549.21115	475.64486	-309.38218	1
276	O	74.17200	83.36028	78.85505	556.06106	-390.37755	-78.24250	1
277	O	74.13545	81.66083	80.36518	-572.27940	-310.19032	-209.75862	1
278	H	74.85013	81.45180	81.02960	-1380.08193	2212.14486	790.85944	1

Listing 44: C00044.xmolout

1		276						
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750 11100
		0.2500	300.00	0.00	0.00	0.00	-1293.7722 0.0000	300.0000
3	H	65.03120	79.95604	82.05380	-2043.14101	-1757.64893	399.89339	1
4	N	64.97378	80.60698	82.83598	426.75047	490.45733	-334.42467	1
5	H	64.82898	79.97577	83.62896	442.25559	-1110.30854	-2448.52907	1
6	C	66.12690	81.41037	83.00294	415.32972	-666.39213	83.73172	1
7	H	66.68481	81.27106	82.05167	879.32219	2491.00447	667.35213	1
8	C	65.70781	82.95337	83.22529	31.35357	477.41777	628.23362	1

9	H	65.33133	83.08305	84.26782	1168.38489	2240.25337	-1019.71136	1
10	H	66.60407	83.61356	83.14245	-360.43770	2534.90498	931.67112	1
11	C	64.65296	83.37007	82.23717	463.18208	512.70242	-382.34388	1
12	H	63.78093	82.68725	82.35357	1725.29117	1863.52247	-987.07854	1
13	C	64.20427	84.79795	82.52595	710.42801	-144.27427	-313.15367	1
14	H	63.38021	85.12096	81.83942	364.20195	-1033.13725	2494.72524	1
15	H	63.82684	84.90974	83.57493	2567.61904	335.80679	847.48802	1
16	H	65.04579	85.52661	82.39838	-2587.99029	680.92867	-512.16411	1
17	C	65.15515	83.27353	80.80278	268.17616	741.64379	-40.42634	1
18	H	64.37841	83.61401	80.07051	1283.54314	-1945.37420	-1411.27812	1
19	H	66.06540	83.90608	80.64015	-1258.57796	1317.15249	-2026.02085	1
20	H	65.42809	82.22139	80.53102	-2502.84526	909.80597	575.92391	1
21	C	66.87647	80.78444	84.28757	619.36578	-458.64843	-172.09273	1
22	O	66.54856	79.68210	84.75154	-81.40433	433.87611	522.34594	1
23	N	67.78490	81.62874	84.71772	175.23996	-622.20190	341.55523	1
24	H	67.83878	82.47593	84.14868	-876.57256	-303.22879	-2561.90213	1
25	C	69.00998	81.26722	85.37686	-571.88214	-534.10783	-106.15033	1
26	H	69.02877	81.88095	86.30394	-2713.20841	-16.25800	-248.80809	1
27	C	69.04154	79.70808	85.70384	166.60354	288.16399	-716.09568	1
28	H	68.76963	79.17746	84.74405	-2097.85574	1636.78449	-586.18044	1
29	O	68.09876	79.30205	86.69543	-317.80580	-363.38227	484.43082	1
30	H	67.27784	79.14344	86.08732	1863.74748	-1451.84923	1357.29467	1
31	C	70.53470	79.37705	86.06422	503.80731	517.99032	318.51606	1
32	H	70.69263	78.27703	86.15455	640.61020	-2157.10410	-1536.29104	1
33	H	71.26197	79.75268	85.29311	1687.88455	465.60692	2087.56452	1
34	H	70.82697	79.82996	87.04173	-1293.07895	-1899.88581	-1463.57452	1
35	C	70.11631	81.78367	84.31224	-153.07550	-733.68902	248.70981	1
36	O	69.81468	81.90739	83.15113	186.15459	-480.78787	-449.34387	1
37	N	71.29830	82.02072	84.90129	-487.53139	543.18517	42.03850	1
38	C	72.46994	82.23933	84.10423	-699.35871	69.34393	360.10701	1
39	H	72.17613	82.95031	83.29970	2.81126	-221.99807	-2715.58072	1
40	C	73.50187	82.81141	85.16141	-507.46439	-592.59194	122.07761	1
41	H	74.55803	82.57905	84.89925	-1975.08116	525.87560	-1801.71556	1
42	H	73.43509	83.92040	85.22933	1588.27743	-1913.22100	1113.83566	1
43	C	73.03809	82.14128	86.49195	-613.62442	-457.55993	-194.14490	1
44	H	73.36323	81.07776	86.54108	1707.54637	-721.27992	1996.92523	1
45	H	73.42507	82.64232	87.40765	758.23357	2100.81767	1560.55011	1
46	C	71.46065	82.26144	86.32676	-352.41524	704.96076	49.21465	1
47	H	70.86274	81.51926	86.90676	1714.76886	-2070.42778	443.35792	1
48	H	71.05270	83.28387	86.51207	1224.15040	1801.50881	1636.97633	1
49	C	72.95420	80.79762	83.49183	566.85117	537.05831	117.62814	1
50	O	72.99315	79.79950	84.17404	-550.26779	-406.08867	4.21666	1
51	N	73.24105	80.95112	82.20011	566.34832	-425.77725	180.18749	1
52	H	73.13688	81.90695	81.85751	644.44502	2646.80550	-52.73430	1
53	C	74.22599	80.12769	81.56591	612.34801	-281.48662	411.56221	1
54	H	74.32459	80.62045	80.57257	1667.23498	-1490.75142	1556.16753	1
55	C	75.59064	80.21985	82.39230	-714.45746	-175.43074	286.98927	1
56	H	75.46408	79.65329	83.35420	-787.09484	1763.03619	-1922.46060	1
57	O	76.01763	81.54912	82.74367	-429.46514	516.51932	-128.40526	1
58	H	76.05921	81.47905	83.71803	1981.82785	436.16847	-1818.18182	1
59	C	76.57837	79.44215	81.44637	630.79189	-468.94448	76.03230	1
60	H	77.59569	79.36280	81.89524	-1775.71861	2062.30353	131.89849	1
61	H	76.21898	78.39538	81.23969	-1855.14608	88.94118	1993.53760	1
62	H	76.69303	79.95679	80.46377	-1504.82350	-780.94249	-2132.90992	1
63	C	73.64929	78.61490	81.45296	288.57638	618.62814	-397.00270	1
64	O	74.37367	77.63408	81.48306	321.70495	-185.26452	574.37218	1
65	N	72.35543	78.65909	81.13604	-447.05792	-446.53431	367.76425	1
66	H	71.92174	79.57526	81.24860	350.31316	1975.63644	-1843.31522	1
67	C	71.61948	77.44259	81.21197	-511.23061	374.03917	-471.51480	1
68	H	72.36844	76.64107	81.01555	2234.79579	-898.70890	-1273.45190	1
69	C	71.08344	77.38157	82.72759	529.53781	-159.34528	563.72604	1
70	H	70.51466	76.42014	82.83753	654.59388	2347.94251	1217.51488	1

71	H	71.99351	77.30499	83.38225	-1526.55661	2103.42026	817.87394	1
72	O	70.25716	78.48816	83.15761	-554.84278	14.12789	399.58769	1
73	H	70.96930	79.13824	83.35860	1297.06236	2061.84854	1220.68812	1
74	C	70.38394	77.45249	80.16423	-662.15484	-412.13544	123.62687	1
75	O	69.65291	76.49082	80.09595	-540.01537	-317.05804	274.91456	1
76	N	70.33225	78.55795	79.41536	-202.76299	-690.00100	-131.49145	1
77	H	71.06373	79.24626	79.58129	-702.62132	-2617.37191	281.70413	1
78	C	69.26255	78.76410	78.45421	-491.73914	576.34187	222.73509	1
79	H	68.55013	77.94440	78.71728	1977.17978	-1823.58850	-434.68928	1
80	C	68.72295	80.17094	78.63531	-649.50797	-328.66843	306.11224	1
81	H	69.56204	80.88102	78.45840	2075.07803	1452.16490	-1004.45904	1
82	C	67.62703	80.48284	77.63292	-615.18735	-489.99689	-70.96352	1
83	H	67.23442	81.52956	77.75703	-1226.32661	-1724.38906	-1716.47170	1
84	H	68.00474	80.38836	76.57508	2381.64273	-969.84735	900.46860	1
85	H	66.75308	79.78326	77.74098	2122.74991	1702.23946	-141.36228	1
86	C	68.21756	80.40260	80.04805	-501.86074	-479.61276	-376.42482	1
87	H	67.89521	81.46826	80.20609	993.79261	-2246.95401	-1177.81305	1
88	H	67.33460	79.74696	80.28298	42.71279	-626.15391	-2651.37258	1
89	H	69.00922	80.17358	80.81539	-2026.39012	-1590.33709	-887.82922	1
90	C	69.96769	78.55836	76.94363	-672.89153	382.57394	-156.34072	1
91	O	70.06768	79.48653	76.17685	410.04627	221.86223	500.35950	1
92	N	70.33292	77.30011	76.78658	-378.11782	-443.79414	-441.10984	1
93	H	70.11436	76.71499	77.59184	2404.15973	-568.14894	1149.30085	1
94	C	70.92843	76.79899	75.59384	-544.54484	466.16019	331.29119	1
95	H	70.98853	75.70183	75.78091	-1409.80988	-170.17955	2325.32679	1
96	C	69.93035	77.18939	74.41186	-184.48284	116.78282	-758.89137	1
97	H	68.88051	76.97544	74.71325	1893.78641	1861.14652	611.04528	1
98	H	69.97420	78.28993	74.23113	-2170.79665	-974.19311	1327.50117	1
99	C	70.30780	76.39324	73.12788	389.51668	672.81878	-138.49152	1
100	H	71.33287	76.68480	72.78303	510.64577	1933.03327	1851.02484	1
101	H	70.39533	75.30884	73.36101	-2302.30869	-1105.72939	-948.89774	1
102	C	69.28735	76.58844	71.94262	-559.93427	-126.34590	542.30857	1
103	O	69.45306	75.97631	70.91988	-670.36003	-111.83166	76.36448	1
104	N	68.28813	77.45830	72.20351	-216.06729	-537.07037	446.51379	1
105	H	68.12912	78.04182	73.03331	-1251.96487	1074.12894	-2168.52500	1
106	H	67.57065	77.72628	71.52070	-2451.83023	-720.73851	944.84612	1
107	C	72.36540	77.46322	75.26894	546.24052	-563.88337	-85.11809	1
108	O	72.64171	77.62360	74.08677	71.70702	-307.40463	606.69673	1
109	N	73.15506	77.64419	76.31961	479.90863	-504.50129	222.86849	1
110	C	74.29447	78.52448	76.25217	75.51268	-600.91904	506.73700	1
111	H	73.94482	79.40274	75.66195	-2033.61562	1795.30103	254.89480	1
112	C	74.58964	78.78641	77.78942	523.79067	517.99274	284.45581	1
113	H	75.62564	79.14702	77.97840	1599.61665	-1127.00911	1895.98173	1
114	H	73.89656	79.54029	78.22667	-1881.83093	1275.82488	-1501.55016	1
115	C	74.31654	77.36195	78.36141	-600.05639	-404.05026	316.64485	1
116	H	75.13127	76.65878	78.07188	-2597.05260	496.36221	657.73249	1
117	H	74.24079	77.33435	79.48028	-1666.24518	1294.38985	-1723.90591	1
118	C	72.95181	77.02177	77.62214	493.57570	-129.95376	-602.56394	1
119	H	72.73278	75.93864	77.47250	-1469.08415	-637.84797	2204.22581	1
120	H	72.05869	77.52543	78.06191	-1038.97840	1068.88701	-2280.71789	1
121	C	75.54073	77.75349	75.53554	188.88100	241.05089	-727.87821	1
122	O	76.50791	77.45170	76.17972	531.88613	-49.19943	427.07960	1
123	N	75.29839	77.59317	74.23385	708.14833	26.93417	-179.73509	1
124	H	74.35006	77.85616	73.86178	-2232.69501	-1179.09831	1023.94816	1
125	C	76.30241	77.04329	73.32097	-738.32412	259.92548	104.42456	1
126	H	75.86763	77.30009	72.32645	2028.89123	1260.02983	1311.33324	1
127	C	77.63820	77.71545	73.56643	-258.65678	-345.52513	661.28459	1
128	H	77.94112	77.49043	74.62049	-1826.06090	-1801.46097	-918.64554	1
129	C	78.72371	77.19888	72.64087	-541.23400	531.92970	-218.41428	1
130	H	79.71484	77.68930	72.84542	1311.73218	-2219.18200	882.19023	1
131	H	78.86745	76.08180	72.76007	-1048.71298	1223.58118	-2196.97971	1
132	H	78.47429	77.38971	71.56112	419.06414	1903.92898	1903.44670	1

133	C	77.53678	79.22503	73.42655	-423.86431	152.66566	-648.55262	1
134	H	78.51097	79.73320	73.66348	105.68386	-2342.50080	1387.51238	1
135	H	77.24973	79.52445	72.38176	-1695.63603	-1484.73621	-1531.02793	1
136	H	76.75884	79.64907	74.11851	-1853.57121	-487.39031	1936.59343	1
137	C	76.35805	75.39925	73.53319	539.71428	-510.58232	267.58633	1
138	O	77.37791	74.77769	73.34043	-15.93758	-278.34085	-624.49402	1
139	N	75.10719	74.87635	73.66422	-676.81886	12.05292	276.17960	1
140	H	74.55755	75.72618	73.84940	-1694.44250	-373.84189	-2100.66098	1
141	C	74.98597	73.77966	74.60842	412.33078	-664.70360	108.35451	1
142	H	75.24566	74.20787	75.60051	1765.77476	1294.44366	1621.76594	1
143	C	73.47640	73.36603	74.47988	-179.66635	-721.95667	-264.73915	1
144	H	72.80653	74.11094	74.96631	-607.34922	2587.87032	-598.10018	1
145	H	73.18622	73.36751	73.40482	-359.69332	-1479.13954	-2259.74260	1
146	C	73.27550	71.93543	75.08972	-240.01076	616.02425	431.85322	1
147	H	74.14088	71.28046	74.83286	-1359.17131	782.54425	2227.99181	1
148	H	73.23437	71.96529	76.20122	-820.36667	85.81767	-2596.78715	1
149	C	71.95270	71.33449	74.46847	-513.07015	236.18570	-551.87280	1
150	H	71.04977	71.86869	74.84417	1816.11944	-1183.11722	-1650.94321	1
151	H	71.94556	71.46086	73.36077	-1800.04429	-1361.53473	1526.34643	1
152	C	71.91237	69.82927	74.82460	726.08972	-253.19732	-179.64713	1
153	H	72.75497	69.23934	74.41043	1224.27271	-456.51798	-2390.90304	1
154	H	71.78704	69.60796	75.90368	1206.40339	-1150.93514	-2154.90344	1
155	N	70.64819	69.22060	74.13368	329.70796	-633.68968	-155.67358	1
156	H	70.49416	68.18158	74.28258	1348.31305	1938.76845	1359.00643	1
157	H	69.70046	69.61611	74.40257	2096.92035	1446.54551	-966.48890	1
158	H	70.62427	69.28514	73.07518	-1197.07217	-2303.53719	827.28733	1
159	C	75.93365	72.52163	74.21556	-378.01186	-556.17301	-413.96481	1
160	O	76.35431	71.79138	75.08614	-409.44433	-307.55053	-453.30833	1
161	N	75.91204	72.24871	72.86437	-429.02477	524.70884	274.08502	1
162	H	75.49225	73.12454	72.51383	1706.34263	-1425.96036	1574.38926	1
163	C	77.20026	71.90929	72.28002	-45.25864	-626.22952	478.93267	1
164	H	77.63074	72.90911	72.04718	1988.63164	570.90773	1772.87287	1
165	C	78.07795	71.08463	73.28126	551.77128	-20.49526	-564.54996	1
166	H	78.42534	71.73251	74.12121	1434.61535	-1753.10253	1513.99471	1
167	H	77.46967	70.28932	73.77295	-714.67738	1819.09770	1898.36494	1
168	C	79.29150	70.47439	72.49168	446.99263	-555.77305	338.97221	1
169	H	78.93704	69.89636	71.60917	1953.68466	1892.25957	-161.67766	1
170	H	79.95272	71.27162	72.08534	-403.03785	2688.07032	-188.43591	1
171	C	80.08062	69.53532	73.48517	567.86262	335.74681	434.04421	1
172	H	80.50348	70.12060	74.33389	-1080.02275	1568.26081	-1948.78900	1
173	H	79.40009	68.78234	73.94621	-919.54108	2111.34692	1456.13463	1
174	C	81.20103	68.83678	72.67616	195.81897	173.33862	-745.11536	1
175	H	80.84145	68.09448	71.93317	1405.67949	-2301.21089	-390.08113	1
176	H	81.93854	69.52463	72.20410	-940.37328	-1118.32446	2299.72133	1
177	N	82.03274	67.97664	73.68200	319.26422	656.36007	-42.02424	1
178	H	82.83411	67.44269	73.23762	1961.03633	619.91968	1787.09422	1
179	H	82.52767	68.48497	74.47147	854.14343	-2156.80752	1429.08711	1
180	H	81.52628	67.19934	74.19862	1237.02905	-1378.50857	-1998.28500	1
181	C	76.81633	71.06685	70.93829	532.53319	-268.57236	517.55729	1
182	O	76.81193	71.62840	69.86940	266.16714	-290.73804	-558.88002	1
183	N	76.57747	69.77067	71.22163	-226.25352	640.49678	-270.32839	1
184	H	76.57032	69.57683	72.22415	2007.69063	-1035.27229	1523.50231	1
185	C	75.61676	69.05356	70.43229	-540.76542	-573.33303	49.50000	1
186	H	75.44053	68.13115	71.02762	-2374.20950	-1036.76023	843.75774	1
187	C	74.31048	69.96006	70.40691	-77.09082	666.87422	-415.84136	1
188	H	74.60107	70.92973	69.91667	-985.81834	617.19825	2463.91927	1
189	O	73.79639	70.30787	71.72070	293.29899	-391.65602	-477.80926	1
190	H	74.35702	71.07445	71.93399	2528.72714	-681.76262	-751.27122	1
191	C	73.29911	69.16956	69.50404	252.47363	-605.14473	440.05134	1
192	H	72.36821	69.75650	69.32223	-2052.65063	1456.49051	-1043.51830	1
193	H	73.74567	68.91844	68.49945	-2152.98800	-1661.97574	-161.70652	1
194	H	72.99263	68.20982	69.98313	-473.12726	-1584.27339	2165.61725	1

195	C	76.31824	68.71908	68.99988	360.36307	488.46713	505.10056	1
196	O	75.65784	68.67956	67.97923	-200.08817	-528.03552	-385.82850	1
197	N	77.58398	68.37706	69.19601	-597.54095	-226.44775	355.20479	1
198	H	77.89838	68.44948	70.16379	2179.23655	-1300.70981	-991.33835	1
199	C	78.46282	67.97788	68.16959	-687.68921	297.39807	-249.45179	1
200	H	79.32469	67.53232	68.71523	-349.16256	-2467.37713	-1101.72831	1
201	C	77.74312	67.01282	67.11365	672.47345	361.54328	-201.62880	1
202	H	76.80032	67.49550	66.73867	1541.41502	582.18425	2169.97026	1
203	H	78.41459	66.88236	66.23030	-2534.67717	60.25153	997.72295	1
204	C	77.43938	65.66643	67.78455	574.26774	-389.43119	-377.02542	1
205	C	78.49239	64.73511	68.02880	688.82679	-287.33580	-257.96133	1
206	H	79.53416	64.97074	67.74407	331.14182	1470.38163	2269.80013	1
207	C	76.09813	65.36734	68.16969	-383.52382	-675.04808	144.24917	1
208	H	75.28834	66.09941	67.99345	4.09847	1517.59662	2262.86397	1
209	C	78.17496	63.52089	68.63604	-134.76730	428.45285	-649.50303	1
210	H	78.98666	62.79697	68.82555	-903.23433	1600.49020	2011.53387	1
211	C	75.83071	64.13481	68.76996	-335.53281	-615.00040	-364.39058	1
212	H	74.78899	63.90703	69.05608	1596.45398	-1369.33862	1732.02659	1
213	C	76.84895	63.16951	69.02261	585.48547	-340.24194	-406.23938	1
214	O	76.58975	61.91467	69.63293	-419.15649	-173.04408	-511.94141	1
215	H	75.61244	61.98306	69.74528	-1071.84350	1559.71507	-1960.13012	1
216	C	78.89349	69.24315	67.22431	291.41878	-183.13091	710.72246	1
217	O	78.79609	69.14883	66.01918	379.87695	523.47396	-222.23622	1
218	N	79.42986	70.22630	67.93848	564.30591	373.09380	277.24371	1
219	H	79.44260	70.13444	68.95410	-120.59931	-2436.07824	-1214.35098	1
220	C	79.75677	71.43060	67.24749	404.07514	-299.37480	608.84009	1
221	H	79.82087	71.11861	66.17752	-1071.07882	-841.69025	2359.66467	1
222	C	78.54656	72.42285	67.52178	-683.12807	68.71770	-390.13096	1
223	H	77.58321	71.95348	67.21771	2068.88918	1596.58590	770.89603	1
224	H	78.42857	72.64067	68.60883	1379.86429	2342.49779	-179.85638	1
225	C	78.83556	73.71687	66.70283	-176.39967	537.49466	550.97268	1
226	H	79.79346	74.18420	67.02469	-396.28051	1942.22168	1869.33314	1
227	H	78.96545	73.48050	65.62313	-94.44700	586.00678	-2659.20016	1
228	C	77.60442	74.71058	66.92429	-291.69381	-718.18079	-150.72929	1
229	H	76.60052	74.32192	66.61640	-2303.38776	1089.76242	964.62032	1
230	H	77.50965	75.13002	67.95831	884.16729	2568.80533	-207.74283	1
231	N	77.94263	75.75933	66.05510	-594.49522	-252.81478	342.29276	1
232	H	78.85445	75.71908	65.62639	-1735.17426	2084.05705	-263.71605	1
233	C	77.18766	76.74388	65.77818	595.23177	-271.52487	442.22352	1
234	N	75.92910	76.78972	66.38765	585.53813	-424.79750	-105.81303	1
235	H	75.50376	76.13646	67.04426	959.88797	1327.56823	-2177.11905	1
236	H	75.23652	77.52514	66.24367	1578.48647	16.27378	-2220.76233	1
237	N	77.81004	77.61921	64.87684	-452.17763	-390.33541	-421.51853	1
238	H	78.72391	77.57922	64.42799	470.26107	1974.25629	-1817.92087	1
239	H	77.36442	78.46712	64.52426	1856.67307	-1573.97321	-1224.35416	1
240	C	81.16105	72.01303	67.84950	-531.47271	-581.45780	-55.06206	1
241	O	82.14660	72.06448	67.12552	-243.00837	192.73507	609.52485	1
242	N	81.05308	72.43184	69.09745	343.49288	-644.25607	38.09164	1
243	H	80.15686	72.23287	69.53407	-1691.16043	-1535.97525	-1484.73099	1
244	C	82.21221	72.94737	69.81925	542.66492	350.14337	454.42563	1
245	H	82.76521	73.46580	68.99920	1209.57979	-2396.95920	463.86744	1
246	C	81.74837	73.85469	70.94741	-737.14309	145.93010	242.71942	1
247	H	81.14685	73.24369	71.65639	-1050.18303	159.36419	-2509.06125	1
248	C	82.93240	74.42457	71.70620	-706.77696	-252.88343	-245.16230	1
249	H	82.60578	75.07248	72.56567	-1624.64039	-1665.49085	1417.86935	1
250	H	83.57725	73.60056	72.12770	2566.10521	598.51109	693.22305	1
251	H	83.58667	75.05513	71.04264	-1972.69758	107.10018	-1876.34312	1
252	C	80.86175	74.97564	70.43695	412.85148	672.58832	-27.69222	1
253	H	80.49142	75.62867	71.27350	1447.02277	1762.76533	-1490.78944	1
254	H	81.41192	75.63940	69.71458	1320.77379	-145.20455	2378.68491	1
255	H	79.95994	74.57631	69.89593	-1512.10848	1470.52031	1724.75147	1
256	C	83.05882	71.61491	70.36310	-607.11113	499.56689	73.73769	1

257	O	83.22287	71.42117	71.53740	357.97126	460.81534	356.68785	1
258	N	83.51792	70.96897	69.30707	536.55407	-368.62270	332.76306	1
259	H	83.26083	71.32721	68.36342	524.38866	2297.69985	1367.20941	1
260	C	84.07205	69.67012	69.43173	46.50277	-774.29190	-147.97904	1
261	H	84.37111	69.42340	68.38896	1676.51875	1883.29066	1032.55549	1
262	C	85.33000	69.72520	70.44461	-559.41456	-34.19198	-556.30433	1
263	H	84.96524	70.04571	71.45257	-64.66664	395.18769	2695.05373	1
264	H	85.78246	68.71502	70.58461	-2703.44278	-60.40056	333.79418	1
265	C	86.35281	70.69796	69.92686	-519.76435	377.31045	459.42366	1
266	H	85.82557	71.64012	69.65310	-1746.74323	1667.50644	-1261.73691	1
267	C	87.38077	71.01604	71.00656	570.95554	16.46261	-545.27700	1
268	H	88.13794	71.76139	70.65077	2391.58273	28.05277	-1305.07271	1
269	H	86.89862	71.44337	71.92322	175.75588	917.63458	2559.43867	1
270	H	87.94258	70.09999	71.32338	-1063.97851	-2155.34650	1283.00462	1
271	C	87.06904	70.16231	68.69401	193.76014	2.62946	-765.53141	1
272	H	87.84115	70.88320	68.31999	507.39394	-846.55087	2539.60089	1
273	H	87.59541	69.19696	68.90921	1337.57841	1818.19054	1526.01994	1
274	H	86.35849	69.97263	67.84924	1100.88635	-1172.91350	-2199.08909	1
275	C	82.94606	68.66221	69.98014	-549.21115	475.64486	-309.38218	1
276	O	81.76680	68.90987	70.00801	556.06106	-390.37755	-78.24250	1
277	O	83.40385	67.37905	70.37164	-572.27940	-310.19032	-209.75862	1
278	H	84.36135	67.47863	70.11653	-1380.08193	2212.14486	790.85944	1

Listing 45: C00045.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	1.7062	6825
		0.2500	300.00	0.00	0.00	0.00	-1293.7502	0.0000	300.0000
3	H	79.81510	83.67426	78.64968	-2043.14101	-1757.64893	399.89339		1
4	N	80.48079	83.44081	77.91540	426.75047	490.45733	-334.42467		1
5	H	80.78883	82.51091	78.19175	442.25559	-1110.30854	-2448.52907		1
6	C	81.52316	84.37474	77.73452	415.32972	-666.39213	83.73172		1
7	H	81.01395	85.35656	77.82982	879.32219	2491.00447	667.35213		1
8	C	82.67335	84.13389	78.83060	31.35357	477.41777	628.23362		1
9	H	83.10774	83.11525	78.68514	1168.38489	2240.25337	-1019.71136		1
10	H	83.51399	84.84836	78.65774	-360.43770	2534.90498	931.67112		1
11	C	82.13054	84.28012	80.23128	463.18208	512.70242	-382.34388		1
12	H	81.24365	83.61705	80.33979	1725.29117	1863.52247	-987.07854		1
13	C	83.17679	83.84821	81.25085	710.42801	-144.27427	-313.15367		1
14	H	82.78808	83.92251	82.29940	364.20195	-1033.13725	2494.72524		1
15	H	83.49955	82.78707	81.09011	2567.61904	335.80679	847.48802		1
16	H	84.09619	84.48638	81.19296	-2587.99029	680.92867	-512.16411		1
17	C	81.70459	85.71359	80.51542	268.17616	741.64379	-40.42634		1
18	H	81.31824	85.82990	81.56110	1283.54314	-1945.37420	-1411.27812		1
19	H	82.55978	86.42828	80.39713	-1258.57796	1317.15249	-2026.02085		1
20	H	80.89146	86.05181	79.82287	-2502.84526	909.80597	575.92391		1
21	C	82.15241	84.09692	76.24359	619.36578	-458.64843	-172.09273		1
22	O	83.19054	83.49314	76.10104	-81.40433	433.87611	522.34594		1
23	N	81.33807	84.61524	75.33173	175.23996	-622.20190	341.55523		1
24	H	80.52245	85.11651	75.68322	-876.57256	-303.22879	-2561.90213		1
25	C	81.63483	84.59875	73.94445	-571.88214	-534.10783	-106.15033		1
26	H	80.80131	85.19364	73.50824	-2713.20841	-16.25800	-248.80809		1
27	C	83.06028	85.31737	73.79223	166.60354	288.16399	-716.09568		1
28	H	83.82831	84.60890	74.21454	-2097.85574	1636.78449	-586.18044		1
29	O	83.21004	86.56041	74.50296	-317.80580	-363.38227	484.43082		1
30	H	83.87091	86.30483	75.17809	1863.74748	-1451.84923	1357.29467		1
31	C	83.24378	85.44418	72.23616	503.80731	517.99032	318.51606		1
32	H	84.24054	85.87374	71.98085	640.61020	-2157.10410	-1536.29104		1
33	H	83.16795	84.45312	71.71889	1687.88455	465.60692	2087.56452		1
34	H	82.47384	86.11551	71.78936	-1293.07895	-1899.88581	-1463.57452		1
35	C	81.66085	83.05908	73.40927	-153.07550	-733.68902	248.70981		1
36	O	82.61655	82.71742	72.75732	186.15459	-480.78787	-449.34387		1

37	N	80.55510	82.35355	73.68671	-487.53139	543.18517	42.03850	1
38	C	80.42589	80.98994	73.26950	-699.35871	69.34393	360.10701	1
39	H	81.44086	80.52928	73.29481	2.81126	-221.99807	-2715.58072	1
40	C	79.37033	80.43228	74.32309	-507.46439	-592.59194	122.07761	1
41	H	78.86834	79.50001	73.98005	-1975.08116	525.87560	-1801.71556	1
42	H	79.84766	80.20141	75.30127	1588.27743	-1913.22100	1113.83566	1
43	C	78.40075	81.64710	74.43264	-613.62442	-457.55993	-194.14490	1
44	H	77.74794	81.71285	73.53222	1707.54637	-721.27992	1996.92523	1
45	H	77.72538	81.60553	75.31664	758.23357	2100.81767	1560.55011	1
46	C	79.44611	82.84466	74.49252	-352.41524	704.96076	49.21465	1
47	H	79.09577	83.81052	74.05896	1714.76886	-2070.42778	443.35792	1
48	H	79.87782	83.02908	75.50534	1224.15040	1801.50881	1636.97633	1
49	C	79.71829	80.91930	71.79727	566.85117	537.05831	117.62814	1
50	O	79.06537	81.82023	71.33976	-550.26779	-406.08867	4.21666	1
51	N	79.81070	79.64288	71.37857	566.34832	-425.77725	180.18749	1
52	H	80.50038	79.08613	71.88840	644.44502	2646.80550	-52.73430	1
53	C	79.72704	79.41644	69.94860	612.34801	-281.48662	411.56221	1
54	H	80.42092	80.15858	69.49578	1667.23498	-1490.75142	1556.16753	1
55	C	80.19249	77.91123	69.74377	-714.45746	-175.43074	286.98927	1
56	H	79.36449	77.22842	70.07965	-787.09484	1763.03619	-1922.46060	1
57	O	81.36051	77.50532	70.49314	-429.46514	516.51932	-128.40526	1
58	H	81.00591	76.75003	71.00060	1981.82785	436.16847	-1818.18182	1
59	C	80.32399	77.83564	68.17800	630.79189	-468.94448	76.03230	1
60	H	80.53630	76.79591	67.83637	-1775.71861	2062.30353	131.89849	1
61	H	79.39154	78.17321	67.66316	-1855.14608	88.94118	1993.53760	1
62	H	81.15703	78.47899	67.81027	-1504.82350	-780.94249	-2132.90992	1
63	C	78.19870	79.61535	69.46576	288.57638	618.62814	-397.00270	1
64	O	77.94825	79.76895	68.29374	321.70495	-185.26452	574.37218	1
65	N	77.31524	79.39399	70.47488	-447.05792	-446.53431	367.76425	1
66	H	77.79577	79.33978	71.37642	350.31316	1975.63644	-1843.31522	1
67	C	76.17979	80.30800	70.45473	-511.23061	374.03917	-471.51480	1
68	H	76.56964	81.26659	70.04248	2234.79579	-898.70890	-1273.45190	1
69	C	75.13713	79.61316	69.45885	529.53781	-159.34528	563.72604	1
70	H	74.30802	80.34214	69.25159	654.59388	2347.94251	1217.51488	1
71	H	75.69357	79.46541	68.49263	-1526.55661	2103.42026	817.87394	1
72	O	74.54367	78.36863	69.91244	-554.84278	14.12789	399.58769	1
73	H	75.33063	77.79303	69.85282	1297.06236	2061.84854	1220.68812	1
74	C	75.64942	80.42218	71.95285	-662.15484	-412.13544	123.62687	1
75	O	75.99650	79.64830	72.86173	-540.01537	-317.05804	274.91456	1
76	N	74.80093	81.42537	72.03314	-202.76299	-690.00100	-131.49145	1
77	H	74.59068	81.92487	71.17008	-702.62132	-2617.37191	281.70413	1
78	C	74.21369	81.80860	73.29811	-491.73914	576.34187	222.73509	1
79	H	74.78651	81.21843	74.05567	1977.17978	-1823.58850	-434.68928	1
80	C	74.33889	83.32470	73.42542	-649.50797	-328.66843	306.11224	1
81	H	73.83238	83.77893	72.54500	2075.07803	1452.16490	-1004.45904	1
82	C	73.65249	83.83047	74.67897	-615.18735	-489.99689	-70.96352	1
83	H	73.69916	84.95227	74.75572	-1226.32661	-1724.38906	-1716.47170	1
84	H	72.56537	83.53711	74.70123	2381.64273	-969.84735	900.46860	1
85	H	74.12822	83.41160	75.60881	2122.74991	1702.23946	-141.36228	1
86	C	75.78983	83.76549	73.39803	-501.86074	-479.61276	-376.42482	1
87	H	75.88747	84.88588	73.37407	993.79261	-2246.95401	-1177.81305	1
88	H	76.34858	83.40207	74.30413	42.71279	-626.15391	-2651.37258	1
89	H	76.32639	83.36135	72.49446	-2026.39012	-1590.33709	-887.82922	1
90	C	72.58661	81.39750	73.22030	-672.89153	382.57394	-156.34072	1
91	O	71.85517	81.85436	72.37787	410.04627	221.86223	500.35950	1
92	N	72.29741	80.61157	74.24178	-378.11782	-443.79414	-441.10984	1
93	H	73.05063	80.35371	74.87578	2404.15973	-568.14894	1149.30085	1
94	C	70.98747	80.07892	74.36761	-544.54484	466.16019	331.29119	1
95	H	70.41312	80.52460	73.52431	-1409.80988	-170.17955	2325.32679	1
96	C	71.16652	78.50329	74.27742	-184.48284	116.78282	-758.89137	1
97	H	71.68772	78.26135	73.32403	1893.78641	1861.14652	611.04528	1
98	H	71.83455	78.13568	75.08890	-2170.79665	-974.19311	1327.50117	1

99	C	69.78587	77.78159	74.34177	389.51668	672.81878	-138.49152	1
100	H	69.35345	77.85477	75.36771	510.64577	1933.03327	1851.02484	1
101	H	69.04656	78.30464	73.69549	-2302.30869	-1105.72939	-948.89774	1
102	C	69.87230	76.26613	73.91154	-559.93427	-126.34590	542.30857	1
103	O	68.88016	75.58308	73.90702	-670.36003	-111.83166	76.36448	1
104	N	71.11434	75.85860	73.56822	-216.06729	-537.07037	446.51379	1
105	H	71.97530	76.40994	73.48759	-1251.96487	1074.12894	-2168.52500	1
106	H	71.32685	74.93354	73.17933	-2451.83023	-720.73851	944.84612	1
107	C	70.46882	80.48972	75.86972	546.24052	-563.88337	-85.11809	1
108	O	70.98602	79.97820	76.83045	71.70702	-307.40463	606.69673	1
109	N	69.46314	81.37589	75.81811	479.90863	-504.50129	222.86849	1
110	C	68.98147	82.04572	76.98902	75.51268	-600.91904	506.73700	1
111	H	69.87092	82.24598	77.62961	-2033.61562	1795.30103	254.89480	1
112	C	68.26697	83.33288	76.39230	523.79067	517.99274	284.45581	1
113	H	67.49866	83.75429	77.07945	1599.61665	-1127.00911	1895.98173	1
114	H	68.99463	84.14930	76.18541	-1881.83093	1275.82488	-1501.55016	1
115	C	67.66652	82.75928	75.07158	-600.05639	-404.05026	316.64485	1
116	H	66.74505	82.16974	75.27653	-2597.05260	496.36221	657.73249	1
117	H	67.38555	83.54221	74.33157	-1666.24518	1294.38985	-1723.90591	1
118	C	68.85272	81.82455	74.57454	493.57570	-129.95376	-602.56394	1
119	H	68.53470	80.92613	73.99493	-1469.08415	-637.84797	2204.22581	1
120	H	69.65988	82.35878	74.01758	-1038.97840	1068.88701	-2280.71789	1
121	C	67.87176	81.12447	77.75756	188.88100	241.05089	-727.87821	1
122	O	67.06227	81.64281	78.49497	531.88613	-49.19943	427.07960	1
123	N	68.00351	79.83879	77.43208	708.14833	26.93417	-179.73509	1
124	H	68.80397	79.62870	76.82545	-2232.69501	-1179.09831	1023.94816	1
125	C	67.56242	78.87015	78.39755	-738.32412	259.92548	104.42456	1
126	H	67.62318	79.38599	79.38113	2028.89123	1260.02983	1311.33324	1
127	C	66.06845	78.50553	78.00271	-258.65678	-345.52513	661.28459	1
128	H	65.90823	78.68417	76.91760	-1826.06090	-1801.46097	-918.64554	1
129	C	65.73719	77.02260	78.38570	-541.23400	531.92970	-218.41428	1
130	H	64.66967	76.77308	78.18003	1311.73218	-2219.18200	882.19023	1
131	H	66.36485	76.30511	77.80277	-1048.71298	1223.58118	-2196.97971	1
132	H	65.92481	76.82556	79.46729	419.06414	1903.92898	1903.44670	1
133	C	65.12763	79.40830	78.87244	-423.86431	152.66566	-648.55262	1
134	H	64.06817	79.36183	78.52603	105.68386	-2342.50080	1387.51238	1
135	H	65.13944	79.09954	79.94449	-1695.63603	-1484.73621	-1531.02793	1
136	H	65.45879	80.48715	78.83400	-1853.57121	-487.39031	1936.59343	1
137	C	68.53624	77.57320	78.24368	539.71428	-510.58232	267.58633	1
138	O	68.50882	76.86203	77.24338	-15.93758	-278.34085	-624.49402	1
139	N	69.24319	77.45293	79.34472	-676.81886	12.05292	276.17960	1
140	H	69.11775	78.18674	80.04184	-1694.44250	-373.84189	-2100.66098	1
141	C	69.95375	76.27482	79.68984	412.33078	-664.70360	108.35451	1
142	H	70.28686	76.46963	80.73388	1765.77476	1294.44366	1621.76594	1
143	C	68.94217	75.06113	79.56358	-179.66635	-721.95667	-264.73915	1
144	H	68.04803	75.20808	80.20962	-607.34922	2587.87032	-598.10018	1
145	H	68.54602	74.98459	78.52494	-359.69332	-1479.13954	-2259.74260	1
146	C	69.73032	73.76777	79.95615	-240.01076	616.02425	431.85322	1
147	H	70.71152	73.73235	79.42425	-1359.17131	782.54425	2227.99181	1
148	H	69.96847	73.75379	81.04354	-820.36667	85.81767	-2596.78715	1
149	C	68.84993	72.52570	79.54270	-513.07015	236.18570	-551.87280	1
150	H	67.89907	72.49016	80.12194	1816.11944	-1183.11722	-1650.94321	1
151	H	68.55425	72.58698	78.47008	-1800.04429	-1361.53473	1526.34643	1
152	C	69.71971	71.26184	79.79579	726.08972	-253.19732	-179.64713	1
153	H	70.66984	71.24231	79.22001	1224.27271	-456.51798	-2390.90304	1
154	H	69.92036	71.04452	80.86595	1206.40339	-1150.93514	-2154.90344	1
155	N	68.92269	70.06329	79.26543	329.70796	-633.68968	-155.67358	1
156	H	69.37277	69.12372	79.43415	1348.31305	1938.76845	1359.00643	1
157	H	67.96991	69.89414	79.68563	2096.92035	1446.54551	-966.48890	1
158	H	68.75055	70.08316	78.11416	-1197.07217	-2303.53719	827.28733	1
159	C	71.22821	75.99142	78.68401	-378.01186	-556.17301	-413.96481	1
160	O	72.33404	76.11059	79.14375	-409.44433	-307.55053	-453.30833	1

161	N	70.84518	75.64678	77.46473	-429.02477	524.70884	274.08502	1
162	H	69.84173	75.76610	77.17490	1706.34263	-1425.96036	1574.38926	1
163	C	71.71563	74.89736	76.62719	-45.25864	-626.22952	478.93267	1
164	H	71.20864	74.96814	75.63963	1988.63164	570.90773	1772.87287	1
165	C	73.13002	75.60150	76.69326	551.77128	-20.49526	-564.54996	1
166	H	72.99130	76.69972	76.81851	1434.61535	-1753.10253	1513.99471	1
167	H	73.70138	75.27146	77.59445	-714.67738	1819.09770	1898.36494	1
168	C	73.91969	75.27794	75.37970	446.99263	-555.77305	338.97221	1
169	H	74.39166	74.27023	75.43263	1953.68466	1892.25957	-161.67766	1
170	H	73.23711	75.24513	74.50332	-403.03785	2688.07032	-188.43591	1
171	C	74.99890	76.41764	75.19837	567.86262	335.74681	434.04421	1
172	H	74.52102	77.42419	75.22619	-1080.02275	1568.26081	-1948.78900	1
173	H	75.72460	76.40172	76.04981	-919.54108	2111.34692	1456.13463	1
174	C	75.73007	76.20469	73.84691	195.81897	173.33862	-745.11536	1
175	H	76.24846	75.22787	73.76330	1405.67949	-2301.21089	-390.08113	1
176	H	75.10126	76.37487	72.94812	-940.37328	-1118.32446	2299.72133	1
177	N	76.85831	77.25785	73.74465	319.26422	656.36007	-42.02424	1
178	H	77.57055	77.06056	72.98521	1961.03633	619.91968	1787.09422	1
179	H	76.53240	78.31893	73.53205	854.14343	-2156.80752	1429.08711	1
180	H	77.49674	77.33304	74.58584	1237.02905	-1378.50857	-1998.28500	1
181	C	71.83172	73.34618	77.16109	532.53319	-268.57236	517.55729	1
182	O	72.42096	73.02310	78.16587	266.16714	-290.73804	-558.88002	1
183	N	71.13652	72.54963	76.33690	-226.25352	640.49678	-270.32839	1
184	H	70.76587	73.01187	75.50602	2007.69063	-1035.27229	1523.50231	1
185	C	71.66416	71.20290	76.22483	-540.76542	-573.33303	49.50000	1
186	H	72.00868	70.93438	77.25207	-2374.20950	-1036.76023	843.75774	1
187	C	70.53861	70.29663	75.66509	-77.09082	666.87422	-415.84136	1
188	H	70.01584	70.76868	74.80676	-985.81834	617.19825	2463.91927	1
189	O	69.23875	70.08246	76.68861	293.29899	-391.65602	-477.80926	1
190	H	68.62027	70.64641	76.22888	2528.72714	-681.76262	-751.27122	1
191	C	71.13702	68.92400	75.30270	252.47363	-605.14473	440.05134	1
192	H	70.36355	68.24741	74.86134	-2052.65063	1456.49051	-1043.51830	1
193	H	71.97051	69.01391	74.55989	-2152.98800	-1661.97574	-161.70652	1
194	H	71.55273	68.41284	76.20670	-473.12726	-1584.27339	2165.61725	1
195	C	72.90841	71.27359	75.13755	360.36307	488.46713	505.10056	1
196	O	72.93296	72.05248	74.21654	-200.08817	-528.03552	-385.82850	1
197	N	73.74611	70.28895	75.43917	-597.54095	-226.44775	355.20479	1
198	H	73.53907	69.72238	76.26010	2179.23655	-1300.70981	-991.33835	1
199	C	74.84062	70.03714	74.58489	-687.68921	297.39807	-249.45179	1
200	H	74.78866	70.83355	73.80764	-349.16256	-2467.37713	-1101.72831	1
201	C	76.16762	70.07021	75.48238	672.47345	361.54328	-201.62880	1
202	H	76.11194	69.30105	76.28584	1541.41502	582.18425	2169.97026	1
203	H	77.05652	69.82061	74.85849	-2534.67717	60.25153	997.72295	1
204	C	76.28867	71.47674	76.08536	574.26774	-389.43119	-377.02542	1
205	C	77.00281	72.49433	75.38463	688.82679	-287.33580	-257.96133	1
206	H	77.48223	72.27815	74.41291	331.14182	1470.38163	2269.80013	1
207	C	75.64756	71.77541	77.32556	-383.52382	-675.04808	144.24917	1
208	H	75.06643	71.00053	77.85705	4.09847	1517.59662	2262.86397	1
209	C	77.08802	73.76565	75.95491	-134.76730	428.45285	-649.50303	1
210	H	77.65049	74.54799	75.41657	-903.23433	1600.49020	2011.53387	1
211	C	75.75437	73.06601	77.85157	-335.53281	-615.00040	-364.39058	1
212	H	75.24517	73.28198	78.80773	1596.45398	-1369.33862	1732.02659	1
213	C	76.48477	74.10201	77.20094	585.48547	-340.24194	-406.23938	1
214	O	76.61176	75.41718	77.73558	-419.15649	-173.04408	-511.94141	1
215	H	76.10525	75.30091	78.57303	-1071.84350	1559.71507	-1960.13012	1
216	C	74.72359	68.51228	73.97669	291.41878	-183.13091	710.72246	1
217	O	74.77887	68.36756	72.77664	379.87695	523.47396	-222.23622	1
218	N	74.53273	67.60078	74.92267	564.30591	373.09380	277.24371	1
219	H	74.48559	67.96430	75.87313	-120.59931	-2436.07824	-1214.35098	1
220	C	74.86264	66.22892	74.71450	404.07514	-299.37480	608.84009	1
221	H	74.33544	65.68740	75.53113	-1071.07882	-841.69025	2359.66467	1
222	C	74.36306	65.85888	73.25939	-683.12807	68.71770	-390.13096	1

223	H	73.48364	66.49873	73.01180	2068.88918	1596.58590	770.89603	1
224	H	75.14019	66.13872	72.50944	1379.86429	2342.49779	-179.85638	1
225	C	73.99217	64.35099	73.11025	-176.39967	537.49466	550.97268	1
226	H	74.88894	63.69395	73.15800	-396.28051	1942.22168	1869.33314	1
227	H	73.31824	64.00972	73.92667	-94.44700	586.00678	-2659.20016	1
228	C	73.26814	64.26452	71.68469	-291.69381	-718.18079	-150.72929	1
229	H	72.36803	64.91642	71.55635	-2303.38776	1089.76242	964.62032	1
230	H	73.96243	64.44491	70.82437	884.16729	2568.80533	-207.74283	1
231	N	72.85160	62.93113	71.61039	-594.49522	-252.81478	342.29276	1
232	H	73.39207	62.26513	72.14090	-1735.17426	2084.05705	-263.71605	1
233	C	71.88103	62.50563	70.90722	595.23177	-271.52487	442.22352	1
234	N	71.15066	63.42923	70.15194	585.53813	-424.79750	-105.81303	1
235	H	71.28327	64.43363	70.04261	959.88797	1327.56823	-2177.11905	1
236	H	70.36596	63.19149	69.54433	1578.48647	16.27378	-2220.76233	1
237	N	71.73666	61.11726	71.03510	-452.17763	-390.33541	-421.51853	1
238	H	72.26714	60.43477	71.57432	470.26107	1974.25629	-1817.92087	1
239	H	71.01724	60.58603	70.54278	1856.67307	-1573.97321	-1224.35416	1
240	C	76.48557	66.05806	74.80792	-531.47271	-581.45780	-55.06206	1
241	O	77.28247	66.96814	74.76144	-243.00837	192.73507	609.52485	1
242	N	76.79304	64.72586	74.97814	343.49288	-644.25607	38.09164	1
243	H	75.85136	64.31259	74.94398	-1691.16043	-1535.97525	-1484.73099	1
244	C	77.74111	64.21309	73.99926	542.66492	350.14337	454.42563	1
245	H	77.28506	64.41599	73.00721	1209.57979	-2396.95920	463.86744	1
246	C	79.10005	64.98655	74.21751	-737.14309	145.93010	242.71942	1
247	H	79.05350	65.57967	75.15897	-1050.18303	159.36419	-2509.06125	1
248	C	80.31999	63.99906	74.23534	-706.77696	-252.88343	-245.16230	1
249	H	81.28845	64.54197	74.33978	-1624.64039	-1665.49085	1417.86935	1
250	H	80.25046	63.27960	75.08511	2566.10521	598.51109	693.22305	1
251	H	80.37284	63.39729	73.29803	-1972.69758	107.10018	-1876.34312	1
252	C	79.34698	65.91588	72.97719	412.85148	672.58832	-27.69222	1
253	H	80.30555	66.47801	73.07116	1447.02277	1762.76533	-1490.78944	1
254	H	79.39433	65.33342	72.02748	1320.77379	-145.20455	2378.68491	1
255	H	78.53056	66.67071	72.86871	-1512.10848	1470.52031	1724.75147	1
256	C	77.82637	62.63005	74.32625	-607.11113	499.56689	73.73769	1
257	O	77.72573	61.80471	73.44407	357.97126	460.81534	356.68785	1
258	N	78.10496	62.46648	75.61580	536.55407	-368.62270	332.76306	1
259	H	78.13545	63.28227	76.25564	524.38866	2297.69985	1367.20941	1
260	C	77.85758	61.19934	76.24970	46.50277	-774.29190	-147.97904	1
261	H	76.84016	60.89218	75.92210	1676.51875	1883.29066	1032.55549	1
262	C	78.97079	60.10565	75.83734	-559.41456	-34.19198	-556.30433	1
263	H	79.90779	60.62306	75.52055	-64.66664	395.18769	2695.05373	1
264	H	79.24701	59.46817	76.71128	-2703.44278	-60.40056	333.79418	1
265	C	78.41698	59.25734	74.72733	-519.76435	377.31045	459.42366	1
266	H	78.01041	59.95316	73.93086	-1746.74323	1667.50644	-1261.73691	1
267	C	79.51134	58.39632	74.10919	570.95554	16.46261	-545.27700	1
268	H	79.11506	57.76289	73.27389	2391.58273	28.05277	-1305.07271	1
269	H	80.34093	59.02045	73.68760	175.75588	917.63458	2559.43867	1
270	H	79.96613	57.70314	74.86313	-1063.97851	-2155.34650	1283.00462	1
271	C	77.29942	58.35363	75.23141	193.76014	2.62946	-765.53141	1
272	H	76.86665	57.73294	74.40515	507.39394	-846.55087	2539.60089	1
273	H	77.66709	57.64599	76.01864	1337.57841	1818.19054	1526.01994	1
274	H	76.45661	58.93745	75.68185	1100.88635	-1172.91350	-2199.08909	1
275	C	77.96341	61.63438	77.77407	-549.21115	475.64486	-309.38218	1
276	O	78.10419	62.80561	78.06622	556.06106	-390.37755	-78.24250	1
277	O	77.86954	60.64843	78.77202	-572.27940	-310.19032	-209.75862	1
278	H	77.73779	59.84515	78.18968	-1380.08193	2212.14486	790.85944	1

Listing 46: C00046.xmolout

1	276								
2	150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.7550	3020	
	0.2500	300.00	0.00	0.00	0.00	-1293.7445	0.0000	300.0000	

3	H	87.38199	78.63726	71.23284	-2043.14101	-1757.64893	399.89339	1
4	N	87.26963	78.73093	70.22582	426.75047	490.45733	-334.42467	1
5	H	86.26341	78.86670	70.15689	442.25559	-1110.30854	-2448.52907	1
6	C	88.04032	79.77897	69.65540	415.32972	-666.39213	83.73172	1
7	H	89.03757	79.55975	70.09902	879.32219	2491.00447	667.35213	1
8	C	88.03448	79.66078	68.04247	31.35357	477.41777	628.23362	1
9	H	87.03891	79.97152	67.64606	1168.38489	2240.25337	-1019.71136	1
10	H	88.77469	80.37219	67.60513	-360.43770	2534.90498	931.67112	1
11	C	88.33299	78.24841	67.62728	463.18208	512.70242	-382.34388	1
12	H	87.57039	77.58373	68.09375	1725.29117	1863.52247	-987.07854	1
13	C	88.23856	78.12170	66.11063	710.42801	-144.27427	-313.15367	1
14	H	88.38582	77.06391	65.77328	364.20195	-1033.13725	2494.72524	1
15	H	87.24087	78.45825	65.72836	2567.61904	335.80679	847.48802	1
16	H	89.01618	78.74424	65.59809	-2587.99029	680.92867	-512.16411	1
17	C	89.71118	77.79236	68.08808	268.17616	741.64379	-40.42634	1
18	H	89.93384	76.74784	67.74934	1283.54314	-1945.37420	-1411.27812	1
19	H	90.52199	78.45225	67.68574	-1258.57796	1317.15249	-2026.02085	1
20	H	89.79652	77.80123	69.20505	-2502.84526	909.80597	575.92391	1
21	C	87.42201	81.12261	70.23958	619.36578	-458.64843	-172.09273	1
22	O	87.27320	81.29788	71.50661	-81.40433	433.87611	522.34594	1
23	N	87.09350	82.00872	69.35253	175.23996	-622.20190	341.55523	1
24	H	87.26665	81.85438	68.36306	-876.57256	-303.22879	-2561.90213	1
25	C	86.75403	83.28795	69.90692	-571.88214	-534.10783	-106.15033	1
26	H	87.66148	83.90490	69.74573	-2713.20841	-16.25800	-248.80809	1
27	C	85.50300	83.83748	69.12791	166.60354	288.16399	-716.09568	1
28	H	84.65696	83.10832	69.26384	-2097.85574	1636.78449	-586.18044	1
29	O	85.66451	83.98910	67.69617	-317.80580	-363.38227	484.43082	1
30	H	84.95992	83.40502	67.35966	1863.74748	-1451.84923	1357.29467	1
31	C	85.17497	85.15664	69.92823	503.80731	517.99032	318.51606	1
32	H	84.23427	85.62975	69.56301	640.61020	-2157.10410	-1536.29104	1
33	H	85.03962	84.96098	71.01985	1687.88455	465.60692	2087.56452	1
34	H	85.98618	85.91285	69.82434	-1293.07895	-1899.88581	-1463.57452	1
35	C	86.35484	83.01086	71.52722	-153.07550	-733.68902	248.70981	1
36	O	85.11550	82.79822	71.71878	186.15459	-480.78787	-449.34387	1
37	N	87.14549	83.82227	72.28988	-487.53139	543.18517	42.03850	1
38	C	87.21104	83.65144	73.70138	-699.35871	69.34393	360.10701	1
39	H	87.20376	82.54979	73.87817	2.81126	-221.99807	-2715.58072	1
40	C	88.55237	84.39925	74.13278	-507.46439	-592.59194	122.07761	1
41	H	88.46560	84.88625	75.12990	-1975.08116	525.87560	-1801.71556	1
42	H	89.40406	83.68737	74.20878	1588.27743	-1913.22100	1113.83566	1
43	C	88.77647	85.42211	72.98118	-613.62442	-457.55993	-194.14490	1
44	H	88.17493	86.34557	73.13509	1707.54637	-721.27992	1996.92523	1
45	H	89.83511	85.74665	72.87329	758.23357	2100.81767	1560.55011	1
46	C	88.25019	84.57250	71.73235	-352.41524	704.96076	49.21465	1
47	H	87.87679	85.17063	70.86423	1714.76886	-2070.42778	443.35792	1
48	H	88.97514	83.80431	71.36582	1224.15040	1801.50881	1636.97633	1
49	C	85.89679	84.35839	74.37279	566.85117	537.05831	117.62814	1
50	O	85.37234	83.88082	75.37143	-550.26779	-406.08867	4.21666	1
51	N	85.60187	85.48439	73.75584	566.34832	-425.77725	180.18749	1
52	H	86.14575	85.70303	72.92474	644.44502	2646.80550	-52.73430	1
53	C	84.51868	86.26090	74.26756	612.34801	-281.48662	411.56221	1
54	H	84.57627	86.02336	75.35630	1667.23498	-1490.75142	1556.16753	1
55	C	84.73307	87.79548	73.88532	-714.45746	-175.43074	286.98927	1
56	H	84.56234	87.92297	72.78175	-787.09484	1763.03619	-1922.46060	1
57	O	86.03436	88.33825	74.16687	-429.46514	516.51932	-128.40526	1
58	H	86.31082	88.64333	73.27930	1981.82785	436.16847	-1818.18182	1
59	C	83.53231	88.43747	74.67510	630.79189	-468.94448	76.03230	1
60	H	83.44605	89.52970	74.47181	-1775.71861	2062.30353	131.89849	1
61	H	82.55832	87.96693	74.39607	-1855.14608	88.94118	1993.53760	1
62	H	83.65917	88.31620	75.77614	-1504.82350	-780.94249	-2132.90992	1
63	C	83.15972	85.65156	73.58014	288.57638	618.62814	-397.00270	1
64	O	82.46148	86.29814	72.83688	321.70495	-185.26452	574.37218	1

65	N	83.01286	84.39503	73.98570	-447.05792	-446.53431	367.76425	1
66	H	83.71686	83.94841	74.60731	350.31316	1975.63644	-1843.31522	1
67	C	81.78128	83.76969	73.62772	-511.23061	374.03917	-471.51480	1
68	H	81.01577	84.55944	73.79260	2234.79579	-898.70890	-1273.45190	1
69	C	81.91486	83.44114	72.06321	529.53781	-159.34528	563.72604	1
70	H	80.87361	83.37099	71.63486	654.59388	2347.94251	1217.51488	1
71	H	82.39152	84.36286	71.62491	-1526.55661	2103.42026	817.87394	1
72	O	82.59216	82.24847	71.69538	-554.84278	14.12789	399.58769	1
73	H	83.57975	82.53424	71.95489	1297.06236	2061.84854	1220.68812	1
74	C	81.63462	82.44987	74.56741	-662.15484	-412.13544	123.62687	1
75	O	82.46740	81.57489	74.65195	-540.01537	-317.05804	274.91456	1
76	N	80.47630	82.54335	75.21487	-202.76299	-690.00100	-131.49145	1
77	H	79.84067	83.33413	75.09720	-702.62132	-2617.37191	281.70413	1
78	C	79.95286	81.33130	75.76614	-491.73914	576.34187	222.73509	1
79	H	80.33009	80.50226	75.12615	1977.17978	-1823.58850	-434.68928	1
80	C	80.50871	81.20967	77.24975	-649.50797	-328.66843	306.11224	1
81	H	80.19043	82.08173	77.86040	2075.07803	1452.16490	-1004.45904	1
82	C	79.95857	79.86799	77.84147	-615.18735	-489.99689	-70.96352	1
83	H	80.32262	79.69719	78.88177	-1226.32661	-1724.38906	-1716.47170	1
84	H	78.84281	79.86147	77.87212	2381.64273	-969.84735	900.46860	1
85	H	80.27635	78.99065	77.23028	2122.74991	1702.23946	-141.36228	1
86	C	82.07379	81.11035	77.21318	-501.86074	-479.61276	-376.42482	1
87	H	82.49982	80.87248	78.21609	993.79261	-2246.95401	-1177.81305	1
88	H	82.41846	80.31604	76.50448	42.71279	-626.15391	-2651.37258	1
89	H	82.53628	82.07085	76.87578	-2026.39012	-1590.33709	-887.82922	1
90	C	78.33480	81.57763	75.73965	-672.89153	382.57394	-156.34072	1
91	O	77.83718	82.64486	76.01892	410.04627	221.86223	500.35950	1
92	N	77.73845	80.44358	75.38721	-378.11782	-443.79414	-441.10984	1
93	H	78.29722	79.60489	75.22956	2404.15973	-568.14894	1149.30085	1
94	C	76.32001	80.38549	75.42108	-544.54484	466.16019	331.29119	1
95	H	75.96310	81.41490	75.65883	-1409.80988	-170.17955	2325.32679	1
96	C	75.87553	79.82722	73.99666	-184.48284	116.78282	-758.89137	1
97	H	76.21026	80.50682	73.18136	1893.78641	1861.14652	611.04528	1
98	H	76.36891	78.84941	73.79812	-2170.79665	-974.19311	1327.50117	1
99	C	74.32569	79.67133	74.00476	389.51668	672.81878	-138.49152	1
100	H	73.99089	79.17930	74.94395	510.64577	1933.03327	1851.02484	1
101	H	73.83843	80.67096	74.02625	-2302.30869	-1105.72939	-948.89774	1
102	C	73.80526	78.83207	72.77326	-559.93427	-126.34590	542.30857	1
103	O	72.70320	78.34879	72.81270	-670.36003	-111.83166	76.36448	1
104	N	74.68367	78.75180	71.75252	-216.06729	-537.07037	446.51379	1
105	H	75.61573	79.17356	71.66255	-1251.96487	1074.12894	-2168.52500	1
106	H	74.48315	78.29698	70.85527	-2451.83023	-720.73851	944.84612	1
107	C	75.94173	79.22550	76.51191	546.24052	-563.88337	-85.11809	1
108	O	76.50890	78.16322	76.46013	71.70702	-307.40463	606.69673	1
109	N	74.93103	79.61127	77.29864	479.90863	-504.50129	222.86849	1
110	C	74.61245	78.84770	78.47119	75.51268	-600.91904	506.73700	1
111	H	75.59813	78.55642	78.89953	-2033.61562	1795.30103	254.89480	1
112	C	73.78083	79.86433	79.35412	523.79067	517.99274	284.45581	1
113	H	73.00865	79.35645	79.97484	1599.61665	-1127.00911	1895.98173	1
114	H	74.44311	80.40494	80.06680	-1881.83093	1275.82488	-1501.55016	1
115	C	73.16664	80.85114	78.30992	-600.05639	-404.05026	316.64485	1
116	H	72.23930	80.43705	77.85566	-2597.05260	496.36221	657.73249	1
117	H	72.89149	81.83985	78.74197	-1666.24518	1294.38985	-1723.90591	1
118	C	74.34461	80.94455	77.24945	493.57570	-129.95376	-602.56394	1
119	H	74.02437	81.16083	76.20366	-1469.08415	-637.84797	2204.22581	1
120	H	75.16658	81.64361	77.53591	-1038.97840	1068.88701	-2280.71789	1
121	C	73.74849	77.50141	78.12156	188.88100	241.05089	-727.87821	1
122	O	73.93468	76.50788	78.82680	531.88613	-49.19943	427.07960	1
123	N	72.82034	77.68741	77.19871	708.14833	26.93417	-179.73509	1
124	H	72.95255	78.64126	76.85554	-2232.69501	-1179.09831	1023.94816	1
125	C	72.19308	76.65364	76.39213	-738.32412	259.92548	104.42456	1
126	H	71.72426	77.23020	75.55824	2028.89123	1260.02983	1311.33324	1

127	C	73.25911	75.68074	75.91430	-258.65678	-345.52513	661.28459	1
128	H	73.77793	75.27867	76.81498	-1826.06090	-1801.46097	-918.64554	1
129	C	72.64557	74.52113	75.15092	-541.23400	531.92970	-218.41428	1
130	H	73.41532	73.75055	74.87059	1311.73218	-2219.18200	882.19023	1
131	H	71.85000	73.99898	75.75226	-1048.71298	1223.58118	-2196.97971	1
132	H	72.16005	74.87012	74.19778	419.06414	1903.92898	1903.44670	1
133	C	74.29913	76.36922	75.05111	-423.86431	152.66566	-648.55262	1
134	H	75.05477	75.64081	74.64685	105.68386	-2342.50080	1387.51238	1
135	H	73.82559	76.88924	74.16814	-1695.63603	-1484.73621	-1531.02793	1
136	H	74.87220	77.14906	75.63848	-1853.57121	-487.39031	1936.59343	1
137	C	71.04498	75.80164	77.25851	539.71428	-510.58232	267.58633	1
138	O	69.99343	75.58786	76.71773	-15.93758	-278.34085	-624.49402	1
139	N	71.50328	75.37967	78.41479	-676.81886	12.05292	276.17960	1
140	H	72.47819	75.65150	78.70695	-1694.44250	-373.84189	-2100.66098	1
141	C	70.64292	74.79237	79.39235	412.33078	-664.70360	108.35451	1
142	H	71.08726	75.15051	80.34895	1765.77476	1294.44366	1621.76594	1
143	C	69.14480	75.26647	79.18594	-179.66635	-721.95667	-264.73915	1
144	H	69.00456	76.35452	78.95504	-607.34922	2587.87032	-598.10018	1
145	H	68.69705	74.75147	78.30120	-359.69332	-1479.13954	-2259.74260	1
146	C	68.35679	74.91708	80.49122	-240.01076	616.02425	431.85322	1
147	H	68.53532	73.84342	80.76644	-1359.17131	782.54425	2227.99181	1
148	H	68.72013	75.52082	81.35342	-820.36667	85.81767	-2596.78715	1
149	C	66.81621	75.16554	80.23735	-513.07015	236.18570	-551.87280	1
150	H	66.59522	76.25217	80.12737	1816.11944	-1183.11722	-1650.94321	1
151	H	66.48665	74.69000	79.28485	-1800.04429	-1361.53473	1526.34643	1
152	C	66.06449	74.55350	81.44272	726.08972	-253.19732	-179.64713	1
153	H	66.14875	73.45120	81.52434	1224.27271	-456.51798	-2390.90304	1
154	H	66.29790	75.02278	82.41912	1206.40339	-1150.93514	-2154.90344	1
155	N	64.53591	74.81747	81.23213	329.70796	-633.68968	-155.67358	1
156	H	63.89539	74.43363	81.98574	1348.31305	1938.76845	1359.00643	1
157	H	64.22400	75.83121	81.19164	2096.92035	1446.54551	-966.48890	1
158	H	64.09186	74.41639	80.35530	-1197.07217	-2303.53719	827.28733	1
159	C	70.68463	73.16745	79.30759	-378.01186	-556.17301	-413.96481	1
160	O	69.89307	72.52152	80.00309	-409.44433	-307.55053	-453.30833	1
161	N	71.61528	72.73296	78.49297	-429.02477	524.70884	274.08502	1
162	H	72.11376	73.49100	78.02875	1706.34263	-1425.96036	1574.38926	1
163	C	72.03389	71.38245	78.36968	-45.25864	-626.22952	478.93267	1
164	H	72.98377	71.45566	77.79382	1988.63164	570.90773	1772.87287	1
165	C	72.21377	70.77284	79.82099	551.77128	-20.49526	-564.54996	1
166	H	72.97801	71.34087	80.39791	1434.61535	-1753.10253	1513.99471	1
167	H	71.26791	70.86728	80.40725	-714.67738	1819.09770	1898.36494	1
168	C	72.62233	69.27115	79.66495	446.99263	-555.77305	338.97221	1
169	H	71.86827	68.71950	79.06042	1953.68466	1892.25957	-161.67766	1
170	H	73.58419	69.17622	79.11311	-403.03785	2688.07032	-188.43591	1
171	C	72.73572	68.64407	81.11255	567.86262	335.74681	434.04421	1
172	H	73.48840	69.19111	81.72543	-1080.02275	1568.26081	-1948.78900	1
173	H	71.77070	68.73810	81.66191	-919.54108	2111.34692	1456.13463	1
174	C	73.13334	67.15888	80.94621	195.81897	173.33862	-745.11536	1
175	H	72.33510	66.50900	80.53544	1405.67949	-2301.21089	-390.08113	1
176	H	74.07804	66.99373	80.39056	-940.37328	-1118.32446	2299.72133	1
177	N	73.42359	66.59434	82.37763	319.26422	656.36007	-42.02424	1
178	H	73.71575	65.57545	82.42166	1961.03633	619.91968	1787.09422	1
179	H	74.20719	67.05773	82.92382	854.14343	-2156.80752	1429.08711	1
180	H	72.62704	66.61687	83.07866	1237.02905	-1378.50857	-1998.28500	1
181	C	70.92782	70.45849	77.58284	532.53319	-268.57236	517.55729	1
182	O	71.34179	69.70824	76.72499	266.16714	-290.73804	-558.88002	1
183	N	69.72481	70.57000	78.10743	-226.25352	640.49678	-270.32839	1
184	H	69.61076	71.22368	78.92442	2007.69063	-1035.27229	1523.50231	1
185	C	68.54528	70.18425	77.41110	-540.76542	-573.33303	49.50000	1
186	H	67.76273	70.83794	77.85639	-2374.20950	-1036.76023	843.75774	1
187	C	68.72274	70.42780	75.83993	-77.09082	666.87422	-415.84136	1
188	H	69.56290	69.77158	75.47139	-985.81834	617.19825	2463.91927	1

189	O	69.04971	71.78055	75.47066	293.29899	-391.65602	-477.80926	1
190	H	69.98178	71.67285	75.19279	2528.72714	-681.76262	-751.27122	1
191	C	67.36998	69.88863	75.24791	252.47363	-605.14473	440.05134	1
192	H	67.35694	69.96126	74.13615	-2052.65063	1456.49051	-1043.51830	1
193	H	67.19818	68.81731	75.50834	-2152.98800	-1661.97574	-161.70652	1
194	H	66.49823	70.46963	75.62915	-473.12726	-1584.27339	2165.61725	1
195	C	68.23416	68.61292	77.72142	360.36307	488.46713	505.10056	1
196	O	67.07415	68.23100	77.71293	-200.08817	-528.03552	-385.82850	1
197	N	69.34988	67.92163	77.86377	-597.54095	-226.44775	355.20479	1
198	H	70.22390	68.45419	77.73901	2179.23655	-1300.70981	-991.33835	1
199	C	69.41663	66.61308	78.39222	-687.68921	297.39807	-249.45179	1
200	H	70.46940	66.51275	78.73594	-349.16256	-2467.37713	-1101.72831	1
201	C	68.33322	66.39225	79.54894	672.47345	361.54328	-201.62880	1
202	H	67.30982	66.49764	79.11452	1541.41502	582.18425	2169.97026	1
203	H	68.41807	65.34969	79.93357	-2534.67717	60.25153	997.72295	1
204	C	68.51895	67.39940	80.69225	574.26774	-389.43119	-377.02542	1
205	C	69.49726	67.18359	81.70887	688.82679	-287.33580	-257.96133	1
206	H	70.16427	66.30317	81.67559	331.14182	1470.38163	2269.80013	1
207	C	67.66989	68.54643	80.73779	-383.52382	-675.04808	144.24917	1
208	H	66.92216	68.72040	79.93985	4.09847	1517.59662	2262.86397	1
209	C	69.57985	68.10179	82.75558	-134.76730	428.45285	-649.50303	1
210	H	70.32515	67.92872	83.55109	-903.23433	1600.49020	2011.53387	1
211	C	67.79387	69.43933	81.80385	-335.53281	-615.00040	-364.39058	1
212	H	67.12666	70.31886	81.82974	1596.45398	-1369.33862	1732.02659	1
213	C	68.74197	69.25074	82.85162	585.48547	-340.24194	-406.23938	1
214	O	68.86757	70.14613	83.94543	-419.15649	-173.04408	-511.94141	1
215	H	68.15808	70.79157	83.71349	-1071.84350	1559.71507	-1960.13012	1
216	C	69.02806	65.49696	77.26302	291.41878	-183.13091	710.72246	1
217	O	69.47405	64.37670	77.32426	379.87695	523.47396	-222.23622	1
218	N	68.08533	65.96816	76.44573	564.30591	373.09380	277.24371	1
219	H	67.77965	66.95000	76.55700	-120.59931	-2436.07824	-1214.35098	1
220	C	67.91125	65.28132	75.20349	404.07514	-299.37480	608.84009	1
221	H	68.06180	64.20147	75.43537	-1071.07882	-841.69025	2359.66467	1
222	C	66.46375	65.68504	74.70563	-683.12807	68.71770	-390.13096	1
223	H	65.73150	65.57130	75.53661	2068.88918	1596.58590	770.89603	1
224	H	66.42780	66.76130	74.42253	1379.86429	2342.49779	-179.85638	1
225	C	66.07416	64.77886	73.49745	-176.39967	537.49466	550.97268	1
226	H	66.70708	64.99665	72.60178	-396.28051	1942.22168	1869.33314	1
227	H	66.23856	63.70474	73.73737	-94.44700	586.00678	-2659.20016	1
228	C	64.53120	65.07761	73.20769	-291.69381	-718.18079	-150.72929	1
229	H	63.85612	65.02627	74.10006	-2303.38776	1089.76242	964.62032	1
230	H	64.31612	66.03788	72.67359	884.16729	2568.80533	-207.74283	1
231	N	64.17349	64.01547	72.36504	-594.49522	-252.81478	342.29276	1
232	H	64.89814	63.35164	72.14009	-1735.17426	2084.05705	-263.71605	1
233	C	63.01209	63.83627	71.88104	595.23177	-271.52487	442.22352	1
234	N	62.02113	64.77036	72.20189	585.53813	-424.79750	-105.81303	1
235	H	62.08587	65.61294	72.77189	959.88797	1327.56823	-2177.11905	1
236	H	61.05781	64.73791	71.86648	1578.48647	16.27378	-2220.76233	1
237	N	62.96969	62.67738	71.09349	-452.17763	-390.33541	-421.51853	1
238	H	63.69368	61.99842	70.86277	470.26107	1974.25629	-1817.92087	1
239	H	62.12569	62.35720	70.61695	1856.67307	-1573.97321	-1224.35416	1
240	C	69.00416	65.86829	74.13636	-531.47271	-581.45780	-55.06206	1
241	O	69.40745	67.00397	74.14027	-243.00837	192.73507	609.52485	1
242	N	69.28434	64.88417	73.27072	343.49288	-644.25607	38.09164	1
243	H	68.74763	64.02896	73.41044	-1691.16043	-1535.97525	-1484.73099	1
244	C	69.98245	65.17569	72.01646	542.66492	350.14337	454.42563	1
245	H	70.90312	65.72310	72.32654	1209.57979	-2396.95920	463.86744	1
246	C	70.22847	63.88081	71.26977	-737.14309	145.93010	242.71942	1
247	H	69.23568	63.43460	71.03419	-1050.18303	159.36419	-2509.06125	1
248	C	70.95390	64.13874	69.96034	-706.77696	-252.88343	-245.16230	1
249	H	71.05496	63.20219	69.34647	-1624.64039	-1665.49085	1417.86935	1
250	H	70.41461	64.89810	69.32855	2566.10521	598.51109	693.22305	1

251	H	71.99103	64.53781	70.13269	-1972.69758	107.10018	-1876.34312	1
252	C	71.00046	62.86804	72.09602	412.85148	672.58832	-27.69222	1
253	H	71.13392	61.89623	71.54587	1447.02277	1762.76533	-1490.78944	1
254	H	72.02610	63.24662	72.35852	1320.77379	-145.20455	2378.68491	1
255	H	70.47718	62.63717	73.06413	-1512.10848	1470.52031	1724.75147	1
256	C	68.95127	66.11702	71.10908	-607.11113	499.56689	73.73769	1
257	O	67.82492	65.77390	70.84617	357.97126	460.81534	356.68785	1
258	N	69.60133	67.21442	70.73932	536.55407	-368.62270	332.76306	1
259	H	70.56737	67.31432	71.05120	524.38866	2297.69985	1367.20941	1
260	C	69.18749	67.86581	69.54511	46.50277	-774.29190	-147.97904	1
261	H	68.33672	67.24993	69.17227	1676.51875	1883.29066	1032.55549	1
262	C	68.75939	69.38058	69.91914	-559.41456	-34.19198	-556.30433	1
263	H	69.57704	69.86551	70.50377	-64.66664	395.18769	2695.05373	1
264	H	68.62153	70.00198	69.00286	-2703.44278	-60.40056	333.79418	1
265	C	67.49082	69.31869	70.72422	-519.76435	377.31045	459.42366	1
266	H	67.59500	68.50041	71.47378	-1746.74323	1667.50644	-1261.73691	1
267	C	67.26080	70.62984	71.46556	570.95554	16.46261	-545.27700	1
268	H	66.32315	70.60011	72.07820	2391.58273	28.05277	-1305.07271	1
269	H	68.10642	70.86626	72.16217	175.75588	917.63458	2559.43867	1
270	H	67.16524	71.49223	70.75674	-1063.97851	-2155.34650	1283.00462	1
271	C	66.29272	69.01955	69.83226	193.76014	2.62946	-765.53141	1
272	H	65.33612	69.00497	70.41507	507.39394	-846.55087	2539.60089	1
273	H	66.17742	69.78825	69.02503	1337.57841	1818.19054	1526.01994	1
274	H	66.38762	68.02232	69.33042	1100.88635	-1172.91350	-2199.08909	1
275	C	70.47675	67.90316	68.58413	-549.21115	475.64486	-309.38218	1
276	O	71.51716	67.36543	68.86271	556.06106	-390.37755	-78.24250	1
277	O	70.33161	68.59552	67.35710	-572.27940	-310.19032	-209.75862	1
278	H	69.37586	68.86151	67.44273	-1380.08193	2212.14486	790.85944	1

Listing 47: C00047.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.7078	0.0000	300.0000
3	H	76.71315	73.25631	82.38942	-2043.14101	-1757.64893	399.89339		1
4	N	77.61161	72.89208	82.07683	426.75047	490.45733	-334.42467		1
5	H	77.32416	72.32704	81.27854	442.25559	-1110.30854	-2448.52907		1
6	C	78.54684	73.90031	81.72965	415.32972	-666.39213	83.73172		1
7	H	77.89164	74.72760	81.38330	879.32219	2491.00447	667.35213		1
8	C	79.37578	74.31727	83.04416	31.35357	477.41777	628.23362		1
9	H	79.89793	73.41561	83.44579	1168.38489	2240.25337	-1019.71136		1
10	H	80.17602	75.04920	82.77590	-360.43770	2534.90498	931.67112		1
11	C	78.48071	74.90339	84.10654	463.18208	512.70242	-382.34388		1
12	H	77.65750	74.18264	84.30967	1725.29117	1863.52247	-987.07854		1
13	C	79.26264	75.11867	85.39692	710.42801	-144.27427	-313.15367		1
14	H	78.61438	75.53700	86.20985	364.20195	-1033.13725	2494.72524		1
15	H	79.70179	74.16238	85.78186	2567.61904	335.80679	847.48802		1
16	H	80.11051	75.83663	85.25025	-2587.99029	680.92867	-512.16411		1
17	C	77.87494	76.22915	83.66693	268.17616	741.64379	-40.42634		1
18	H	77.25296	76.68773	84.47894	1283.54314	-1945.37420	-1411.27812		1
19	H	78.66755	76.97458	83.39809	-1258.57796	1317.15249	-2026.02085		1
20	H	77.21269	76.10974	82.77138	-2502.84526	909.80597	575.92391		1
21	C	79.41965	73.27712	80.50520	619.36578	-458.64843	-172.09273		1
22	O	78.88612	72.90865	79.47654	-81.40433	433.87611	522.34594		1
23	N	80.71533	73.27954	80.79156	175.23996	-622.20190	341.55523		1
24	H	81.03178	73.59340	81.70639	-876.57256	-303.22879	-2561.90213		1
25	C	81.63591	72.72131	79.86072	-571.88214	-534.10783	-106.15033		1
26	H	81.03800	72.54026	78.93911	-2713.20841	-16.25800	-248.80809		1
27	C	82.83023	73.78150	79.70289	166.60354	288.16399	-716.09568		1
28	H	83.33753	73.88913	80.69980	-2097.85574	1636.78449	-586.18044		1
29	O	82.42125	75.10943	79.31616	-317.80580	-363.38227	484.43082		1
30	H	82.71196	75.62416	80.09493	1863.74748	-1451.84923	1357.29467		1

31	C	83.80025	73.04361	78.71306	503.80731	517.99032	318.51606	1
32	H	84.71925	73.64487	78.52023	640.61020	-2157.10410	-1536.29104	1
33	H	84.12982	72.05430	79.11460	1687.88455	465.60692	2087.56452	1
34	H	83.31766	72.84806	77.72214	-1293.07895	-1899.88581	-1463.57452	1
35	C	82.25374	71.37402	80.53557	-153.07550	-733.68902	248.70981	1
36	O	83.29937	71.46316	81.15942	186.15459	-480.78787	-449.34387	1
37	N	81.49819	70.29989	80.31469	-487.53139	543.18517	42.03850	1
38	C	81.86865	69.00916	80.82400	-699.35871	69.34393	360.10701	1
39	H	82.27816	69.19515	81.84322	2.81126	-221.99807	-2715.58072	1
40	C	80.50560	68.20572	80.75292	-507.46439	-592.59194	122.07761	1
41	H	80.65624	67.10250	80.72826	-1975.08116	525.87560	-1801.71556	1
42	H	79.85385	68.42300	81.62885	1588.27743	-1913.22100	1113.83566	1
43	C	79.89449	68.77871	79.43545	-613.62442	-457.55993	-194.14490	1
44	H	80.41103	68.35676	78.54301	1707.54637	-721.27992	1996.92523	1
45	H	78.80955	68.56583	79.31115	758.23357	2100.81767	1560.55011	1
46	C	80.21565	70.32367	79.62224	-352.41524	704.96076	49.21465	1
47	H	80.33169	70.90160	78.67992	1714.76886	-2070.42778	443.35792	1
48	H	79.51400	70.87043	80.29849	1224.15040	1801.50881	1636.97633	1
49	C	82.99703	68.39564	79.80081	566.85117	537.05831	117.62814	1
50	O	82.75467	67.39945	79.16674	-550.26779	-406.08867	4.21666	1
51	N	84.07891	69.15282	79.85725	566.34832	-425.77725	180.18749	1
52	H	84.07302	69.97783	80.49669	644.44502	2646.80550	-52.73430	1
53	C	85.22429	68.92116	79.04723	612.34801	-281.48662	411.56221	1
54	H	86.04670	69.37111	79.64686	1667.23498	-1490.75142	1556.16753	1
55	C	85.42883	67.35130	78.83070	-714.45746	-175.43074	286.98927	1
56	H	84.56276	66.96615	78.21424	-787.09484	1763.03619	-1922.46060	1
57	O	85.44985	66.58405	80.05665	-429.46514	516.51932	-128.40526	1
58	H	84.51932	66.27272	80.07078	1981.82785	436.16847	-1818.18182	1
59	C	86.73533	67.23270	77.96632	630.79189	-468.94448	76.03230	1
60	H	86.97610	66.16672	77.74436	-1775.71861	2062.30353	131.89849	1
61	H	86.64156	67.76071	76.98585	-1855.14608	88.94118	1993.53760	1
62	H	87.61536	67.66632	78.49589	-1504.82350	-780.94249	-2132.90992	1
63	C	85.05396	69.73969	77.64866	288.57638	618.62814	-397.00270	1
64	O	86.02481	69.86589	76.93168	321.70495	-185.26452	574.37218	1
65	N	83.83055	70.23311	77.44563	-447.05792	-446.53431	367.76425	1
66	H	83.10539	69.98526	78.11809	350.31316	1975.63644	-1843.31522	1
67	C	83.57187	70.69161	76.12216	-511.23061	374.03917	-471.51480	1
68	H	84.56882	71.04316	75.76738	2234.79579	-898.70890	-1273.45190	1
69	C	83.07037	69.40963	75.31028	529.53781	-159.34528	563.72604	1
70	H	83.15047	69.66926	74.22212	654.59388	2347.94251	1217.51488	1
71	H	83.80927	68.58480	75.50740	-1526.55661	2103.42026	817.87394	1
72	O	81.75761	68.89116	75.63951	-554.84278	14.12789	399.58769	1
73	H	81.19376	69.53460	75.15777	1297.06236	2061.84854	1220.68812	1
74	C	82.41301	71.85433	76.10008	-662.15484	-412.13544	123.62687	1
75	O	82.67285	72.89530	75.53071	-540.01537	-317.05804	274.91456	1
76	N	81.32388	71.51768	76.77824	-202.76299	-690.00100	-131.49145	1
77	H	81.36535	70.56128	77.13511	-702.62132	-2617.37191	281.70413	1
78	C	80.06501	72.17530	76.62628	-491.73914	576.34187	222.73509	1
79	H	79.56360	72.11576	77.62652	1977.17978	-1823.58850	-434.68928	1
80	C	80.23032	73.66573	76.12418	-649.50797	-328.66843	306.11224	1
81	H	80.75716	73.70364	75.13897	2075.07803	1452.16490	-1004.45904	1
82	C	78.78430	74.26538	76.01936	-615.18735	-489.99689	-70.96352	1
83	H	78.80331	75.33485	75.70422	-1226.32661	-1724.38906	-1716.47170	1
84	H	78.16408	73.71195	75.27541	2381.64273	-969.84735	900.46860	1
85	H	78.25069	74.21530	76.99778	2122.74991	1702.23946	-141.36228	1
86	C	80.97889	74.54805	77.18725	-501.86074	-479.61276	-376.42482	1
87	H	80.93531	75.63247	76.93039	993.79261	-2246.95401	-1177.81305	1
88	H	80.54229	74.43108	78.20975	42.71279	-626.15391	-2651.37258	1
89	H	82.05980	74.27182	77.24668	-2026.39012	-1590.33709	-887.82922	1
90	C	79.23581	71.32798	75.49387	-672.89153	382.57394	-156.34072	1
91	O	79.72850	70.89961	74.47059	410.04627	221.86223	500.35950	1
92	N	77.98805	71.22965	75.92685	-378.11782	-443.79414	-441.10984	1

93	H	77.75742	71.73028	76.78370	2404.15973	-568.14894	1149.30085	1
94	C	76.94262	70.80104	75.03133	-544.54484	466.16019	331.29119	1
95	H	76.92818	71.58505	74.24234	-1409.80988	-170.17955	2325.32679	1
96	C	77.33026	69.38989	74.42882	-184.48284	116.78282	-758.89137	1
97	H	78.33283	69.43221	73.92926	1893.78641	1861.14652	611.04528	1
98	H	77.42293	68.62857	75.23796	-2170.79665	-974.19311	1327.50117	1
99	C	76.20294	68.99933	73.42143	389.51668	672.81878	-138.49152	1
100	H	75.20649	69.07251	73.91750	510.64577	1933.03327	1851.02484	1
101	H	76.14470	69.74716	72.59992	-2302.30869	-1105.72939	-948.89774	1
102	C	76.39001	67.55896	72.81223	-559.93427	-126.34590	542.30857	1
103	O	75.55613	67.11558	72.06509	-670.36003	-111.83166	76.36448	1
104	N	77.52563	66.93901	73.20042	-216.06729	-537.07037	446.51379	1
105	H	78.28613	67.27578	73.80234	-1251.96487	1074.12894	-2168.52500	1
106	H	77.81336	66.01225	72.86811	-2451.83023	-720.73851	944.84612	1
107	C	75.53623	70.68105	75.82621	546.24052	-563.88337	-85.11809	1
108	O	74.54519	70.87032	75.16445	71.70702	-307.40463	606.69673	1
109	N	75.60587	70.23347	77.09054	479.90863	-504.50129	222.86849	1
110	C	74.39933	70.17850	77.85817	75.51268	-600.91904	506.73700	1
111	H	73.57495	70.15265	77.10620	-2033.61562	1795.30103	254.89480	1
112	C	74.62426	68.86474	78.71928	523.79067	517.99274	284.45581	1
113	H	73.99567	68.83589	79.63719	1599.61665	-1127.00911	1895.98173	1
114	H	74.38527	67.94727	78.13642	-1881.83093	1275.82488	-1501.55016	1
115	C	76.15175	68.96307	79.02249	-600.05639	-404.05026	316.64485	1
116	H	76.34875	69.73448	79.80372	-2597.05260	496.36221	657.73249	1
117	H	76.60119	68.01081	79.38408	-1666.24518	1294.38985	-1723.90591	1
118	C	76.70295	69.42267	77.60627	493.57570	-129.95376	-602.56394	1
119	H	77.62654	70.04407	77.64720	-1469.08415	-637.84797	2204.22581	1
120	H	76.84916	68.60138	76.86453	-1038.97840	1068.88701	-2280.71789	1
121	C	74.33572	71.49433	78.84233	188.88100	241.05089	-727.87821	1
122	O	74.93199	71.52620	79.89641	531.88613	-49.19943	427.07960	1
123	N	73.57581	72.43686	78.29968	708.14833	26.93417	-179.73509	1
124	H	73.19652	72.27646	77.36783	-2232.69501	-1179.09831	1023.94816	1
125	C	73.39041	73.61542	79.08058	-738.32412	259.92548	104.42456	1
126	H	73.41659	73.22658	80.12452	2028.89123	1260.02983	1311.33324	1
127	C	74.61955	74.59144	78.82207	-258.65678	-345.52513	661.28459	1
128	H	74.66897	74.88622	77.75155	-1826.06090	-1801.46097	-918.64554	1
129	C	74.40731	75.83623	79.74883	-541.23400	531.92970	-218.41428	1
130	H	75.19588	76.60935	79.59413	1311.73218	-2219.18200	882.19023	1
131	H	73.41677	76.31882	79.55734	-1048.71298	1223.58118	-2196.97971	1
132	H	74.42739	75.55014	80.82694	419.06414	1903.92898	1903.44670	1
133	C	75.94811	73.88902	79.26929	-423.86431	152.66566	-648.55262	1
134	H	76.82903	74.56911	79.18964	105.68386	-2342.50080	1387.51238	1
135	H	75.88459	73.54817	80.33056	-1695.63603	-1484.73621	-1531.02793	1
136	H	76.16918	72.98660	78.64789	-1853.57121	-487.39031	1936.59343	1
137	C	72.02076	74.43007	78.67750	539.71428	-510.58232	267.58633	1
138	O	71.49497	75.08089	79.55508	-15.93758	-278.34085	-624.49402	1
139	N	71.76353	74.42277	77.37777	-676.81886	12.05292	276.17960	1
140	H	72.38883	73.81370	76.85404	-1694.44250	-373.84189	-2100.66098	1
141	C	70.47221	74.75365	76.83841	412.33078	-664.70360	108.35451	1
142	H	70.09245	73.80393	76.40032	1765.77476	1294.44366	1621.76594	1
143	C	69.52541	75.36737	77.93882	-179.66635	-721.95667	-264.73915	1
144	H	69.38646	74.65275	78.78388	-607.34922	2587.87032	-598.10018	1
145	H	70.00589	76.26698	78.39280	-359.69332	-1479.13954	-2259.74260	1
146	C	68.15142	75.75585	77.29264	-240.01076	616.02425	431.85322	1
147	H	68.30814	76.43024	76.41991	-1359.17131	782.54425	2227.99181	1
148	H	67.62120	74.86119	76.89724	-820.36667	85.81767	-2596.78715	1
149	C	67.30542	76.47119	78.42100	-513.07015	236.18570	-551.87280	1
150	H	67.09274	75.76787	79.25879	1816.11944	-1183.11722	-1650.94321	1
151	H	67.88349	77.30938	78.87380	-1800.04429	-1361.53473	1526.34643	1
152	C	65.99022	76.99902	77.80294	726.08972	-253.19732	-179.64713	1
153	H	66.12360	77.79873	77.04735	1224.27271	-456.51798	-2390.90304	1
154	H	65.31559	76.21346	77.40838	1206.40339	-1150.93514	-2154.90344	1

155	N	65.17424	77.67875	78.95540	329.70796	-633.68968	-155.67358	1
156	H	64.24413	78.10358	78.67323	1348.31305	1938.76845	1359.00643	1
157	H	64.88290	77.06161	79.76829	2096.92035	1446.54551	-966.48890	1
158	H	65.63323	78.49521	79.45473	-1197.07217	-2303.53719	827.28733	1
159	C	70.69986	75.87776	75.68339	-378.01186	-556.17301	-413.96481	1
160	O	69.96744	75.91487	74.69462	-409.44433	-307.55053	-453.30833	1
161	N	71.66117	76.70805	76.02893	-429.02477	524.70884	274.08502	1
162	H	72.15487	76.46964	76.88728	1706.34263	-1425.96036	1574.38926	1
163	C	71.91952	77.87766	75.25338	-45.25864	-626.22952	478.93267	1
164	H	70.90313	78.15346	74.89017	1988.63164	570.90773	1772.87287	1
165	C	72.61661	78.94511	76.18505	551.77128	-20.49526	-564.54996	1
166	H	71.96903	79.18796	77.05756	1434.61535	-1753.10253	1513.99471	1
167	H	73.56320	78.54443	76.61167	-714.67738	1819.09770	1898.36494	1
168	C	72.88802	80.21693	75.31286	446.99263	-555.77305	338.97221	1
169	H	73.61762	79.98329	74.50191	1953.68466	1892.25957	-161.67766	1
170	H	71.95049	80.56037	74.79930	-403.03785	2688.07032	-188.43591	1
171	C	73.43428	81.36837	76.24730	567.86262	335.74681	434.04421	1
172	H	72.70466	81.60271	77.05657	-1080.02275	1568.26081	-1948.78900	1
173	H	74.37474	81.06079	76.75951	-919.54108	2111.34692	1456.13463	1
174	C	73.66234	82.60290	75.34252	195.81897	173.33862	-745.11536	1
175	H	74.45001	82.47182	74.57344	1405.67949	-2301.21089	-390.08113	1
176	H	72.73876	83.00802	74.87666	-940.37328	-1118.32446	2299.72133	1
177	N	74.17741	83.76471	76.25194	319.26422	656.36007	-42.02424	1
178	H	74.41189	84.67188	75.75443	1961.03633	619.91968	1787.09422	1
179	H	73.50115	84.10665	76.99406	854.14343	-2156.80752	1429.08711	1
180	H	75.06139	83.59570	76.81546	1237.02905	-1378.50857	-1998.28500	1
181	C	72.88600	77.44030	73.99970	532.53319	-268.57236	517.55729	1
182	O	74.01102	77.84135	73.84668	266.16714	-290.73804	-558.88002	1
183	N	72.12655	76.69216	73.19923	-226.25352	640.49678	-270.32839	1
184	H	71.16541	76.42435	73.53281	2007.69063	-1035.27229	1523.50231	1
185	C	72.82075	75.83775	72.29123	-540.76542	-573.33303	49.50000	1
186	H	73.86390	76.23066	72.25345	-2374.20950	-1036.76023	843.75774	1
187	C	72.73255	74.39805	72.98444	-77.09082	666.87422	-415.84136	1
188	H	71.64355	74.13580	73.08669	-985.81834	617.19825	2463.91927	1
189	O	73.26076	74.33480	74.32810	293.29899	-391.65602	-477.80926	1
190	H	72.45557	74.51274	74.85436	2528.72714	-681.76262	-751.27122	1
191	C	73.41918	73.43592	71.95216	252.47363	-605.14473	440.05134	1
192	H	73.43451	72.38450	72.32454	-2052.65063	1456.49051	-1043.51830	1
193	H	72.89260	73.42986	70.96641	-2152.98800	-1661.97574	-161.70652	1
194	H	74.47712	73.73291	71.76037	-473.12726	-1584.27339	2165.61725	1
195	C	72.06586	75.85856	70.84601	360.36307	488.46713	505.10056	1
196	O	72.59997	75.35156	69.88499	-200.08817	-528.03552	-385.82850	1
197	N	70.83394	76.37561	70.90094	-597.54095	-226.44775	355.20479	1
198	H	70.57126	76.82551	71.77644	2179.23655	-1300.70981	-991.33835	1
199	C	70.25490	76.78044	69.66735	-687.68921	297.39807	-249.45179	1
200	H	70.66257	76.07877	68.90229	-349.16256	-2467.37713	-1101.72831	1
201	C	68.66466	76.78387	69.83987	672.47345	361.54328	-201.62880	1
202	H	68.39864	77.55627	70.59277	1541.41502	582.18425	2169.97026	1
203	H	68.18785	77.08731	68.87983	-2534.67717	60.25153	997.72295	1
204	C	68.12895	75.42109	70.29703	574.26774	-389.43119	-377.02542	1
205	C	67.82525	74.40615	69.34008	688.82679	-287.33580	-257.96133	1
206	H	68.01298	74.56975	68.26347	331.14182	1470.38163	2269.80013	1
207	C	67.90647	75.19296	71.68959	-383.52382	-675.04808	144.24917	1
208	H	68.16564	75.96596	72.43599	4.09847	1517.59662	2262.86397	1
209	C	67.27268	73.20841	69.79331	-134.76730	428.45285	-649.50303	1
210	H	67.02777	72.42618	69.05372	-903.23433	1600.49020	2011.53387	1
211	C	67.34668	73.97849	72.09201	-335.53281	-615.00040	-364.39058	1
212	H	67.16635	73.81967	73.16966	1596.45398	-1369.33862	1732.02659	1
213	C	67.00232	72.94814	71.16835	585.48547	-340.24194	-406.23938	1
214	O	66.42664	71.71389	71.56741	-419.15649	-173.04408	-511.94141	1
215	H	66.35334	71.87050	72.53851	-1071.84350	1559.71507	-1960.13012	1
216	C	70.63209	78.34893	69.40818	291.41878	-183.13091	710.72246	1

217	O	70.99169	79.11093	70.27262	379.87695	523.47396	-222.23622	1
218	N	70.25160	78.62206	68.14479	564.30591	373.09380	277.24371	1
219	H	70.04818	77.77239	67.61699	-120.59931	-2436.07824	-1214.35098	1
220	C	70.92042	79.71924	67.47427	404.07514	-299.37480	608.84009	1
221	H	72.00767	79.48868	67.50427	-1071.07882	-841.69025	2359.66467	1
222	C	70.30548	79.74028	66.02721	-683.12807	68.71770	-390.13096	1
223	H	70.47487	78.77305	65.50177	2068.88918	1596.58590	770.89603	1
224	H	69.19973	79.85494	66.09677	1379.86429	2342.49779	-179.85638	1
225	C	70.92846	80.92792	65.22347	-176.39967	537.49466	550.97268	1
226	H	70.91510	81.86761	65.82016	-396.28051	1942.22168	1869.33314	1
227	H	71.99722	80.73845	64.97996	-94.44700	586.00678	-2659.20016	1
228	C	70.03687	81.08139	63.90782	-291.69381	-718.18079	-150.72929	1
229	H	70.02242	80.18664	63.23441	-2303.38776	1089.76242	964.62032	1
230	H	68.97534	81.39528	64.07810	884.16729	2568.80533	-207.74283	1
231	N	70.67815	82.11852	63.21633	-594.49522	-252.81478	342.29276	1
232	H	71.53981	82.46265	63.61026	-1735.17426	2084.05705	-263.71605	1
233	C	70.25033	82.63828	62.13793	595.23177	-271.52487	442.22352	1
234	N	69.05357	82.14488	61.60559	585.53813	-424.79750	-105.81303	1
235	H	68.44429	81.40794	61.95786	959.88797	1327.56823	-2177.11905	1
236	H	68.61250	82.48149	60.74936	1578.48647	16.27378	-2220.76233	1
237	N	71.11388	83.64600	61.68473	-452.17763	-390.33541	-421.51853	1
238	H	71.98549	84.00426	62.07166	470.26107	1974.25629	-1817.92087	1
239	H	70.94644	84.18090	60.83179	1856.67307	-1573.97321	-1224.35416	1
240	C	70.51872	81.10245	68.22465	-531.47271	-581.45780	-55.06206	1
241	O	69.38191	81.38869	68.51637	-243.00837	192.73507	609.52485	1
242	N	71.62100	81.93788	68.31484	343.49288	-644.25607	38.09164	1
243	H	72.31069	81.36954	67.79575	-1691.16043	-1535.97525	-1484.73099	1
244	C	72.05779	82.32593	69.68171	542.66492	350.14337	454.42563	1
245	H	72.43032	81.36788	70.11113	1209.57979	-2396.95920	463.86744	1
246	C	73.12976	83.36780	69.49363	-737.14309	145.93010	242.71942	1
247	H	72.76727	84.07755	68.71494	-1050.18303	159.36419	-2509.06125	1
248	C	73.37968	84.15797	70.76665	-706.77696	-252.88343	-245.16230	1
249	H	74.15758	84.95613	70.61606	-1624.64039	-1665.49085	1417.86935	1
250	H	72.43807	84.66872	71.11943	2566.10521	598.51109	693.22305	1
251	H	73.73447	83.49700	71.60454	-1972.69758	107.10018	-1876.34312	1
252	C	74.43772	82.77045	69.00360	412.85148	672.58832	-27.69222	1
253	H	75.21449	83.56375	68.82440	1447.02277	1762.76533	-1490.78944	1
254	H	74.86731	82.04767	69.75050	1320.77379	-145.20455	2378.68491	1
255	H	74.30409	82.21076	68.03781	-1512.10848	1470.52031	1724.75147	1
256	C	70.79755	82.94925	70.54416	-607.11113	499.56689	73.73769	1
257	O	70.38118	84.06145	70.32662	357.97126	460.81534	356.68785	1
258	N	70.44326	82.10072	71.50085	536.55407	-368.62270	332.76306	1
259	H	70.90251	81.19106	71.55897	524.38866	2297.69985	1367.20941	1
260	C	69.34327	82.45504	72.31756	46.50277	-774.29190	-147.97904	1
261	H	68.86402	83.31901	71.80226	1676.51875	1883.29066	1032.55549	1
262	C	68.40461	81.15680	72.52845	-559.41456	-34.19198	-556.30433	1
263	H	68.93551	80.42293	73.18183	-64.66664	395.18769	2695.05373	1
264	H	67.48039	81.44470	73.08442	-2703.44278	-60.40056	333.79418	1
265	C	68.06472	80.51927	71.20834	-519.76435	377.31045	459.42366	1
266	H	69.00831	80.14581	70.73989	-1746.74323	1667.50644	-1261.73691	1
267	C	67.11563	79.34868	71.42967	570.95554	16.46261	-545.27700	1
268	H	66.84580	78.84523	70.46524	2391.58273	28.05277	-1305.07271	1
269	H	67.56391	78.57332	72.10428	175.75588	917.63458	2559.43867	1
270	H	66.15725	79.68147	71.90566	-1063.97851	-2155.34650	1283.00462	1
271	C	67.43441	81.51972	70.24679	193.76014	2.62946	-765.53141	1
272	H	67.23953	81.05505	69.24283	507.39394	-846.55087	2539.60089	1
273	H	66.45930	81.91692	70.63425	1337.57841	1818.19054	1526.01994	1
274	H	68.11208	82.39939	70.06732	1100.88635	-1172.91350	-2199.08909	1
275	C	69.92105	82.81853	73.78446	-549.21115	475.64486	-309.38218	1
276	O	70.69985	82.10639	74.37166	556.06106	-390.37755	-78.24250	1
277	O	69.35515	83.94172	74.41819	-572.27940	-310.19032	-209.75862	1
278	H	68.77531	84.26934	73.67158	-1380.08193	2212.14486	790.85944	1

Listing 48: C00048.xmolout

1	276							
2	150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
	0.2500	300.00	0.00	0.00	0.00	-1293.7071	0.0000	300.0000
3	H	60.08894	78.48963	69.93480	-2043.14101	-1757.64893	399.89339	1
4	N	59.97632	79.50315	69.93002	426.75047	490.45733	-334.42467	1
5	H	59.71229	79.72098	70.90112	442.25559	-1110.30854	-2448.52907	1
6	C	61.14284	80.20622	69.56222	415.32972	-666.39213	83.73172	1
7	H	61.78246	79.52905	68.95599	879.32219	2491.00447	667.35213	1
8	C	60.70163	81.54069	68.77378	31.35357	477.41777	628.23362	1
9	H	60.07683	82.17260	69.44967	1168.38489	2240.25337	-1019.71136	1
10	H	61.59548	82.15722	68.51309	-360.43770	2534.90498	931.67112	1
11	C	59.92105	81.16474	67.54034	463.18208	512.70242	-382.34388	1
12	H	59.13179	80.43833	67.83990	1725.29117	1863.52247	-987.07854	1
13	C	59.24685	82.39459	66.94540	710.42801	-144.27427	-313.15367	1
14	H	58.63795	82.13623	66.04085	364.20195	-1033.13725	2494.72524	1
15	H	58.55834	82.88595	67.68056	2567.61904	335.80679	847.48802	1
16	H	59.99835	83.16377	66.63023	-2587.99029	680.92867	-512.16411	1
17	C	60.81099	80.51254	66.49155	268.17616	741.64379	-40.42634	1
18	H	60.23535	80.25430	65.56522	1283.54314	-1945.37420	-1411.27812	1
19	H	61.64881	81.18971	66.18287	-1258.57796	1317.15249	-2026.02085	1
20	H	61.27162	79.56393	66.86990	-2502.84526	909.80597	575.92391	1
21	C	61.77046	80.63628	71.00728	619.36578	-458.64843	-172.09273	1
22	O	61.05916	80.66637	71.99599	-81.40433	433.87611	522.34594	1
23	N	63.03400	80.98329	70.83993	175.23996	-622.20190	341.55523	1
24	H	63.37978	80.92707	69.88157	-876.57256	-303.22879	-2561.90213	1
25	C	63.91854	81.38846	71.86915	-571.88214	-534.10783	-106.15033	1
26	H	64.75117	81.86083	71.30529	-2713.20841	-16.25800	-248.80809	1
27	C	63.16351	82.39827	72.85617	166.60354	288.16399	-716.09568	1
28	H	62.25203	81.86930	73.26565	-2097.85574	1636.78449	-586.18044	1
29	O	62.70850	83.62153	72.25236	-317.80580	-363.38227	484.43082	1
30	H	61.73792	83.49335	72.28842	1863.74748	-1451.84923	1357.29467	1
31	C	64.22822	82.55029	74.00344	503.80731	517.99032	318.51606	1
32	H	63.84474	83.18756	74.83397	640.61020	-2157.10410	-1536.29104	1
33	H	64.50265	81.55930	74.44364	1687.88455	465.60692	2087.56452	1
34	H	65.16751	83.02208	73.63131	-1293.07895	-1899.88581	-1463.57452	1
35	C	64.40027	80.06844	72.71390	-153.07550	-733.68902	248.70981	1
36	O	63.67946	79.61557	73.56451	186.15459	-480.78787	-449.34387	1
37	N	65.63438	79.67921	72.35887	-487.53139	543.18517	42.03850	1
38	C	66.24665	78.54103	72.96937	-699.35871	69.34393	360.10701	1
39	H	65.44806	77.78980	73.16418	2.81126	-221.99807	-2715.58072	1
40	C	67.33167	78.14999	71.87771	-507.46439	-592.59194	122.07761	1
41	H	68.14251	77.50503	72.28440	-1975.08116	525.87560	-1801.71556	1
42	H	66.87879	77.59838	71.02377	1588.27743	-1913.22100	1113.83566	1
43	C	67.82451	79.56553	71.44701	-613.62442	-457.55993	-194.14490	1
44	H	68.48247	80.00688	72.23263	1707.54637	-721.27992	1996.92523	1
45	H	68.40317	79.57242	70.49581	758.23357	2100.81767	1560.55011	1
46	C	66.44713	80.35198	71.35439	-352.41524	704.96076	49.21465	1
47	H	66.50627	81.43401	71.61847	1714.76886	-2070.42778	443.35792	1
48	H	65.90356	80.23422	70.38685	1224.15040	1801.50881	1636.97633	1
49	C	67.02221	79.02197	74.33761	566.85117	537.05831	117.62814	1
50	O	67.69588	80.02345	74.37934	-550.26779	-406.08867	4.21666	1
51	N	66.85032	78.09007	75.26519	566.34832	-425.77725	180.18749	1
52	H	66.28971	77.26725	75.04744	644.44502	2646.80550	-52.73430	1
53	C	67.50215	78.23880	76.51389	612.34801	-281.48662	411.56221	1
54	H	67.96305	79.25473	76.51679	1667.23498	-1490.75142	1556.16753	1
55	C	66.37290	78.00247	77.63373	-714.45746	-175.43074	286.98927	1
56	H	65.86166	77.02788	77.40366	-787.09484	1763.03619	-1922.46060	1
57	O	65.33682	78.99737	77.67580	-429.46514	516.51932	-128.40526	1

58	H	64.56691	78.48235	77.36078	1981.82785	436.16847	-1818.18182	1
59	C	67.21218	77.84227	78.95234	630.79189	-468.94448	76.03230	1
60	H	66.56080	77.59444	79.82222	-1775.71861	2062.30353	131.89849	1
61	H	67.97208	77.02951	78.86666	-1855.14608	88.94118	1993.53760	1
62	H	67.75838	78.78065	79.20420	-1504.82350	-780.94249	-2132.90992	1
63	C	68.56672	77.00241	76.62729	288.57638	618.62814	-397.00270	1
64	O	68.28845	75.87859	76.28642	321.70495	-185.26452	574.37218	1
65	N	69.64043	77.42048	77.31598	-447.05792	-446.53431	367.76425	1
66	H	69.72187	78.42858	77.45238	350.31316	1975.63644	-1843.31522	1
67	C	70.83906	76.63004	77.10265	-511.23061	374.03917	-471.51480	1
68	H	70.42966	75.59423	77.03653	2234.79579	-898.70890	-1273.45190	1
69	C	71.45262	77.10710	75.74924	529.53781	-159.34528	563.72604	1
70	H	72.15705	76.32721	75.36459	654.59388	2347.94251	1217.51488	1
71	H	70.65768	77.25538	74.98026	-1526.55661	2103.42026	817.87394	1
72	O	72.17057	78.53293	75.64668	-554.84278	14.12789	399.58769	1
73	H	73.01929	78.18800	75.38590	1297.06236	2061.84854	1220.68812	1
74	C	71.77275	76.87276	78.42081	-662.15484	-412.13544	123.62687	1
75	O	71.70547	76.08925	79.33034	-540.01537	-317.05804	274.91456	1
76	N	72.57021	77.92866	78.25618	-202.76299	-690.00100	-131.49145	1
77	H	72.46875	78.43151	77.33326	-702.62132	-2617.37191	281.70413	1
78	C	73.09255	78.72673	79.38394	-491.73914	576.34187	222.73509	1
79	H	72.44589	79.63085	79.30714	1977.17978	-1823.58850	-434.68928	1
80	C	72.96522	78.04521	80.72055	-649.50797	-328.66843	306.11224	1
81	H	73.18655	76.95820	80.58649	2075.07803	1452.16490	-1004.45904	1
82	C	73.92586	78.58933	81.76415	-615.18735	-489.99689	-70.96352	1
83	H	73.76878	78.10526	82.76707	-1226.32661	-1724.38906	-1716.47170	1
84	H	75.00588	78.41091	81.47192	2381.64273	-969.84735	900.46860	1
85	H	73.79802	79.69756	81.90553	2122.74991	1702.23946	-141.36228	1
86	C	71.55406	78.17366	81.27535	-501.86074	-479.61276	-376.42482	1
87	H	71.43023	77.59181	82.22907	993.79261	-2246.95401	-1177.81305	1
88	H	71.29342	79.24330	81.50192	42.71279	-626.15391	-2651.37258	1
89	H	70.78534	77.79022	80.54835	-2026.39012	-1590.33709	-887.82922	1
90	C	74.62907	79.09666	78.88903	-672.89153	382.57394	-156.34072	1
91	O	75.60032	78.75674	79.54705	410.04627	221.86223	500.35950	1
92	N	74.58610	79.79671	77.78020	-378.11782	-443.79414	-441.10984	1
93	H	73.64471	79.93254	77.41960	2404.15973	-568.14894	1149.30085	1
94	C	75.71445	80.36831	77.12430	-544.54484	466.16019	331.29119	1
95	H	75.21907	81.03616	76.38615	-1409.80988	-170.17955	2325.32679	1
96	C	76.52763	81.19621	78.20151	-184.48284	116.78282	-758.89137	1
97	H	75.86269	81.90754	78.74193	1893.78641	1861.14652	611.04528	1
98	H	76.93087	80.52999	78.99619	-2170.79665	-974.19311	1327.50117	1
99	C	77.66012	81.95754	77.44239	389.51668	672.81878	-138.49152	1
100	H	78.13147	81.29541	76.68281	510.64577	1933.03327	1851.02484	1
101	H	77.22733	82.78273	76.83549	-2302.30869	-1105.72939	-948.89774	1
102	C	78.77521	82.52600	78.39791	-559.93427	-126.34590	542.30857	1
103	O	79.74209	83.06584	77.92487	-670.36003	-111.83166	76.36448	1
104	N	78.52733	82.34318	79.71339	-216.06729	-537.07037	446.51379	1
105	H	77.70995	81.93071	80.17758	-1251.96487	1074.12894	-2168.52500	1
106	H	79.14020	82.68344	80.46252	-2451.83023	-720.73851	944.84612	1
107	C	76.47378	79.18120	76.28868	546.24052	-563.88337	-85.11809	1
108	O	75.98427	78.97151	75.20123	71.70702	-307.40463	606.69673	1
109	N	77.50584	78.54584	76.84747	479.90863	-504.50129	222.86849	1
110	C	78.06451	77.38833	76.18137	75.51268	-600.91904	506.73700	1
111	H	77.96251	77.63636	75.09910	-2033.61562	1795.30103	254.89480	1
112	C	79.56416	77.37070	76.75105	523.79067	517.99274	284.45581	1
113	H	80.05685	76.38044	76.63529	1599.61665	-1127.00911	1895.98173	1
114	H	80.20617	78.11559	76.23174	-1881.83093	1275.82488	-1501.55016	1
115	C	79.31250	77.76921	78.23374	-600.05639	-404.05026	316.64485	1
116	H	78.95576	76.89575	78.82429	-2597.05260	496.36221	657.73249	1
117	H	80.22288	78.14949	78.74922	-1666.24518	1294.38985	-1723.90591	1
118	C	78.17168	78.87163	78.09302	493.57570	-129.95376	-602.56394	1
119	H	77.36119	78.81980	78.88907	-1469.08415	-637.84797	2204.22581	1

120	H	78.55268	79.91483	78.00237	-1038.97840	1068.88701	-2280.71789	1
121	C	77.31553	76.04584	76.59106	188.88100	241.05089	-727.87821	1
122	O	77.80987	74.82113	76.32565	531.88613	-49.19943	427.07960	1
123	N	76.20006	76.23459	77.19436	708.14833	26.93417	-179.73509	1
124	H	76.07939	77.24385	77.33272	-2232.69501	-1179.09831	1023.94816	1
125	C	75.21887	75.21565	77.28875	-738.32412	259.92548	104.42456	1
126	H	75.78293	74.26035	77.20100	2028.89123	1260.02983	1311.33324	1
127	C	74.43446	75.39171	78.64219	-258.65678	-345.52513	661.28459	1
128	H	73.87041	76.35217	78.64448	-1826.06090	-1801.46097	-918.64554	1
129	C	73.44624	74.18259	78.81080	-541.23400	531.92970	-218.41428	1
130	H	72.92260	74.21294	79.79760	1311.73218	-2219.18200	882.19023	1
131	H	72.65571	74.19455	78.01791	-1048.71298	1223.58118	-2196.97971	1
132	H	73.97444	73.20322	78.74027	419.06414	1903.92898	1903.44670	1
133	C	75.45602	75.37201	79.83418	-423.86431	152.66566	-648.55262	1
134	H	74.94089	75.44232	80.82064	105.68386	-2342.50080	1387.51238	1
135	H	76.06233	74.43618	79.83796	-1695.63603	-1484.73621	-1531.02793	1
136	H	76.16590	76.23033	79.76581	-1853.57121	-487.39031	1936.59343	1
137	C	74.12484	75.42883	76.03403	539.71428	-510.58232	267.58633	1
138	O	73.18642	74.61972	75.90693	-15.93758	-278.34085	-624.49402	1
139	N	74.34638	76.44841	75.29407	-676.81886	12.05292	276.17960	1
140	H	75.14667	76.99915	75.54905	-1694.44250	-373.84189	-2100.66098	1
141	C	74.93767	74.86294	72.52554	412.33078	-664.70360	108.35451	1
142	H	74.60439	75.04681	71.47913	1765.77476	1294.44366	1621.76594	1
143	C	77.23500	74.48708	71.64100	-179.66635	-721.95667	-264.73915	1
144	H	78.28497	74.86230	71.64756	-607.34922	2587.87032	-598.10018	1
145	H	77.30226	73.39434	71.83948	-359.69332	-1479.13954	-2259.74260	1
146	C	76.58691	74.73363	70.22569	-240.01076	616.02425	431.85322	1
147	H	75.88509	73.90797	69.97141	-1359.17131	782.54425	2227.99181	1
148	H	75.98068	75.66691	70.22677	-820.36667	85.81767	-2596.78715	1
149	C	77.73376	74.85524	69.15005	-513.07015	236.18570	-551.87280	1
150	H	78.23617	75.84742	69.22682	1816.11944	-1183.11722	-1650.94321	1
151	H	78.53135	74.09644	69.32185	-1800.04429	-1361.53473	1526.34643	1
152	C	77.09194	74.66523	67.75368	726.08972	-253.19732	-179.64713	1
153	H	76.83475	73.61612	67.50564	1224.27271	-456.51798	-2390.90304	1
154	H	76.22640	75.32589	67.54577	1206.40339	-1150.93514	-2154.90344	1
155	N	78.15421	75.08355	66.68301	329.70796	-633.68968	-155.67358	1
156	H	77.87400	74.92175	65.67262	1348.31305	1938.76845	1359.00643	1
157	H	78.42855	76.10900	66.65833	2096.92035	1446.54551	-966.48890	1
158	H	79.10001	74.60309	66.71786	-1197.07217	-2303.53719	827.28733	1
159	C	74.87939	73.32295	72.95043	-378.01186	-556.17301	-413.96481	1
160	O	75.74859	72.97353	73.88301	-409.44433	-307.55053	-453.30833	1
161	N	74.08341	72.57149	72.29491	-429.02477	524.70884	274.08502	1
162	H	73.56871	73.15538	71.63116	1706.34263	-1425.96036	1574.38926	1
163	C	73.86170	71.18029	72.54649	-45.25864	-626.22952	478.93267	1
164	H	73.64325	71.12753	73.63632	1988.63164	570.90773	1772.87287	1
165	C	72.63481	70.80172	71.63111	551.77128	-20.49526	-564.54996	1
166	H	71.78513	71.49627	71.81907	1434.61535	-1753.10253	1513.99471	1
167	H	72.90503	70.94953	70.56128	-714.67738	1819.09770	1898.36494	1
168	C	72.18893	69.31985	71.87096	446.99263	-555.77305	338.97221	1
169	H	73.03704	68.61687	71.69735	1953.68466	1892.25957	-161.67766	1
170	H	71.86211	69.15775	72.92249	-403.03785	2688.07032	-188.43591	1
171	C	71.00940	69.05150	70.85165	567.86262	335.74681	434.04421	1
172	H	70.13603	69.70502	71.07943	-1080.02275	1568.26081	-1948.78900	1
173	H	71.32147	69.31731	69.81560	-919.54108	2111.34692	1456.13463	1
174	C	70.60908	67.56007	70.92015	195.81897	173.33862	-745.11536	1
175	H	71.40879	66.85350	70.62085	1405.67949	-2301.21089	-390.08113	1
176	H	70.16278	67.24236	71.88343	-940.37328	-1118.32446	2299.72133	1
177	N	69.47563	67.34156	69.86012	319.26422	656.36007	-42.02424	1
178	H	69.10610	66.35089	69.77728	1961.03633	619.91968	1787.09422	1
179	H	68.57621	67.88915	69.99352	854.14343	-2156.80752	1429.08711	1
180	H	69.71557	67.55882	68.84920	1237.02905	-1378.50857	-1998.28500	1
181	C	75.18340	70.28991	72.18898	532.53319	-268.57236	517.55729	1

182	O	75.14441	69.09364	72.37761	266.16714	-290.73804	-558.88002	1
183	N	76.16267	71.00294	71.63004	-226.25352	640.49678	-270.32839	1
184	H	75.99067	72.00642	71.59678	2007.69063	-1035.27229	1523.50231	1
185	C	77.47146	70.44314	71.59914	-540.76542	-573.33303	49.50000	1
186	H	77.28985	69.35518	71.75974	-2374.20950	-1036.76023	843.75774	1
187	C	78.08170	70.79734	70.17153	-77.09082	666.87422	-415.84136	1
188	H	78.09423	71.91573	70.03314	-985.81834	617.19825	2463.91927	1
189	O	77.33734	70.32010	69.02865	293.29899	-391.65602	-477.80926	1
190	H	77.05981	71.16223	68.61989	2528.72714	-681.76262	-751.27122	1
191	C	79.54825	70.24634	70.31111	252.47363	-605.14473	440.05134	1
192	H	80.15671	70.48632	69.40853	-2052.65063	1456.49051	-1043.51830	1
193	H	80.09092	70.67052	71.20048	-2152.98800	-1661.97574	-161.70652	1
194	H	79.55148	69.13698	70.42225	-473.12726	-1584.27339	2165.61725	1
195	C	78.32943	71.12483	72.83016	360.36307	488.46713	505.10056	1
196	O	78.31752	70.58066	73.90722	-200.08817	-528.03552	-385.82850	1
197	N	78.92748	72.24477	72.45363	-597.54095	-226.44775	355.20479	1
198	H	78.83957	72.54387	71.48390	2179.23655	-1300.70981	-991.33835	1
199	C	79.82564	72.93654	73.30635	-687.68921	297.39807	-249.45179	1
200	H	80.14648	73.80167	72.68431	-349.16256	-2467.37713	-1101.72831	1
201	C	79.03197	73.37938	74.61772	672.47345	361.54328	-201.62880	1
202	H	78.41053	72.52087	74.97224	1541.41502	582.18425	2169.97026	1
203	H	79.75708	73.60716	75.43510	-2534.67717	60.25153	997.72295	1
204	C	78.14684	74.63540	74.54769	574.26774	-389.43119	-377.02542	1
205	C	78.86209	75.79330	73.94009	688.82679	-287.33580	-257.96133	1
206	H	79.92556	75.95719	74.16618	331.14182	1470.38163	2269.80013	1
207	C	76.72214	74.49846	74.06792	-383.52382	-675.04808	144.24917	1
208	H	75.99717	74.77017	74.87436	4.09847	1517.59662	2262.86397	1
209	C	78.18452	76.73388	73.20064	-134.76730	428.45285	-649.50303	1
210	H	78.73109	77.65355	72.92583	-903.23433	1600.49020	2011.53387	1
211	C	76.43182	75.16646	72.77640	-335.53281	-615.00040	-364.39058	1
212	H	74.29220	75.50018	73.17722	1596.45398	-1369.33862	1732.02659	1
213	C	76.78857	76.59519	72.79314	585.48547	-340.24194	-406.23938	1
214	O	75.95107	77.51143	72.23025	-419.15649	-173.04408	-511.94141	1
215	H	75.84402	78.12459	73.06116	-1071.84350	1559.71507	-1960.13012	1
216	C	81.06141	71.91209	73.60171	291.41878	-183.13091	710.72246	1
217	O	81.48406	71.18609	72.73003	379.87695	523.47396	-222.23622	1
218	N	81.57155	72.11546	74.80996	564.30591	373.09380	277.24371	1
219	H	81.15546	72.77238	75.47029	-120.59931	-2436.07824	-1214.35098	1
220	C	82.54647	71.21719	75.31569	404.07514	-299.37480	608.84009	1
221	H	82.70658	70.42979	74.54246	-1071.07882	-841.69025	2359.66467	1
222	C	83.81083	72.13926	75.59911	-683.12807	68.71770	-390.13096	1
223	H	84.11241	72.67523	74.67166	2068.88918	1596.58590	770.89603	1
224	H	83.54005	72.93578	76.32791	1379.86429	2342.49779	-179.85638	1
225	C	84.99082	71.28318	76.14499	-176.39967	537.49466	550.97268	1
226	H	84.68145	70.71575	77.05425	-396.28051	1942.22168	1869.33314	1
227	H	85.31190	70.51506	75.40652	-94.44700	586.00678	-2659.20016	1
228	C	86.17978	72.30302	76.47619	-291.69381	-718.18079	-150.72929	1
229	H	86.60683	72.87190	75.61291	-2303.38776	1089.76242	964.62032	1
230	H	85.94465	73.02227	77.30007	884.16729	2568.80533	-207.74283	1
231	N	87.14857	71.43304	76.97609	-594.49522	-252.81478	342.29276	1
232	H	86.77006	70.53842	77.32364	-1735.17426	2084.05705	-263.71605	1
233	C	88.39093	71.70227	77.05434	595.23177	-271.52487	442.22352	1
234	N	88.84151	72.93605	76.59522	585.53813	-424.79750	-105.81303	1
235	H	88.30815	73.71763	76.21355	959.88797	1327.56823	-2177.11905	1
236	H	89.80947	73.26081	76.63316	1578.48647	16.27378	-2220.76233	1
237	N	89.03307	70.60217	77.63148	-452.17763	-390.33541	-421.51853	1
238	H	88.63374	69.74868	78.02336	470.26107	1974.25629	-1817.92087	1
239	H	90.02845	70.57716	77.85636	1856.67307	-1573.97321	-1224.35416	1
240	C	81.99786	70.70738	76.77746	-531.47271	-581.45780	-55.06206	1
241	O	81.40586	71.46513	77.51178	-243.00837	192.73507	609.52485	1
242	N	82.40544	69.46246	77.03032	343.49288	-644.25607	38.09164	1
243	H	82.90369	68.97942	76.28360	-1691.16043	-1535.97525	-1484.73099	1

244	C	81.72338	68.77175	78.07211	542.66492	350.14337	454.42563	1
245	H	81.06503	69.54157	78.54023	1209.57979	-2396.95920	463.86744	1
246	C	80.93446	67.56171	77.40094	-737.14309	145.93010	242.71942	1
247	H	81.62066	66.95970	76.76737	-1050.18303	159.36419	-2509.06125	1
248	C	80.31021	66.67924	78.53423	-706.77696	-252.88343	-245.16230	1
249	H	79.75369	65.80559	78.12086	-1624.64039	-1665.49085	1417.86935	1
250	H	81.09797	66.27950	79.21960	2566.10521	598.51109	693.22305	1
251	H	79.59781	67.26390	79.16244	-1972.69758	107.10018	-1876.34312	1
252	C	79.75489	68.13555	76.54496	412.85148	672.58832	-27.69222	1
253	H	79.17548	67.32395	76.04494	1447.02277	1762.76533	-1490.78944	1
254	H	79.03864	68.71620	77.17282	1320.77379	-145.20455	2378.68491	1
255	H	80.12246	68.82412	75.74702	-1512.10848	1470.52031	1724.75147	1
256	C	82.74483	68.07099	79.14219	-607.11113	499.56689	73.73769	1
257	O	82.35936	67.86950	80.27195	357.97126	460.81534	356.68785	1
258	N	83.86697	67.61160	78.57319	536.55407	-368.62270	332.76306	1
259	H	84.03663	67.94681	77.62494	524.38866	2297.69985	1367.20941	1
260	C	84.96158	67.39483	79.46740	46.50277	-774.29190	-147.97904	1
261	H	84.51679	67.36573	80.49015	1676.51875	1883.29066	1032.55549	1
262	C	85.74806	66.04538	79.05042	-559.41456	-34.19198	-556.30433	1
263	H	86.19801	66.18283	78.03861	-64.66664	395.18769	2695.05373	1
264	H	86.60482	65.86773	79.74352	-2703.44278	-60.40056	333.79418	1
265	C	84.80700	64.87161	79.04663	-519.76435	377.31045	459.42366	1
266	H	83.92285	65.13550	78.42302	-1746.74323	1667.50644	-1261.73691	1
267	C	85.49307	63.65563	78.43534	570.95554	16.46261	-545.27700	1
268	H	84.80884	62.76957	78.39471	2391.58273	28.05277	-1305.07271	1
269	H	85.83866	63.85767	77.38881	175.75588	917.63458	2559.43867	1
270	H	86.39431	63.35126	79.02742	-1063.97851	-2155.34650	1283.00462	1
271	C	84.32453	64.53706	80.45146	193.76014	2.62946	-765.53141	1
272	H	83.65858	63.63578	80.45566	507.39394	-846.55087	2539.60089	1
273	H	85.18047	64.31994	81.14147	1337.57841	1818.19054	1526.01994	1
274	H	83.74015	65.38253	80.89912	1100.88635	-1172.91350	-2199.08909	1
275	C	85.98697	68.59812	79.21864	-549.21115	475.64486	-309.38218	1
276	O	86.00333	69.22660	78.17403	556.06106	-390.37755	-78.24250	1
277	O	86.96129	68.83394	80.19431	-572.27940	-310.19032	-209.75862	1
278	H	86.63401	68.18706	80.89439	-1380.08193	2212.14486	790.85944	1

Listing 49: C00049.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.7032	0.0000	300.0000
3	H	79.11725	85.79260	78.33612	-2043.14101	-1757.64893	399.89339		1
4	N	79.94656	85.78227	78.92696	426.75047	490.45733	-334.42467		1
5	H	79.62704	86.30149	79.74227	442.25559	-1110.30854	-2448.52907		1
6	C	81.10257	86.30588	78.31318	415.32972	-666.39213	83.73172		1
7	H	80.95392	86.13786	77.22600	879.32219	2491.00447	667.35213		1
8	C	81.23918	87.86571	78.68611	31.35357	477.41777	628.23362		1
9	H	81.33613	87.97056	79.79367	1168.38489	2240.25337	-1019.71136		1
10	H	82.18366	88.28165	78.25825	-360.43770	2534.90498	931.67112		1
11	C	80.04241	88.63516	78.18538	463.18208	512.70242	-382.34388		1
12	H	79.11860	88.08067	78.46322	1725.29117	1863.52247	-987.07854		1
13	C	79.98363	90.01048	78.83791	710.42801	-144.27427	-313.15367		1
14	H	79.09136	90.59425	78.49277	364.20195	-1033.13725	2494.72524		1
15	H	79.92157	89.93754	79.95453	2567.61904	335.80679	847.48802		1
16	H	80.89226	90.62006	78.59592	-2587.99029	680.92867	-512.16411		1
17	C	80.08076	88.78979	76.67133	268.17616	741.64379	-40.42634		1
18	H	79.19530	89.36272	76.29200	1283.54314	-1945.37420	-1411.27812		1
19	H	80.99851	89.33968	76.33738	-1258.57796	1317.15249	-2026.02085		1
20	H	80.08171	87.79764	76.15095	-2502.84526	909.80597	575.92391		1
21	C	82.43932	85.56211	78.87537	619.36578	-458.64843	-172.09273		1
22	O	83.48224	85.66381	78.26400	-81.40433	433.87611	522.34594		1
23	N	82.22939	84.95033	80.03998	175.23996	-622.20190	341.55523		1

24	H	81.28797	85.03800	80.41677	-876.57256	-303.22879	-2561.90213	1
25	C	83.31955	84.33941	80.71428	-571.88214	-534.10783	-106.15033	1
26	H	84.20797	84.75830	80.18324	-2713.20841	-16.25800	-248.80809	1
27	C	83.22048	84.74468	82.26200	166.60354	288.16399	-716.09568	1
28	H	82.29780	84.28117	82.70525	-2097.85574	1636.78449	-586.18044	1
29	O	83.12504	86.15355	82.53179	-317.80580	-363.38227	484.43082	1
30	H	82.26614	86.19872	82.99839	1863.74748	-1451.84923	1357.29467	1
31	C	84.48123	84.01775	82.85720	503.80731	517.99032	318.51606	1
32	H	84.51748	84.10545	83.96787	640.61020	-2157.10410	-1536.29104	1
33	H	84.49105	82.92896	82.60709	1687.88455	465.60692	2087.56452	1
34	H	85.42616	84.45582	82.45956	-1293.07895	-1899.88581	-1463.57452	1
35	C	83.27592	82.70590	80.61124	-153.07550	-733.68902	248.70981	1
36	O	84.35554	82.19575	80.44678	186.15459	-480.78787	-449.34387	1
37	N	82.10071	82.09733	80.84582	-487.53139	543.18517	42.03850	1
38	C	82.07121	80.69731	81.12669	-699.35871	69.34393	360.10701	1
39	H	83.02814	80.44699	81.63878	2.81126	-221.99807	-2715.58072	1
40	C	80.75500	80.57982	82.00760	-507.46439	-592.59194	122.07761	1
41	H	80.36194	79.53998	82.06295	-1975.08116	525.87560	-1801.71556	1
42	H	80.92746	80.91729	83.05414	1588.27743	-1913.22100	1113.83566	1
43	C	79.80932	81.55689	81.24345	-613.62442	-457.55993	-194.14490	1
44	H	79.42647	81.08123	80.30791	1707.54637	-721.27992	1996.92523	1
45	H	78.91679	81.86883	81.83145	758.23357	2100.81767	1560.55011	1
46	C	80.80463	82.75689	80.93442	-352.41524	704.96076	49.21465	1
47	H	80.62214	83.28647	79.96965	1714.76886	-2070.42778	443.35792	1
48	H	80.88863	83.50802	81.75268	1224.15040	1801.50881	1636.97633	1
49	C	81.85644	79.80709	79.75525	566.85117	537.05831	117.62814	1
50	O	82.04188	78.61315	79.80706	-550.26779	-406.08867	4.21666	1
51	N	81.44033	80.55868	78.74910	566.34832	-425.77725	180.18749	1
52	H	81.40290	81.55592	78.94803	644.44502	2646.80550	-52.73430	1
53	C	81.00048	80.03220	77.50585	612.34801	-281.48662	411.56221	1
54	H	80.79149	80.94100	76.90000	1667.23498	-1490.75142	1556.16753	1
55	C	82.28289	79.26127	76.94362	-714.45746	-175.43074	286.98927	1
56	H	82.54591	78.45904	77.68915	-787.09484	1763.03619	-1922.46060	1
57	O	83.44862	80.11703	76.83860	-429.46514	516.51932	-128.40526	1
58	H	83.93466	79.85940	77.64242	1981.82785	436.16847	-1818.18182	1
59	C	81.90632	78.58571	75.57953	630.79189	-468.94448	76.03230	1
60	H	82.80578	78.13295	75.10091	-1775.71861	2062.30353	131.89849	1
61	H	81.16449	77.76333	75.69892	-1855.14608	88.94118	1993.53760	1
62	H	81.48944	79.32457	74.85544	-1504.82350	-780.94249	-2132.90992	1
63	C	79.61832	79.23257	77.82290	288.57638	618.62814	-397.00270	1
64	O	79.03114	79.34185	78.87824	321.70495	-185.26452	574.37218	1
65	N	79.20876	78.57965	76.74107	-447.05792	-446.53431	367.76425	1
66	H	79.72543	78.63706	75.86587	350.31316	1975.63644	-1843.31522	1
67	C	78.00318	77.83290	76.81159	-511.23061	374.03917	-471.51480	1
68	H	77.42219	78.27983	77.65239	2234.79579	-898.70890	-1273.45190	1
69	C	77.32661	77.95734	75.35934	529.53781	-159.34528	563.72604	1
70	H	76.33630	77.43639	75.42427	654.59388	2347.94251	1217.51488	1
71	H	77.11353	79.04624	75.17876	-1526.55661	2103.42026	817.87394	1
72	O	78.12511	77.49340	74.24264	-554.84278	14.12789	399.58769	1
73	H	77.95580	76.53426	74.30555	1297.06236	2061.84854	1220.68812	1
74	C	78.24845	76.24011	77.01991	-662.15484	-412.13544	123.62687	1
75	O	77.29052	75.50873	77.22150	-540.01537	-317.05804	274.91456	1
76	N	79.52308	75.84118	76.78637	-202.76299	-690.00100	-131.49145	1
77	H	80.00766	76.73343	76.64093	-702.62132	-2617.37191	281.70413	1
78	C	80.17073	74.80363	77.61106	-491.73914	576.34187	222.73509	1
79	H	81.25883	75.01803	77.49707	1977.17978	-1823.58850	-434.68928	1
80	C	79.69525	74.94913	79.03967	-649.50797	-328.66843	306.11224	1
81	H	78.58345	74.84854	79.02767	2075.07803	1452.16490	-1004.45904	1
82	C	80.26774	73.85883	79.92880	-615.18735	-489.99689	-70.96352	1
83	H	79.87228	73.92397	80.97893	-1226.32661	-1724.38906	-1716.47170	1
84	H	80.01680	72.83273	79.53812	2381.64273	-969.84735	900.46860	1
85	H	81.38864	73.92156	79.98902	2122.74991	1702.23946	-141.36228	1

86	C	80.02405	76.30976	79.62807	-501.86074	-479.61276	-376.42482	1
87	H	79.69149	76.39082	80.69879	993.79261	-2246.95401	-1177.81305	1
88	H	81.12992	76.52618	79.60798	42.71279	-626.15391	-2651.37258	1
89	H	79.51999	77.14280	79.06166	-2026.39012	-1590.33709	-887.82922	1
90	C	79.77782	73.30319	77.05124	-672.89153	382.57394	-156.34072	1
91	O	80.44906	72.34535	77.34677	410.04627	221.86223	500.35950	1
92	N	78.66444	73.33122	76.33356	-378.11782	-443.79414	-441.10984	1
93	H	78.15328	74.22675	76.23957	2404.15973	-568.14894	1149.30085	1
94	C	78.05162	72.06057	76.06342	-544.54484	466.16019	331.29119	1
95	H	78.29626	71.43503	76.95025	-1409.80988	-170.17955	2325.32679	1
96	C	76.52287	72.35493	75.81409	-184.48284	116.78282	-758.89137	1
97	H	76.09894	73.01395	76.60607	1893.78641	1861.14652	611.04528	1
98	H	76.40303	72.91025	74.85660	-2170.79665	-974.19311	1327.50117	1
99	C	75.78552	70.97220	75.76683	389.51668	672.81878	-138.49152	1
100	H	76.31377	70.28744	75.06567	510.64577	1933.03327	1851.02484	1
101	H	75.85157	70.45866	76.75197	-2302.30869	-1105.72939	-948.89774	1
102	C	74.29173	71.09570	75.33747	-559.93427	-126.34590	542.30857	1
103	O	73.54467	70.13347	75.45868	-670.36003	-111.83166	76.36448	1
104	N	73.97793	72.27437	74.78738	-216.06729	-537.07037	446.51379	1
105	H	74.57413	73.09720	74.63863	-1251.96487	1074.12894	-2168.52500	1
106	H	73.08863	72.48954	74.32182	-2451.83023	-720.73851	944.84612	1
107	C	78.66183	71.48540	74.65478	546.24052	-563.88337	-85.11809	1
108	O	78.40385	72.04719	73.62328	71.70702	-307.40463	606.69673	1
109	N	79.29795	70.32560	74.85405	479.90863	-504.50129	222.86849	1
110	C	80.28773	69.84278	73.93196	75.51268	-600.91904	506.73700	1
111	H	80.92632	70.71979	73.68013	-2033.61562	1795.30103	254.89480	1
112	C	81.02351	68.70517	74.75459	523.79067	517.99274	284.45581	1
113	H	81.43533	67.90188	74.10279	1599.61665	-1127.00911	1895.98173	1
114	H	81.88397	69.11539	75.32922	-1881.83093	1275.82488	-1501.55016	1
115	C	79.90177	68.20246	75.71626	-600.05639	-404.05026	316.64485	1
116	H	79.18353	67.53500	75.19010	-2597.05260	496.36221	657.73249	1
117	H	80.28412	67.63362	76.59335	-1666.24518	1294.38985	-1723.90591	1
118	C	79.23104	69.58970	76.10912	493.57570	-129.95376	-602.56394	1
119	H	78.16755	69.52969	76.44130	-1469.08415	-637.84797	2204.22581	1
120	H	79.82422	70.20359	76.83515	-1038.97840	1068.88701	-2280.71789	1
121	C	79.59823	69.22402	72.58921	188.88100	241.05089	-727.87821	1
122	O	80.27887	68.98692	71.61855	531.88613	-49.19943	427.07960	1
123	N	78.29886	68.96593	72.75654	708.14833	26.93417	-179.73509	1
124	H	77.94596	69.19491	73.68435	-2232.69501	-1179.09831	1023.94816	1
125	C	77.51573	68.36263	71.68974	-738.32412	259.92548	104.42456	1
126	H	78.25491	68.24163	70.85877	2028.89123	1260.02983	1311.33324	1
127	C	76.98201	67.03679	72.21299	-258.65678	-345.52513	661.28459	1
128	H	76.39936	67.24650	73.13731	-1826.06090	-1801.46097	-918.64554	1
129	C	76.06430	66.34670	71.22241	-541.23400	531.92970	-218.41428	1
130	H	75.72856	65.33995	71.59654	1311.73218	-2219.18200	882.19023	1
131	H	75.13646	66.95273	71.01825	-1048.71298	1223.58118	-2196.97971	1
132	H	76.57494	66.18210	70.23309	419.06414	1903.92898	1903.44670	1
133	C	78.11888	66.10253	72.58842	-423.86431	152.66566	-648.55262	1
134	H	77.74550	65.16099	73.07730	105.68386	-2342.50080	1387.51238	1
135	H	78.71376	65.79622	71.68402	-1695.63603	-1484.73621	-1531.02793	1
136	H	78.83708	66.59354	73.30073	-1853.57121	-487.39031	1936.59343	1
137	C	76.26668	69.39704	71.28688	539.71428	-510.58232	267.58633	1
138	O	75.55885	69.07880	70.36463	-15.93758	-278.34085	-624.49402	1
139	N	76.16822	70.43416	72.09658	-676.81886	12.05292	276.17960	1
140	H	76.91822	70.52558	72.78223	-1694.44250	-373.84189	-2100.66098	1
141	C	75.29519	71.53692	71.86854	412.33078	-664.70360	108.35451	1
142	H	75.31913	72.06823	72.84678	1765.77476	1294.44366	1621.76594	1
143	C	75.83130	72.40799	70.65644	-179.66635	-721.95667	-264.73915	1
144	H	76.92888	72.58176	70.73176	-607.34922	2587.87032	-598.10018	1
145	H	75.65733	71.87590	69.69147	-359.69332	-1479.13954	-2259.74260	1
146	C	75.01933	73.74479	70.72398	-240.01076	616.02425	431.85322	1
147	H	73.92745	73.52524	70.66820	-1359.17131	782.54425	2227.99181	1

148	H	75.17796	74.25452	71.70086	-820.36667	85.81767	-2596.78715	1
149	C	75.46396	74.68129	69.53105	-513.07015	236.18570	-551.87280	1
150	H	76.54831	74.92823	69.60388	1816.11944	-1183.11722	-1650.94321	1
151	H	75.33320	74.16800	68.55062	-1800.04429	-1361.53473	1526.34643	1
152	C	74.60024	75.96273	69.60345	726.08972	-253.19732	-179.64713	1
153	H	73.52815	75.81294	69.36781	1224.27271	-456.51798	-2390.90304	1
154	H	74.70235	76.53462	70.54730	1206.40339	-1150.93514	-2154.90344	1
155	N	75.11784	76.94214	68.49721	329.70796	-633.68968	-155.67358	1
156	H	74.60153	77.86599	68.42568	1348.31305	1938.76845	1359.00643	1
157	H	76.12241	77.27414	68.58512	2096.92035	1446.54551	-966.48890	1
158	H	75.08429	76.60391	67.49155	-1197.07217	-2303.53719	827.28733	1
159	C	73.81471	71.08056	71.35357	-378.01186	-556.17301	-413.96481	1
160	O	73.47502	71.33634	70.19664	-409.44433	-307.55053	-453.30833	1
161	N	73.10379	70.57957	72.34421	-429.02477	524.70884	274.08502	1
162	H	73.63894	70.56279	73.21887	1706.34263	-1425.96036	1574.38926	1
163	C	72.30432	69.39858	72.10030	-45.25864	-626.22952	478.93267	1
164	H	72.99078	68.74860	71.51390	1988.63164	570.90773	1772.87287	1
165	C	71.99149	68.86955	73.54666	551.77128	-20.49526	-564.54996	1
166	H	72.91387	68.46838	74.02862	1434.61535	-1753.10253	1513.99471	1
167	H	71.68965	69.73006	74.18876	-714.67738	1819.09770	1898.36494	1
168	C	70.86416	67.78224	73.53117	446.99263	-555.77305	338.97221	1
169	H	70.35711	67.74045	72.54001	1953.68466	1892.25957	-161.67766	1
170	H	71.26496	66.76052	73.71783	-403.03785	2688.07032	-188.43591	1
171	C	69.85017	68.23689	74.65693	567.86262	335.74681	434.04421	1
172	H	70.30601	68.13391	75.66898	-1080.02275	1568.26081	-1948.78900	1
173	H	69.60756	69.31898	74.54308	-919.54108	2111.34692	1456.13463	1
174	C	68.55771	67.39765	74.53705	195.81897	173.33862	-745.11536	1
175	H	68.00101	67.54477	73.58986	1405.67949	-2301.21089	-390.08113	1
176	H	68.68124	66.31516	74.74134	-940.37328	-1118.32446	2299.72133	1
177	N	67.58378	67.91397	75.65055	319.26422	656.36007	-42.02424	1
178	H	66.62032	67.46942	75.68415	1961.03633	619.91968	1787.09422	1
179	H	67.90185	67.80289	76.65691	854.14343	-2156.80752	1429.08711	1
180	H	67.33767	68.94505	75.61786	1237.02905	-1378.50857	-1998.28500	1
181	C	70.96433	69.77961	71.24716	532.53319	-268.57236	517.55729	1
182	O	69.87553	69.83493	71.76139	266.16714	-290.73804	-558.88002	1
183	N	71.30406	69.87609	69.96279	-226.25352	640.49678	-270.32839	1
184	H	72.31088	69.88431	69.73507	2007.69063	-1035.27229	1523.50231	1
185	C	70.36985	70.36167	68.99731	-540.76542	-573.33303	49.50000	1
186	H	70.96996	70.35630	68.05891	-2374.20950	-1036.76023	843.75774	1
187	C	69.11082	69.37534	68.94384	-77.09082	666.87422	-415.84136	1
188	H	68.56861	69.46397	69.92668	-985.81834	617.19825	2463.91927	1
189	O	69.41841	67.98344	68.75508	293.29899	-391.65602	-477.80926	1
190	H	69.11798	67.60981	69.60807	2528.72714	-681.76262	-751.27122	1
191	C	68.25437	70.01964	67.79232	252.47363	-605.14473	440.05134	1
192	H	67.29035	69.47844	67.65112	-2052.65063	1456.49051	-1043.51830	1
193	H	68.00783	71.08957	68.00282	-2152.98800	-1661.97574	-161.70652	1
194	H	68.79484	69.98756	66.81758	-473.12726	-1584.27339	2165.61725	1
195	C	69.98119	71.86229	69.48829	360.36307	488.46713	505.10056	1
196	O	68.82490	72.23046	69.64184	-200.08817	-528.03552	-385.82850	1
197	N	71.10771	72.53277	69.57147	-597.54095	-226.44775	355.20479	1
198	H	72.01328	72.02410	69.45217	2179.23655	-1300.70981	-991.33835	1
199	C	71.15057	73.86356	70.05100	-687.68921	297.39807	-249.45179	1
200	H	72.17496	74.19603	69.77926	-349.16256	-2467.37713	-1101.72831	1
201	C	69.99408	74.75224	69.39531	672.47345	361.54328	-201.62880	1
202	H	68.99392	74.43107	69.77337	1541.41502	582.18425	2169.97026	1
203	H	70.12499	75.81416	69.70768	-2534.67717	60.25153	997.72295	1
204	C	70.04210	74.62235	67.86516	574.26774	-389.43119	-377.02542	1
205	C	71.09897	75.21703	67.11334	688.82679	-287.33580	-257.96133	1
206	H	71.89300	75.79872	67.61584	331.14182	1470.38163	2269.80013	1
207	C	69.02124	73.87387	67.20492	-383.52382	-675.04808	144.24917	1
208	H	68.20256	73.41073	67.78757	4.09847	1517.59662	2262.86397	1
209	C	71.10962	75.04148	65.72923	-134.76730	428.45285	-649.50303	1

210	H	71.92617	75.50093	65.14584	-903.23433	1600.49020	2011.53387	1
211	C	69.07647	73.72282	65.81783	-335.53281	-615.00040	-364.39058	1
212	H	68.28279	73.13604	65.32273	1596.45398	-1369.33862	1732.02659	1
213	C	70.11649	74.29644	65.02959	585.48547	-340.24194	-406.23938	1
214	O	70.18587	74.14762	63.61980	-419.15649	-173.04408	-511.94141	1
215	H	69.36656	73.61979	63.46759	-1071.84350	1559.71507	-1960.13012	1
216	C	70.94862	73.81069	71.67944	291.41878	-183.13091	710.72246	1
217	O	71.85989	74.17524	72.38405	379.87695	523.47396	-222.23622	1
218	N	69.75781	73.32794	71.98863	564.30591	373.09380	277.24371	1
219	H	69.13169	72.99835	71.22205	-120.59931	-2436.07824	-1214.35098	1
220	C	69.28007	73.35011	73.32632	404.07514	-299.37480	608.84009	1
221	H	68.43642	72.62355	73.33056	-1071.07882	-841.69025	2359.66467	1
222	C	70.50042	72.91003	74.24052	-683.12807	68.71770	-390.13096	1
223	H	71.03385	72.06597	73.74363	2068.88918	1596.58590	770.89603	1
224	H	71.24754	73.74465	74.30275	1379.86429	2342.49779	-179.85638	1
225	C	70.06063	72.49935	75.67827	-176.39967	537.49466	550.97268	1
226	H	69.56076	73.33733	76.21268	-396.28051	1942.22168	1869.33314	1
227	H	69.32730	71.66261	75.66959	-94.44700	586.00678	-2659.20016	1
228	C	71.42213	72.08288	76.41245	-291.69381	-718.18079	-150.72929	1
229	H	71.94297	71.15635	76.02371	-2303.38776	1089.76242	964.62032	1
230	H	72.15827	72.92513	76.45981	884.16729	2568.80533	-207.74283	1
231	N	70.99282	71.87280	77.72152	-594.49522	-252.81478	342.29276	1
232	H	70.27107	72.50013	78.05007	-1735.17426	2084.05705	-263.71605	1
233	C	71.45563	71.00809	78.53858	595.23177	-271.52487	442.22352	1
234	N	72.46025	70.14831	78.09850	585.53813	-424.79750	-105.81303	1
235	H	72.86297	70.07324	77.14688	959.88797	1327.56823	-2177.11905	1
236	H	72.88538	69.42130	78.68239	1578.48647	16.27378	-2220.76233	1
237	N	70.81272	71.14263	79.77595	-452.17763	-390.33541	-421.51853	1
238	H	70.06180	71.78481	80.04622	470.26107	1974.25629	-1817.92087	1
239	H	71.01374	70.55796	80.58913	1856.67307	-1573.97321	-1224.35416	1
240	C	68.77546	74.87225	73.64448	-531.47271	-581.45780	-55.06206	1
241	O	68.93284	75.82551	72.91082	-243.00837	192.73507	609.52485	1
242	N	68.13450	74.85752	74.80989	343.49288	-644.25607	38.09164	1
243	H	68.03266	73.97057	75.29896	-1691.16043	-1535.97525	-1484.73099	1
244	C	67.75950	76.13411	75.33373	542.66492	350.14337	454.42563	1
245	H	68.52690	76.83106	74.92394	1209.57979	-2396.95920	463.86744	1
246	C	66.31272	76.49047	74.76966	-737.14309	145.93010	242.71942	1
247	H	65.57408	75.71399	75.06272	-1050.18303	159.36419	-2509.06125	1
248	C	65.91794	77.88882	75.35204	-706.77696	-252.88343	-245.16230	1
249	H	64.88434	78.18523	75.05536	-1624.64039	-1665.49085	1417.86935	1
250	H	65.96244	77.88900	76.46954	2566.10521	598.51109	693.22305	1
251	H	66.60995	78.68862	74.99730	-1972.69758	107.10018	-1876.34312	1
252	C	66.40763	76.60513	73.20933	412.85148	672.58832	-27.69222	1
253	H	65.44746	76.95219	72.75921	1447.02277	1762.76533	-1490.78944	1
254	H	67.20614	77.32376	72.90139	1320.77379	-145.20455	2378.68491	1
255	H	66.66174	75.62161	72.74414	-1512.10848	1470.52031	1724.75147	1
256	C	67.65671	76.08835	76.96115	-607.11113	499.56689	73.73769	1
257	O	67.79365	77.11176	77.59584	357.97126	460.81534	356.68785	1
258	N	67.31125	74.88498	77.39944	536.55407	-368.62270	332.76306	1
259	H	67.17543	74.11332	76.74692	524.38866	2297.69985	1367.20941	1
260	C	67.20930	74.67544	78.79601	46.50277	-774.29190	-147.97904	1
261	H	67.62806	75.59492	79.26659	1676.51875	1883.29066	1032.55549	1
262	C	65.65581	74.41283	79.16296	-559.41456	-34.19198	-556.30433	1
263	H	65.36508	73.39710	78.80448	-64.66664	395.18769	2695.05373	1
264	H	65.51581	74.39473	80.26967	-2703.44278	-60.40056	333.79418	1
265	C	64.78447	75.45638	78.51951	-519.76435	377.31045	459.42366	1
266	H	65.02705	75.48940	77.43281	-1746.74323	1667.50644	-1261.73691	1
267	C	63.31313	75.09056	78.67292	570.95554	16.46261	-545.27700	1
268	H	62.64613	75.84034	78.17476	2391.58273	28.05277	-1305.07271	1
269	H	63.08606	74.09120	78.21996	175.75588	917.63458	2559.43867	1
270	H	63.01065	75.04197	79.75042	-1063.97851	-2155.34650	1283.00462	1
271	C	65.03868	76.83824	79.10485	193.76014	2.62946	-765.53141	1

272	H	64.35124	77.60625	78.66489	507.39394	-846.55087	2539.60089	1
273	H	64.88679	76.85352	80.21493	1337.57841	1818.19054	1526.01994	1
274	H	66.09285	77.17964	78.90047	1100.88635	-1172.91350	-2199.08909	1
275	C	68.01606	73.30734	79.07995	-549.21115	475.64486	-309.38218	1
276	O	68.00603	72.37342	78.32228	556.06106	-390.37755	-78.24250	1
277	O	68.69014	73.21582	80.33052	-572.27940	-310.19032	-209.75862	1
278	H	68.44464	74.11113	80.69302	-1380.08193	2212.14486	790.85944	1

Listing 50: C00050.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.6872	0.0000	300.0000
3	H	61.16985	80.83259	69.48001	-2043.14101	-1757.64893	399.89339		1
4	N	62.12888	80.50896	69.61162	426.75047	490.45733	-334.42467		1
5	H	62.20793	79.68091	68.99573	442.25559	-1110.30854	-2448.52907		1
6	C	63.10329	81.48350	69.30867	415.32972	-666.39213	83.73172		1
7	H	62.63764	82.49151	69.36073	879.32219	2491.00447	667.35213		1
8	C	64.34844	81.29317	70.31870	31.35357	477.41777	628.23362		1
9	H	64.73368	80.24967	70.22318	1168.38489	2240.25337	-1019.71136		1
10	H	65.19229	81.96625	70.02632	-360.43770	2534.90498	931.67112		1
11	C	63.92514	81.54983	71.74042	463.18208	512.70242	-382.34388		1
12	H	63.00945	80.94968	71.94434	1725.29117	1863.52247	-987.07854		1
13	C	65.02548	81.10247	72.69544	710.42801	-144.27427	-313.15367		1
14	H	64.73283	81.25511	73.76608	364.20195	-1033.13725	2494.72524		1
15	H	65.26849	80.01541	72.56930	2567.61904	335.80679	847.48802		1
16	H	65.97434	81.67402	72.52650	-2587.99029	680.92867	-512.16411		1
17	C	63.60926	83.02084	71.97234	268.17616	741.64379	-40.42634		1
18	H	63.31798	83.21735	73.03650	1283.54314	-1945.37420	-1411.27812		1
19	H	64.49171	83.67277	71.74415	-1258.57796	1317.15249	-2026.02085		1
20	H	62.76231	83.36981	71.32724	-2502.84526	909.80597	575.92391		1
21	C	63.55442	81.00194	67.82950	619.36578	-458.64843	-172.09273		1
22	O	63.25721	79.87023	67.46349	-81.40433	433.87611	522.34594		1
23	N	64.30842	81.90308	67.21579	175.23996	-622.20190	341.55523		1
24	H	64.47509	82.80181	67.66836	-876.57256	-303.22879	-2561.90213		1
25	C	64.90282	81.55689	65.97551	-571.88214	-534.10783	-106.15033		1
26	H	64.45678	80.55605	65.75477	-2713.20841	-16.25800	-248.80809		1
27	C	64.56767	82.71205	64.91234	166.60354	288.16399	-716.09568		1
28	H	65.23168	83.59522	65.13080	-2097.85574	1636.78449	-586.18044		1
29	O	63.21890	83.20807	64.92094	-317.80580	-363.38227	484.43082		1
30	H	63.36361	84.14898	65.14945	1863.74748	-1451.84923	1357.29467		1
31	C	65.02120	82.04716	63.56082	503.80731	517.99032	318.51606		1
32	H	64.95401	82.76720	62.71238	640.61020	-2157.10410	-1536.29104		1
33	H	66.07666	81.68500	63.60704	1687.88455	465.60692	2087.56452		1
34	H	64.37867	81.17327	63.30297	-1293.07895	-1899.88581	-1463.57452		1
35	C	66.53420	81.56215	66.12717	-153.07550	-733.68902	248.70981		1
36	O	67.13758	82.39536	65.50266	186.15459	-480.78787	-449.34387		1
37	N	67.00394	80.66518	67.01023	-487.53139	543.18517	42.03850		1
38	C	68.33207	80.14871	66.94693	-699.35871	69.34393	360.10701		1
39	H	68.87898	80.80338	66.22894	2.81126	-221.99807	-2715.58072		1
40	C	68.75825	80.26518	68.47549	-507.46439	-592.59194	122.07761		1
41	H	69.67352	79.68116	68.72643	-1975.08116	525.87560	-1801.71556		1
42	H	68.96688	81.32120	68.75634	1588.27743	-1913.22100	1113.83566		1
43	C	67.46751	79.73761	69.17612	-613.62442	-457.55993	-194.14490		1
44	H	67.40943	78.62718	69.13716	1707.54637	-721.27992	1996.92523		1
45	H	67.39706	80.01763	70.25158	758.23357	2100.81767	1560.55011		1
46	C	66.33653	80.40214	68.28154	-352.41524	704.96076	49.21465		1
47	H	65.45991	79.74372	68.06241	1714.76886	-2070.42778	443.35792		1
48	H	65.97991	81.39868	68.63679	1224.15040	1801.50881	1636.97633		1
49	C	68.21302	78.58539	66.45544	566.85117	537.05831	117.62814		1
50	O	67.56094	78.32174	65.47461	-550.26779	-406.08867	4.21666		1
51	N	68.95763	77.77095	67.19986	566.34832	-425.77725	180.18749		1

52	H	69.48029	78.16149	67.98380	644.44502	2646.80550	-52.73430	1
53	C	68.66267	76.38176	67.12954	612.34801	-281.48662	411.56221	1
54	H	68.22923	76.23260	66.11341	1667.23498	-1490.75142	1556.16753	1
55	C	70.01057	75.58173	67.43604	-714.45746	-175.43074	286.98927	1
56	H	70.35338	75.83500	68.47890	-787.09484	1763.03619	-1922.46060	1
57	O	71.14333	75.87455	66.59766	-429.46514	516.51932	-128.40526	1
58	H	71.76391	76.26308	67.24764	1981.82785	436.16847	-1818.18182	1
59	C	69.47928	74.10114	67.39617	630.79189	-468.94448	76.03230	1
60	H	70.24826	73.37937	67.75663	-1775.71861	2062.30353	131.89849	1
61	H	68.56828	73.96922	68.02984	-1855.14608	88.94118	1993.53760	1
62	H	69.20262	73.80002	66.35915	-1504.82350	-780.94249	-2132.90992	1
63	C	67.61342	75.99050	68.34254	288.57638	618.62814	-397.00270	1
64	O	66.68152	75.25912	68.10186	321.70495	-185.26452	574.37218	1
65	N	68.05321	76.43720	69.50672	-447.05792	-446.53431	367.76425	1
66	H	68.87251	77.03870	69.47927	350.31316	1975.63644	-1843.31522	1
67	C	67.31519	76.20177	70.70998	-511.23061	374.03917	-471.51480	1
68	H	66.31279	76.65084	70.53732	2234.79579	-898.70890	-1273.45190	1
69	C	67.21478	74.61892	70.90928	529.53781	-159.34528	563.72604	1
70	H	66.51718	74.43242	71.77147	654.59388	2347.94251	1217.51488	1
71	H	66.71754	74.20394	69.98808	-1526.55661	2103.42026	817.87394	1
72	O	68.45141	73.91139	71.20829	-554.84278	14.12789	399.58769	1
73	H	68.82523	73.86146	70.31025	1297.06236	2061.84854	1220.68812	1
74	C	68.13521	76.86003	71.94683	-662.15484	-412.13544	123.62687	1
75	O	67.53920	77.26252	72.91667	-540.01537	-317.05804	274.91456	1
76	N	69.44296	76.77582	71.73607	-202.76299	-690.00100	-131.49145	1
77	H	69.84190	76.40148	70.85877	-702.62132	-2617.37191	281.70413	1
78	C	70.40188	77.29867	72.64461	-491.73914	576.34187	222.73509	1
79	H	69.93942	78.14745	73.19735	1977.17978	-1823.58850	-434.68928	1
80	C	70.81459	76.10545	73.61639	-649.50797	-328.66843	306.11224	1
81	H	70.96035	75.17228	73.03003	2075.07803	1452.16490	-1004.45904	1
82	C	72.09587	76.44782	74.44711	-615.18735	-489.99689	-70.96352	1
83	H	72.29355	75.67709	75.22851	-1226.32661	-1724.38906	-1716.47170	1
84	H	73.01756	76.49417	73.78230	2381.64273	-969.84735	900.46860	1
85	H	72.00111	77.42928	74.96902	2122.74991	1702.23946	-141.36228	1
86	C	69.66817	75.91835	74.66765	-501.86074	-479.61276	-376.42482	1
87	H	69.86831	75.05864	75.35018	993.79261	-2246.95401	-1177.81305	1
88	H	69.54241	76.82678	75.30266	42.71279	-626.15391	-2651.37258	1
89	H	68.68800	75.72944	74.16458	-2026.39012	-1590.33709	-887.82922	1
90	C	71.56558	77.67605	71.56313	-672.89153	382.57394	-156.34072	1
91	O	71.46634	77.28497	70.40967	410.04627	221.86223	500.35950	1
92	N	72.49010	78.44674	72.11963	-378.11782	-443.79414	-441.10984	1
93	H	72.39497	78.60443	73.12265	2404.15973	-568.14894	1149.30085	1
94	C	73.76381	78.59081	71.47326	-544.54484	466.16019	331.29119	1
95	H	73.52893	78.89344	70.42896	-1409.80988	-170.17955	2325.32679	1
96	C	74.52429	79.68062	72.33541	-184.48284	116.78282	-758.89137	1
97	H	73.91279	80.60838	72.40530	1893.78641	1861.14652	611.04528	1
98	H	74.64729	79.32151	73.38201	-2170.79665	-974.19311	1327.50117	1
99	C	75.91628	79.99068	71.70235	389.51668	672.81878	-138.49152	1
100	H	76.53589	79.06496	71.66470	510.64577	1933.03327	1851.02484	1
101	H	75.79915	80.28539	70.63461	-2302.30869	-1105.72939	-948.89774	1
102	C	76.69909	81.12529	72.46689	-559.93427	-126.34590	542.30857	1
103	O	77.75567	81.50950	72.03624	-670.36003	-111.83166	76.36448	1
104	N	76.07845	81.57795	73.57755	-216.06729	-537.07037	446.51379	1
105	H	75.18943	81.28476	73.99881	-1251.96487	1074.12894	-2168.52500	1
106	H	76.46011	82.30757	74.18958	-2451.83023	-720.73851	944.84612	1
107	C	74.54399	77.16836	71.55015	546.24052	-563.88337	-85.11809	1
108	O	74.49877	76.49993	72.55860	71.70702	-307.40463	606.69673	1
109	N	75.24074	76.95850	70.43124	479.90863	-504.50129	222.86849	1
110	C	75.94222	75.72151	70.21969	75.51268	-600.91904	506.73700	1
111	H	75.22642	74.90183	70.45666	-2033.61562	1795.30103	254.89480	1
112	C	76.36498	75.82042	68.69368	523.79067	517.99274	284.45581	1
113	H	77.28109	75.23202	68.46210	1599.61665	-1127.00911	1895.98173	1

114	H	75.56440	75.43466	68.02365	-1881.83093	1275.82488	-1501.55016	1
115	C	76.55937	77.35665	68.50848	-600.05639	-404.05026	316.64485	1
116	H	77.51197	77.70129	68.97108	-2597.05260	496.36221	657.73249	1
117	H	76.57617	77.68478	67.44473	-1666.24518	1294.38985	-1723.90591	1
118	C	75.29614	77.89036	69.31426	493.57570	-129.95376	-602.56394	1
119	H	75.38588	78.93246	69.70151	-1469.08415	-637.84797	2204.22581	1
120	H	74.32614	77.77708	68.77301	-1038.97840	1068.88701	-2280.71789	1
121	C	77.25851	75.67887	71.18357	188.88100	241.05089	-727.87821	1
122	O	77.86209	76.67828	71.49308	531.88613	-49.19943	427.07960	1
123	N	77.61388	74.39646	71.34832	708.14833	26.93417	-179.73509	1
124	H	76.92513	73.76900	70.92860	-2232.69501	-1179.09831	1023.94816	1
125	C	78.40051	73.90278	72.48329	-738.32412	259.92548	104.42456	1
126	H	78.92517	73.02971	72.03186	2028.89123	1260.02983	1311.33324	1
127	C	79.34635	74.95729	73.00871	-258.65678	-345.52513	661.28459	1
128	H	78.76265	75.88205	73.24359	-1826.06090	-1801.46097	-918.64554	1
129	C	80.03809	74.50673	74.28155	-541.23400	531.92970	-218.41428	1
130	H	80.78757	75.26583	74.63665	1311.73218	-2219.18200	882.19023	1
131	H	79.29184	74.35017	75.13252	-1048.71298	1223.58118	-2196.97971	1
132	H	80.58782	73.53726	74.13479	419.06414	1903.92898	1903.44670	1
133	C	80.38660	75.33698	71.96763	-423.86431	152.66566	-648.55262	1
134	H	81.08104	76.13616	72.34475	105.68386	-2342.50080	1387.51238	1
135	H	81.01747	74.45671	71.66720	-1695.63603	-1484.73621	-1531.02793	1
136	H	79.89389	75.73380	71.03596	-1853.57121	-487.39031	1936.59343	1
137	C	77.30929	73.34974	73.61665	539.71428	-510.58232	267.58633	1
138	O	77.17508	72.15533	73.73131	-15.93758	-278.34085	-624.49402	1
139	N	76.68442	74.32458	74.25351	-676.81886	12.05292	276.17960	1
140	H	76.90814	75.27365	73.96039	-1694.44250	-373.84189	-2100.66098	1
141	C	75.96515	74.05518	75.45622	412.33078	-664.70360	108.35451	1
142	H	75.57179	75.06627	75.70557	1765.77476	1294.44366	1621.76594	1
143	C	74.82349	73.02871	75.07504	-179.66635	-721.95667	-264.73915	1
144	H	74.41270	73.28238	74.07165	-607.34922	2587.87032	-598.10018	1
145	H	75.25355	72.00539	74.96139	-359.69332	-1479.13954	-2259.74260	1
146	C	73.68129	73.06046	76.14494	-240.01076	616.02425	431.85322	1
147	H	74.06565	72.83341	77.16439	-1359.17131	782.54425	2227.99181	1
148	H	73.22864	74.07389	76.21492	-820.36667	85.81767	-2596.78715	1
149	C	72.60226	71.99084	75.70491	-513.07015	236.18570	-551.87280	1
150	H	72.12772	72.28033	74.73897	1816.11944	-1183.11722	-1650.94321	1
151	H	73.07919	71.00016	75.52303	-1800.04429	-1361.53473	1526.34643	1
152	C	71.54619	71.88359	76.82905	726.08972	-253.19732	-179.64713	1
153	H	71.93279	71.48183	77.78700	1224.27271	-456.51798	-2390.90304	1
154	H	70.96878	72.81155	77.01250	1206.40339	-1150.93514	-2154.90344	1
155	N	70.47747	70.83563	76.36646	329.70796	-633.68968	-155.67358	1
156	H	69.69732	70.63537	77.05676	1348.31305	1938.76845	1359.00643	1
157	H	69.92521	71.06707	75.49007	2096.92035	1446.54551	-966.48890	1
158	H	70.82407	69.85514	76.15374	-1197.07217	-2303.53719	827.28733	1
159	C	77.05762	73.54582	76.56050	-378.01186	-556.17301	-413.96481	1
160	O	78.11234	74.16650	76.68977	-409.44433	-307.55053	-453.30833	1
161	N	76.60882	72.55495	77.30119	-429.02477	524.70884	274.08502	1
162	H	75.69902	72.20909	77.00239	1706.34263	-1425.96036	1574.38926	1
163	C	77.40720	71.71290	78.12709	-45.25864	-626.22952	478.93267	1
164	H	76.71395	70.86290	78.33283	1988.63164	570.90773	1772.87287	1
165	C	78.69051	71.25375	77.31360	551.77128	-20.49526	-564.54996	1
166	H	78.44068	71.04561	76.24855	1434.61535	-1753.10253	1513.99471	1
167	H	79.45854	72.05975	77.29483	-714.67738	1819.09770	1898.36494	1
168	C	79.21127	69.97518	78.04852	446.99263	-555.77305	338.97221	1
169	H	79.34901	70.18143	79.13602	1953.68466	1892.25957	-161.67766	1
170	H	78.45176	69.15567	77.99131	-403.03785	2688.07032	-188.43591	1
171	C	80.58152	69.50272	77.42021	567.86262	335.74681	434.04421	1
172	H	80.47475	69.28078	76.33356	-1080.02275	1568.26081	-1948.78900	1
173	H	81.35929	70.30005	77.49750	-919.54108	2111.34692	1456.13463	1
174	C	80.98594	68.23807	78.21701	195.81897	173.33862	-745.11536	1
175	H	81.16714	68.41048	79.29938	1405.67949	-2301.21089	-390.08113	1

176	H	80.30589	67.37111	78.08615	-940.37328	-1118.32446	2299.72133	1
177	N	82.36937	67.76076	77.67221	319.26422	656.36007	-42.02424	1
178	H	82.80857	66.95773	78.20857	1961.03633	619.91968	1787.09422	1
179	H	82.41023	67.40118	76.67398	854.14343	-2156.80752	1429.08711	1
180	H	83.15570	68.47100	77.68608	1237.02905	-1378.50857	-1998.28500	1
181	C	77.94946	72.40464	79.50158	532.53319	-268.57236	517.55729	1
182	O	78.31459	71.66292	80.40577	266.16714	-290.73804	-558.88002	1
183	N	77.97611	73.70696	79.41792	-226.25352	640.49678	-270.32839	1
184	H	77.71683	74.12941	78.50975	2007.69063	-1035.27229	1523.50231	1
185	C	78.15862	74.57134	80.53486	-540.76542	-573.33303	49.50000	1
186	H	77.52924	75.44209	80.24601	-2374.20950	-1036.76023	843.75774	1
187	C	77.69160	73.88293	81.89030	-77.09082	666.87422	-415.84136	1
188	H	78.37554	73.01344	82.11649	-985.81834	617.19825	2463.91927	1
189	O	76.36360	73.29602	81.90294	293.29899	-391.65602	-477.80926	1
190	H	76.59852	72.36668	81.69476	2528.72714	-681.76262	-751.27122	1
191	C	77.94582	75.04669	82.91587	252.47363	-605.14473	440.05134	1
192	H	77.81641	74.70182	83.96770	-2052.65063	1456.49051	-1043.51830	1
193	H	78.97681	75.46314	82.82509	-2152.98800	-1661.97574	-161.70652	1
194	H	77.23573	75.89071	82.75471	-473.12726	-1584.27339	2165.61725	1
195	C	79.74445	75.00124	80.50170	360.36307	488.46713	505.10056	1
196	O	80.11374	75.84264	79.71719	-200.08817	-528.03552	-385.82850	1
197	N	80.46445	74.32209	81.38806	-597.54095	-226.44775	355.20479	1
198	H	80.02681	73.60845	81.96897	2179.23655	-1300.70981	-991.33835	1
199	C	81.85794	74.54008	81.43007	-687.68921	297.39807	-249.45179	1
200	H	82.06512	75.30005	80.63955	-349.16256	-2467.37713	-1101.72831	1
201	C	82.33985	74.95307	82.90508	672.47345	361.54328	-201.62880	1
202	H	82.06826	74.16507	83.64248	1541.41502	582.18425	2169.97026	1
203	H	83.45187	75.03175	82.91711	-2534.67717	60.25153	997.72295	1
204	C	81.68789	76.29093	83.28162	574.26774	-389.43119	-377.02542	1
205	C	82.08249	77.49031	82.61575	688.82679	-287.33580	-257.96133	1
206	H	82.86558	77.47217	81.83619	331.14182	1470.38163	2269.80013	1
207	C	80.67054	76.32227	84.28255	-383.52382	-675.04808	144.24917	1
208	H	80.36082	75.39557	84.79859	4.09847	1517.59662	2262.86397	1
209	C	81.45201	78.68482	82.96201	-134.76730	428.45285	-649.50303	1
210	H	81.75475	79.61192	82.44429	-903.23433	1600.49020	2011.53387	1
211	C	80.06810	77.54367	84.59351	-335.53281	-615.00040	-364.39058	1
212	H	79.28068	77.55506	85.36713	1596.45398	-1369.33862	1732.02659	1
213	C	80.43082	78.76431	83.95289	585.48547	-340.24194	-406.23938	1
214	O	79.82561	80.01030	84.26178	-419.15649	-173.04408	-511.94141	1
215	H	79.19879	79.72128	84.96605	-1071.84350	1559.71507	-1960.13012	1
216	C	82.57772	73.07909	81.23507	291.41878	-183.13091	710.72246	1
217	O	83.53147	72.79819	81.93210	379.87695	523.47396	-222.23622	1
218	N	81.98376	72.36998	80.28387	564.30591	373.09380	277.24371	1
219	H	81.19774	72.82287	79.81575	-120.59931	-2436.07824	-1214.35098	1
220	C	82.52049	71.12710	79.83846	404.07514	-299.37480	608.84009	1
221	H	82.12666	71.03178	78.79970	-1071.07882	-841.69025	2359.66467	1
222	C	84.10665	71.20134	79.92598	-683.12807	68.71770	-390.13096	1
223	H	84.47342	72.18133	79.54531	2068.88918	1596.58590	770.89603	1
224	H	84.43319	71.15219	80.99678	1379.86429	2342.49779	-179.85638	1
225	C	84.72555	70.02028	79.11788	-176.39967	537.49466	550.97268	1
226	H	84.30249	69.04623	79.45951	-396.28051	1942.22168	1869.33314	1
227	H	84.48394	70.09951	78.03479	-94.44700	586.00678	-2659.20016	1
228	C	86.30460	70.07824	79.36682	-291.69381	-718.18079	-150.72929	1
229	H	86.82575	71.00937	79.02985	-2303.38776	1089.76242	964.62032	1
230	H	86.60297	69.86480	80.42538	884.16729	2568.80533	-207.74283	1
231	N	86.74688	69.00763	78.57861	-594.49522	-252.81478	342.29276	1
232	H	86.06985	68.28669	78.38073	-1735.17426	2084.05705	-263.71605	1
233	C	87.92943	68.86671	78.13018	595.23177	-271.52487	442.22352	1
234	N	88.87393	69.85464	78.42807	585.53813	-424.79750	-105.81303	1
235	H	88.77558	70.69747	78.99191	959.88797	1327.56823	-2177.11905	1
236	H	89.85059	69.83540	78.13347	1578.48647	16.27378	-2220.76233	1
237	N	88.04495	67.67939	77.39338	-452.17763	-390.33541	-421.51853	1

238	H	87.36097	66.95579	77.17890	470.26107	1974.25629	-1817.92087	1
239	H	88.91532	67.38009	76.95263	1856.67307	-1573.97321	-1224.35416	1
240	C	81.99731	69.93313	80.80503	-531.47271	-581.45780	-55.06206	1
241	O	82.65074	68.92907	80.95949	-243.00837	192.73507	609.52485	1
242	N	80.73448	70.14710	81.23651	343.49288	-644.25607	38.09164	1
243	H	80.40035	71.08273	80.98905	-1691.16043	-1535.97525	-1484.73099	1
244	C	80.36164	69.54425	82.53079	542.66492	350.14337	454.42563	1
245	H	81.27591	68.97971	82.83511	1209.57979	-2396.95920	463.86744	1
246	C	79.96163	70.66586	83.46932	-737.14309	145.93010	242.71942	1
247	H	79.12854	71.22491	82.98683	-1050.18303	159.36419	-2509.06125	1
248	C	79.45552	70.11943	84.79214	-706.77696	-252.88343	-245.16230	1
249	H	79.06376	70.93473	85.46051	-1624.64039	-1665.49085	1417.86935	1
250	H	78.62236	69.37732	84.64000	2566.10521	598.51109	693.22305	1
251	H	80.26982	69.58634	85.35625	-1972.69758	107.10018	-1876.34312	1
252	C	81.09761	71.64335	83.70498	412.85148	672.58832	-27.69222	1
253	H	80.76323	72.52918	84.31222	1447.02277	1762.76533	-1490.78944	1
254	H	81.94673	71.15874	84.26107	1320.77379	-145.20455	2378.68491	1
255	H	81.52978	72.03615	82.73569	-1512.10848	1470.52031	1724.75147	1
256	C	79.05384	68.56292	82.29224	-607.11113	499.56689	73.73769	1
257	O	78.94003	67.54737	82.93107	357.97126	460.81534	356.68785	1
258	N	78.20428	69.10408	81.43499	536.55407	-368.62270	332.76306	1
259	H	78.39832	70.03056	80.98405	524.38866	2297.69985	1367.20941	1
260	C	77.00624	68.39186	81.17484	46.50277	-774.29190	-147.97904	1
261	H	77.05619	67.47886	81.81571	1676.51875	1883.29066	1032.55549	1
262	C	75.74625	69.35265	81.48975	-559.41456	-34.19198	-556.30433	1
263	H	75.81335	70.26910	80.85670	-64.66664	395.18769	2695.05373	1
264	H	74.79284	68.84812	81.20298	-2703.44278	-60.40056	333.79418	1
265	C	75.74828	69.71169	82.95078	-519.76435	377.31045	459.42366	1
266	H	76.75712	70.10266	83.21488	-1746.74323	1667.50644	-1261.73691	1
267	C	74.71748	70.79674	83.23611	570.95554	16.46261	-545.27700	1
268	H	74.67512	71.04931	84.32693	2391.58273	28.05277	-1305.07271	1
269	H	74.94841	71.74857	82.68543	175.75588	917.63458	2559.43867	1
270	H	73.68790	70.47701	82.93059	-1063.97851	-2155.34650	1283.00462	1
271	C	75.45849	68.49628	83.82199	193.76014	2.62946	-765.53141	1
272	H	75.37980	68.77277	84.90497	507.39394	-846.55087	2539.60089	1
273	H	74.49383	68.00302	83.53590	1337.57841	1818.19054	1526.01994	1
274	H	76.26593	67.72351	83.73788	1100.88635	-1172.91350	-2199.08909	1
275	C	77.05520	68.08740	79.58882	-549.21115	475.64486	-309.38218	1
276	O	76.36386	68.64800	78.77958	556.06106	-390.37755	-78.24250	1
277	O	78.04116	67.15744	79.18406	-572.27940	-310.19032	-209.75862	1
278	H	78.43162	66.94896	80.08314	-1380.08193	2212.14486	790.85944	1

Listing 51: C00051.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.6855	0.0000	300.0000
3	H	64.75932	75.73609	74.33608	-2043.14101	-1757.64893	399.89339		1
4	N	65.63330	75.22322	74.22643	426.75047	490.45733	-334.42467		1
5	H	65.38206	74.48753	73.55695	442.25559	-1110.30854	-2448.52907		1
6	C	66.71825	76.00602	73.76681	415.32972	-666.39213	83.73172		1
7	H	66.38018	77.06232	73.84907	879.32219	2491.00447	667.35213		1
8	C	68.01162	75.71433	74.68881	31.35357	477.41777	628.23362		1
9	H	68.33869	74.65790	74.54022	1168.38489	2240.25337	-1019.71136		1
10	H	68.87167	76.35110	74.37173	-360.43770	2534.90498	931.67112		1
11	C	67.66386	75.95876	76.13193	463.18208	512.70242	-382.34388		1
12	H	66.76618	75.34739	76.37914	1725.29117	1863.52247	-987.07854		1
13	C	68.81414	75.52599	77.03321	710.42801	-144.27427	-313.15367		1
14	H	68.56387	75.66009	78.11704	364.20195	-1033.13725	2494.72524		1
15	H	69.07520	74.44669	76.88322	2567.61904	335.80679	847.48802		1
16	H	69.74065	76.12290	76.83149	-2587.99029	680.92867	-512.16411		1
17	C	67.34078	77.42421	76.39135	268.17616	741.64379	-40.42634		1

18	H	67.12697	77.61440	77.47472	1283.54314	-1945.37420	-1411.27812	1
19	H	68.19123	78.09303	76.09870	-1258.57796	1317.15249	-2026.02085	1
20	H	66.44101	77.75916	75.81424	-2502.84526	909.80597	575.92391	1
21	C	66.95551	75.50732	72.24907	619.36578	-458.64843	-172.09273	1
22	O	66.20626	74.66413	71.72628	-81.40433	433.87611	522.34594	1
23	N	67.95142	76.16497	71.72572	175.23996	-622.20190	341.55523	1
24	H	68.44181	76.80282	72.35058	-876.57256	-303.22879	-2561.90213	1
25	C	68.44205	75.98997	70.38854	-571.88214	-534.10783	-106.15033	1
26	H	69.28162	75.26918	70.50302	-2713.20841	-16.25800	-248.80809	1
27	C	67.30732	75.38505	69.43362	166.60354	288.16399	-716.09568	1
28	H	66.31835	75.81627	69.76244	-2097.85574	1636.78449	-586.18044	1
29	O	67.15769	73.96974	69.51229	-317.80580	-363.38227	484.43082	1
30	H	66.52327	73.91471	70.33026	1863.74748	-1451.84923	1357.29467	1
31	C	67.70255	75.97018	68.02955	503.80731	517.99032	318.51606	1
32	H	67.01538	75.61335	67.22717	640.61020	-2157.10410	-1536.29104	1
33	H	67.67689	77.08740	68.02133	1687.88455	465.60692	2087.56452	1
34	H	68.74051	75.66948	67.74406	-1293.07895	-1899.88581	-1463.57452	1
35	C	69.00174	77.41443	69.86366	-153.07550	-733.68902	248.70981	1
36	O	69.76062	77.33735	68.92697	186.15459	-480.78787	-449.34387	1
37	N	68.45245	78.51598	70.39143	-487.53139	543.18517	42.03850	1
38	C	69.06570	79.78961	70.14416	-699.35871	69.34393	360.10701	1
39	H	69.64838	79.60366	69.21018	2.81126	-221.99807	-2715.58072	1
40	C	67.79024	80.72459	69.98250	-507.46439	-592.59194	122.07761	1
41	H	68.01549	81.80936	70.10070	-1975.08116	525.87560	-1801.71556	1
42	H	67.32866	80.60850	68.97686	1588.27743	-1913.22100	1113.83566	1
43	C	66.85757	80.14842	71.09171	-613.62442	-457.55993	-194.14490	1
44	H	67.19738	80.45729	72.10624	1707.54637	-721.27992	1996.92523	1
45	H	65.79518	80.46772	70.99884	758.23357	2100.81767	1560.55011	1
46	C	67.07035	78.59198	70.85221	-352.41524	704.96076	49.21465	1
47	H	66.96369	77.97018	71.76906	1714.76886	-2070.42778	443.35792	1
48	H	66.45061	78.14825	70.03840	1224.15040	1801.50881	1636.97633	1
49	C	70.04645	80.14588	71.40284	566.85117	537.05831	117.62814	1
50	O	70.94068	79.38172	71.69814	-550.26779	-406.08867	4.21666	1
51	N	69.70502	81.28850	71.98966	566.34832	-425.77725	180.18749	1
52	H	68.94629	81.80852	71.54506	644.44502	2646.80550	-52.73430	1
53	C	70.77429	82.09589	72.54010	612.34801	-281.48662	411.56221	1
54	H	71.57034	82.11590	71.76292	1667.23498	-1490.75142	1556.16753	1
55	C	70.10144	83.51292	72.80324	-714.45746	-175.43074	286.98927	1
56	H	69.30022	83.39949	73.58420	-787.09484	1763.03619	-1922.46060	1
57	O	69.45219	84.10614	71.65856	-429.46514	516.51932	-128.40526	1
58	H	68.54729	84.24198	72.00054	1981.82785	436.16847	-1818.18182	1
59	C	71.31359	84.30894	73.41351	630.79189	-468.94448	76.03230	1
60	H	71.01172	85.33537	73.72638	-1775.71861	2062.30353	131.89849	1
61	H	71.73330	83.79717	74.31091	-1855.14608	88.94118	1993.53760	1
62	H	72.14320	84.41659	72.67642	-1504.82350	-780.94249	-2132.90992	1
63	C	71.26354	81.41413	73.92607	288.57638	618.62814	-397.00270	1
64	O	70.52060	81.13180	74.83033	321.70495	-185.26452	574.37218	1
65	N	72.61521	81.41796	73.91395	-447.05792	-446.53431	367.76425	1
66	H	73.06728	81.70227	73.02373	350.31316	1975.63644	-1843.31522	1
67	C	73.18695	80.29204	74.62833	-511.23061	374.03917	-471.51480	1
68	H	72.42012	80.03060	75.39520	2234.79579	-898.70890	-1273.45190	1
69	C	73.36432	79.15257	73.53094	529.53781	-159.34528	563.72604	1
70	H	73.42199	78.14485	73.99914	654.59388	2347.94251	1217.51488	1
71	H	72.46144	79.15225	72.84077	-1526.55661	2103.42026	817.87394	1
72	O	74.30993	82.41244	71.85120	-554.84278	14.12789	399.58769	2
73	H	74.62929	80.51703	72.34469	1297.06236	2061.84854	1220.68812	1
74	C	74.60087	80.71579	75.25664	-662.15484	-412.13544	123.62687	1
75	O	75.02850	80.09199	76.21965	-540.01537	-317.05804	274.91456	1
76	N	75.19966	81.66858	74.55221	-202.76299	-690.00100	-131.49145	1
77	H	74.67675	81.97303	73.71421	-702.62132	-2617.37191	281.70413	1
78	C	76.02683	82.71219	75.17291	-491.73914	576.34187	222.73509	1
79	H	76.01274	83.52631	74.41053	1977.17978	-1823.58850	-434.68928	1

80	C	75.37144	83.12060	76.47896	-649.50797	-328.66843	306.11224	1
81	H	75.22150	82.19600	77.08481	2075.07803	1452.16490	-1004.45904	1
82	C	76.24949	84.07339	77.26843	-615.18735	-489.99689	-70.96352	1
83	H	75.77733	84.36449	78.24706	-1226.32661	-1724.38906	-1716.47170	1
84	H	77.25080	83.61451	77.50074	2381.64273	-969.84735	900.46860	1
85	H	76.44758	85.02230	76.69726	2122.74991	1702.23946	-141.36228	1
86	C	74.00586	83.74033	76.24280	-501.86074	-479.61276	-376.42482	1
87	H	73.49594	84.01055	77.20797	993.79261	-2246.95401	-1177.81305	1
88	H	74.07797	84.68026	75.62893	42.71279	-626.15391	-2651.37258	1
89	H	73.32652	83.03359	75.68946	-2026.39012	-1590.33709	-887.82922	1
90	C	77.57693	82.17898	75.42662	-672.89153	382.57394	-156.34072	1
91	O	78.49118	82.92290	75.17954	410.04627	221.86223	500.35950	1
92	N	77.60207	80.98748	75.99295	-378.11782	-443.79414	-441.10984	1
93	H	76.70283	80.48780	76.18862	2404.15973	-568.14894	1149.30085	1
94	C	78.87226	80.43098	76.30935	-544.54484	466.16019	331.29119	1
95	H	79.59424	81.25783	76.10129	-1409.80988	-170.17955	2325.32679	1
96	C	78.78224	80.02700	77.84657	-184.48284	116.78282	-758.89137	1
97	H	78.60796	80.92168	78.48532	1893.78641	1861.14652	611.04528	1
98	H	77.89855	79.37613	78.02743	-2170.79665	-974.19311	1327.50117	1
99	C	80.11460	79.31392	78.23278	389.51668	672.81878	-138.49152	1
100	H	80.41725	78.63472	77.40163	510.64577	1933.03327	1851.02484	1
101	H	80.93967	80.05668	78.30328	-2302.30869	-1105.72939	-948.89774	1
102	C	80.03903	78.47637	79.57196	-559.93427	-126.34590	542.30857	1
103	O	81.03334	78.29183	80.22364	-670.36003	-111.83166	76.36448	1
104	N	78.81258	77.92354	79.81000	-216.06729	-537.07037	446.51379	1
105	H	78.05720	77.93584	79.11788	-1251.96487	1074.12894	-2168.52500	1
106	H	78.72510	77.03374	80.32967	-2451.83023	-720.73851	944.84612	1
107	C	79.18823	79.11241	75.39006	546.24052	-563.88337	-85.11809	1
108	O	80.35273	78.93497	75.13678	71.70702	-307.40463	606.69673	1
109	N	78.15905	78.27564	75.17283	479.90863	-504.50129	222.86849	1
110	C	78.26757	77.30771	74.12391	75.51268	-600.91904	506.73700	1
111	H	79.32191	77.41468	73.77520	-2033.61562	1795.30103	254.89480	1
112	C	77.94864	75.96887	74.91181	523.79067	517.99274	284.45581	1
113	H	77.68321	75.11704	74.24580	1599.61665	-1127.00911	1895.98173	1
114	H	78.82963	75.63718	75.50561	-1881.83093	1275.82488	-1501.55016	1
115	C	76.78858	76.42133	75.85582	-600.05639	-404.05026	316.64485	1
116	H	75.80983	76.45964	75.32840	-2597.05260	496.36221	657.73249	1
117	H	76.64610	75.74688	76.72994	-1666.24518	1294.38985	-1723.90591	1
118	C	77.27473	77.87392	76.26497	493.57570	-129.95376	-602.56394	1
119	H	76.45142	78.63809	76.32976	-1469.08415	-637.84797	2204.22581	1
120	H	77.90594	77.90665	77.18319	-1038.97840	1068.88701	-2280.71789	1
121	C	77.17845	77.68030	72.94499	188.88100	241.05089	-727.87821	1
122	O	77.39564	78.66361	72.27378	531.88613	-49.19943	427.07960	1
123	N	76.15994	76.84389	72.89662	708.14833	26.93417	-179.73509	1
124	H	76.15245	76.07794	73.56563	-2232.69501	-1179.09831	1023.94816	1
125	C	75.09501	76.97148	71.96510	-738.32412	259.92548	104.42456	1
126	H	74.23596	76.50940	72.49962	2028.89123	1260.02983	1311.33324	1
127	C	74.88723	78.47506	71.51419	-258.65678	-345.52513	661.28459	1
128	H	75.78313	78.80689	70.93144	-1826.06090	-1801.46097	-918.64554	1
129	C	73.61126	78.50442	70.60148	-541.23400	531.92970	-218.41428	1
130	H	73.34090	79.54417	70.30173	1311.73218	-2219.18200	882.19023	1
131	H	73.77415	77.91545	69.66519	-1048.71298	1223.58118	-2196.97971	1
132	H	72.71894	78.07003	71.11436	419.06414	1903.92898	1903.44670	1
133	C	74.66873	79.45426	72.72281	-423.86431	152.66566	-648.55262	1
134	H	74.26655	82.10899	70.94358	105.68386	-2342.50080	1387.51238	2
135	H	75.55338	79.40826	73.40351	-1695.63603	-1484.73621	-1531.02793	1
136	H	75.15299	82.86807	71.84342	-1853.57121	-487.39031	1936.59343	2
137	C	75.49880	76.13396	70.60298	539.71428	-510.58232	267.58633	1
138	O	75.72575	76.72851	69.57175	-15.93758	-278.34085	-624.49402	1
139	N	75.42385	74.83604	70.83348	-676.81886	12.05292	276.17960	1
140	H	75.18346	74.55938	71.78467	-1694.44250	-373.84189	-2100.66098	1
141	C	75.76704	73.86425	69.85375	412.33078	-664.70360	108.35451	1

142	H	75.19525	72.96977	70.18840	1765.77476	1294.44366	1621.76594	1
143	C	75.40711	74.39294	68.40807	-179.66635	-721.95667	-264.73915	1
144	H	74.36785	74.79271	68.37769	-607.34922	2587.87032	-598.10018	1
145	H	76.07318	75.25241	68.13137	-359.69332	-1479.13954	-2259.74260	1
146	C	75.59669	73.20649	67.40243	-240.01076	616.02425	431.85322	1
147	H	76.64549	72.82914	67.44667	-1359.17131	782.54425	2227.99181	1
148	H	74.94492	72.34564	67.67140	-820.36667	85.81767	-2596.78715	1
149	C	75.25903	73.73951	65.95327	-513.07015	236.18570	-551.87280	1
150	H	74.21155	74.11618	65.90157	1816.11944	-1183.11722	-1650.94321	1
151	H	75.90681	74.60777	65.69091	-1800.04429	-1361.53473	1526.34643	1
152	C	75.47636	72.57450	64.95933	726.08972	-253.19732	-179.64713	1
153	H	76.52821	72.23773	64.86609	1224.27271	-456.51798	-2390.90304	1
154	H	74.81254	71.70149	65.11870	1206.40339	-1150.93514	-2154.90344	1
155	N	75.10118	73.09819	63.53200	329.70796	-633.68968	-155.67358	1
156	H	75.19983	72.39419	62.74464	1348.31305	1938.76845	1359.00643	1
157	H	74.10499	73.43466	63.38662	2096.92035	1446.54551	-966.48890	1
158	H	75.66589	73.91352	63.15387	-1197.07217	-2303.53719	827.28733	1
159	C	77.38770	73.59420	69.87714	-378.01186	-556.17301	-413.96481	1
160	O	78.07441	73.84674	68.91207	-409.44433	-307.55053	-453.30833	1
161	N	77.74754	73.03439	71.02459	-429.02477	524.70884	274.08502	1
162	H	77.03506	72.88351	71.73690	1706.34263	-1425.96036	1574.38926	1
163	C	79.08394	72.54418	71.12305	-45.25864	-626.22952	478.93267	1
164	H	79.51632	72.70280	70.10471	1988.63164	570.90773	1772.87287	1
165	C	79.78448	73.42089	72.25049	551.77128	-20.49526	-564.54996	1
166	H	79.69921	74.50297	72.00497	1434.61535	-1753.10253	1513.99471	1
167	H	79.28001	73.29883	73.23461	-714.67738	1819.09770	1898.36494	1
168	C	81.27901	72.97529	72.32779	446.99263	-555.77305	338.97221	1
169	H	81.35853	71.93343	72.71265	1953.68466	1892.25957	-161.67766	1
170	H	81.74292	72.96431	71.31594	-403.03785	2688.07032	-188.43591	1
171	C	82.03586	73.99239	73.27511	567.86262	335.74681	434.04421	1
172	H	82.00632	75.02473	72.85663	-1080.02275	1568.26081	-1948.78900	1
173	H	81.54082	74.06050	74.27069	-919.54108	2111.34692	1456.13463	1
174	C	83.49226	73.48887	73.40484	195.81897	173.33862	-745.11536	1
175	H	83.59251	72.45449	73.78870	1405.67949	-2301.21089	-390.08113	1
176	H	84.10473	73.60917	72.48903	-940.37328	-1118.32446	2299.72133	1
177	N	84.19954	74.37816	74.48174	319.26422	656.36007	-42.02424	1
178	H	85.21645	74.14573	74.67396	1961.03633	619.91968	1787.09422	1
179	H	84.25990	75.41819	74.27683	854.14343	-2156.80752	1429.08711	1
180	H	83.79467	74.37281	75.46303	1237.02905	-1378.50857	-1998.28500	1
181	C	79.05258	70.97944	71.58846	532.53319	-268.57236	517.55729	1
182	O	79.65454	70.15493	70.90858	266.16714	-290.73804	-558.88002	1
183	N	78.42200	70.82935	72.71091	-226.25352	640.49678	-270.32839	1
184	H	77.97978	71.62560	73.21291	2007.69063	-1035.27229	1523.50231	1
185	C	78.25914	69.56143	73.36412	-540.76542	-573.33303	49.50000	1
186	H	77.46801	69.03055	72.78971	-2374.20950	-1036.76023	843.75774	1
187	C	79.64317	68.77310	73.21037	-77.09082	666.87422	-415.84136	1
188	H	80.41062	69.56562	72.97694	-985.81834	617.19825	2463.91927	1
189	O	79.64412	67.89785	72.07962	293.29899	-391.65602	-477.80926	1
190	H	79.81020	68.58980	71.32977	2528.72714	-681.76262	-751.27122	1
191	C	80.03369	68.12123	74.58178	252.47363	-605.14473	440.05134	1
192	H	81.07056	67.71166	74.55312	-2052.65063	1456.49051	-1043.51830	1
193	H	79.98933	68.85619	75.42064	-2152.98800	-1661.97574	-161.70652	1
194	H	79.35996	67.27049	74.83772	-473.12726	-1584.27339	2165.61725	1
195	C	77.72230	70.08282	74.79805	360.36307	488.46713	505.10056	1
196	O	77.44484	71.27473	74.92344	-200.08817	-528.03552	-385.82850	1
197	N	77.60077	69.09003	75.65980	-597.54095	-226.44775	355.20479	1
198	H	77.83523	68.16228	75.30638	2179.23655	-1300.70981	-991.33835	1
199	C	77.47407	69.26139	77.06071	-687.68921	297.39807	-249.45179	1
200	H	78.01407	68.39363	77.49980	-349.16256	-2467.37713	-1101.72831	1
201	C	78.07050	70.67398	77.51615	672.47345	361.54328	-201.62880	1
202	H	77.53570	71.50735	76.98984	1541.41502	582.18425	2169.97026	1
203	H	77.88967	70.81676	78.60760	-2534.67717	60.25153	997.72295	1

204	C	79.57833	70.73008	77.22084	574.26774	-389.43119	-377.02542	1
205	C	80.48593	69.92328	77.97036	688.82679	-287.33580	-257.96133	1
206	H	80.11504	69.24740	78.76192	331.14182	1470.38163	2269.80013	1
207	C	80.07483	71.59818	76.20193	-383.52382	-675.04808	144.24917	1
208	H	79.38129	72.22608	75.61153	4.09847	1517.59662	2262.86397	1
209	C	81.85201	70.01464	77.69733	-134.76730	428.45285	-649.50303	1
210	H	82.55079	69.39884	78.28981	-903.23433	1600.49020	2011.53387	1
211	C	81.44922	71.65255	75.96122	-335.53281	-615.00040	-364.39058	1
212	H	81.81598	72.32910	75.17173	1596.45398	-1369.33862	1732.02659	1
213	C	82.39043	70.87696	76.69824	585.48547	-340.24194	-406.23938	1
214	O	83.78840	70.93843	76.45890	-419.15649	-173.04408	-511.94141	1
215	H	83.81336	71.67419	75.80143	-1071.84350	1559.71507	-1960.13012	1
216	C	75.88231	69.21869	77.42712	291.41878	-183.13091	710.72246	1
217	O	75.00172	69.66341	76.72745	379.87695	523.47396	-222.23622	1
218	N	75.77598	68.72018	78.66229	564.30591	373.09380	277.24371	1
219	H	76.62321	68.39158	79.12450	-120.59931	-2436.07824	-1214.35098	1
220	C	74.48413	68.26682	79.06914	404.07514	-299.37480	608.84009	1
221	H	73.79292	68.79615	78.36996	-1071.07882	-841.69025	2359.66467	1
222	C	74.42715	66.68873	78.90387	-683.12807	68.71770	-390.13096	1
223	H	74.79975	66.37977	77.90151	2068.88918	1596.58590	770.89603	1
224	H	75.09169	66.18762	79.64279	1379.86429	2342.49779	-179.85638	1
225	C	72.94083	66.26401	79.10925	-176.39967	537.49466	550.97268	1
226	H	72.57616	66.61778	80.10663	-396.28051	1942.22168	1869.33314	1
227	H	72.28420	66.75303	78.35506	-94.44700	586.00678	-2659.20016	1
228	C	72.83376	64.67382	79.00549	-291.69381	-718.18079	-150.72929	1
229	H	73.12306	64.22011	78.02359	-2303.38776	1089.76242	964.62032	1
230	H	73.34973	64.10367	79.81980	884.16729	2568.80533	-207.74283	1
231	N	71.44828	64.51388	79.17283	-594.49522	-252.81478	342.29276	1
232	H	70.92342	65.33868	79.42045	-1735.17426	2084.05705	-263.71605	1
233	C	70.81923	63.41607	79.04567	595.23177	-271.52487	442.22352	1
234	N	71.55496	62.27412	78.71251	585.53813	-424.79750	-105.81303	1
235	H	72.55787	62.17253	78.56294	959.88797	1327.56823	-2177.11905	1
236	H	71.16230	61.33984	78.59282	1578.48647	16.27378	-2220.76233	1
237	N	69.44834	63.59534	79.27937	-452.17763	-390.33541	-421.51853	1
238	H	68.91625	64.42879	79.52475	470.26107	1974.25629	-1817.92087	1
239	H	68.76813	62.83628	79.22840	1856.67307	-1573.97321	-1224.35416	1
240	C	74.27589	68.65054	80.64049	-531.47271	-581.45780	-55.06206	1
241	O	73.59460	67.96792	81.38064	-243.00837	192.73507	609.52485	1
242	N	74.89974	69.78510	80.93007	343.49288	-644.25607	38.09164	1
243	H	75.42805	70.24679	80.19143	-1691.16043	-1535.97525	-1484.73099	1
244	C	74.66016	70.34100	82.22534	542.66492	350.14337	454.42563	1
245	H	73.63448	69.97966	82.46658	1209.57979	-2396.95920	463.86744	1
246	C	75.72807	69.69855	83.20940	-737.14309	145.93010	242.71942	1
247	H	76.76557	69.87121	82.85227	-1050.18303	159.36419	-2509.06125	1
248	C	75.51199	70.31424	84.63340	-706.77696	-252.88343	-245.16230	1
249	H	76.18606	69.84782	85.38962	-1624.64039	-1665.49085	1417.86935	1
250	H	75.71678	71.41028	84.63885	2566.10521	598.51109	693.22305	1
251	H	74.46419	70.16908	84.98710	-1972.69758	107.10018	-1876.34312	1
252	C	75.43350	68.15976	83.29697	412.85148	672.58832	-27.69222	1
253	H	76.05076	67.66277	84.08226	1447.02277	1762.76533	-1490.78944	1
254	H	74.35972	67.96150	83.53419	1320.77379	-145.20455	2378.68491	1
255	H	75.64965	67.64841	82.32763	-1512.10848	1470.52031	1724.75147	1
256	C	74.77489	71.96941	82.07462	-607.11113	499.56689	73.73769	1
257	O	73.75729	72.61098	81.94580	357.97126	460.81534	356.68785	1
258	N	76.02868	72.40299	82.09357	536.55407	-368.62270	332.76306	1
259	H	76.80186	71.74624	82.18840	524.38866	2297.69985	1367.20941	1
260	C	76.25709	73.79079	81.89508	46.50277	-774.29190	-147.97904	1
261	H	75.31243	74.17429	81.44496	1676.51875	1883.29066	1032.55549	1
262	C	76.58012	74.49077	83.32175	-559.41456	-34.19198	-556.30433	1
263	H	77.44635	73.97583	83.80006	-64.66664	395.18769	2695.05373	1
264	H	76.90220	75.54774	83.16869	-2703.44278	-60.40056	333.79418	1
265	C	75.37496	74.43270	84.21514	-519.76435	377.31045	459.42366	1

266	H	75.05619	73.37037	84.31067	-1746.74323	1667.50644	-1261.73691	1
267	C	75.71874	74.96771	85.60075	570.95554	16.46261	-545.27700	1
268	H	74.83820	74.92276	86.29185	2391.58273	28.05277	-1305.07271	1
269	H	76.54633	74.38242	86.07771	175.75588	917.63458	2559.43867	1
270	H	76.05145	76.03663	85.55793	-1063.97851	-2155.34650	1283.00462	1
271	C	74.20939	75.22600	83.63868	193.76014	2.62946	-765.53141	1
272	H	73.35521	75.28803	84.36101	507.39394	-846.55087	2539.60089	1
273	H	74.50665	76.27574	83.38329	1337.57841	1818.19054	1526.01994	1
274	H	73.81215	74.74824	82.70305	1100.88635	-1172.91350	-2199.08909	1
275	C	77.56235	73.96490	80.98040	-549.21115	475.64486	-309.38218	1
276	O	78.27330	73.06469	80.62703	556.06106	-390.37755	-78.24250	1
277	O	77.88085	75.32379	80.64253	-572.27940	-310.19032	-209.75862	1
278	H	77.07296	75.75121	81.03340	-1380.08193	2212.14486	790.85944	1

Listing 52: C00052.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.6794	0.0000	300.0000
3	H	77.25715	83.10635	78.88329	-2043.14101	-1757.64893	399.89339	1	
4	N	78.26404	82.96360	78.86084	426.75047	490.45733	-334.42467	1	
5	H	78.35030	82.14461	78.26200	442.25559	-1110.30854	-2448.52907	1	
6	C	79.03086	84.06656	78.41456	415.32972	-666.39213	83.73172	1	
7	H	78.52172	84.99785	78.75252	879.32219	2491.00447	667.35213	1	
8	C	80.52273	83.88592	79.03341	31.35357	477.41777	628.23362	1	
9	H	80.94988	82.92364	78.66483	1168.38489	2240.25337	-1019.71136	1	
10	H	81.20029	84.68814	78.65725	-360.43770	2534.90498	931.67112	1	
11	C	80.45509	83.89149	80.53269	463.18208	512.70242	-382.34388	1	
12	H	79.61299	83.23203	80.84458	1725.29117	1863.52247	-987.07854	1	
13	C	81.74710	83.33857	81.12372	710.42801	-144.27427	-313.15367	1	
14	H	81.71478	83.31752	82.24333	364.20195	-1033.13725	2494.72524	1	
15	H	81.94542	82.29169	80.77692	2567.61904	335.80679	847.48802	1	
16	H	82.63278	83.95812	80.82899	-2587.99029	680.92867	-512.16411	1	
17	C	80.20877	85.29394	81.07400	268.17616	741.64379	-40.42634	1	
18	H	80.16592	85.30252	82.19363	1283.54314	-1945.37420	-1411.27812	1	
19	H	81.02157	86.00204	80.76849	-1258.57796	1317.15249	-2026.02085	1	
20	H	79.24136	85.71858	80.70188	-2502.84526	909.80597	575.92391	1	
21	C	79.16631	83.91840	76.83373	619.36578	-458.64843	-172.09273	1	
22	O	79.23645	82.80007	76.20587	-81.40433	433.87611	522.34594	1	
23	N	79.30665	85.07515	76.25249	175.23996	-622.20190	341.55523	1	
24	H	79.21058	85.92549	76.80370	-876.57256	-303.22879	-2561.90213	1	
25	C	79.08958	85.00110	74.83449	-571.88214	-534.10783	-106.15033	1	
26	H	78.00090	85.17175	74.73045	-2713.20841	-16.25800	-248.80809	1	
27	C	79.93202	86.15489	74.17748	166.60354	288.16399	-716.09568	1	
28	H	81.00199	86.06071	74.51138	-2097.85574	1636.78449	-586.18044	1	
29	O	79.53490	87.50500	74.52770	-317.80580	-363.38227	484.43082	1	
30	H	80.34975	87.84873	74.93614	1863.74748	-1451.84923	1357.29467	1	
31	C	79.82018	85.75882	72.65650	503.80731	517.99032	318.51606	1	
32	H	80.44164	86.42425	72.01339	640.61020	-2157.10410	-1536.29104	1	
33	H	80.16405	84.70785	72.48345	1687.88455	465.60692	2087.56452	1	
34	H	78.77034	85.83028	72.28857	-1293.07895	-1899.88581	-1463.57452	1	
35	C	79.59178	83.44634	74.38047	-153.07550	-733.68902	248.70981	1	
36	O	80.79547	83.27002	74.14622	186.15459	-480.78787	-449.34387	1	
37	N	78.59008	82.87855	73.60650	-487.53139	543.18517	42.03850	1	
38	C	78.78882	81.62308	73.00367	-699.35871	69.34393	360.10701	1	
39	H	79.65606	81.13232	73.50613	2.81126	-221.99807	-2715.58072	1	
40	C	77.35328	80.93123	73.18518	-507.46439	-592.59194	122.07761	1	
41	H	77.19119	80.07962	72.48793	-1975.08116	525.87560	-1801.71556	1	
42	H	77.21227	80.53803	74.21616	1588.27743	-1913.22100	1113.83566	1	
43	C	76.42898	82.14712	72.90237	-613.62442	-457.55993	-194.14490	1	
44	H	76.38379	82.36255	71.80859	1707.54637	-721.27992	1996.92523	1	
45	H	75.38210	82.00836	73.25271	758.23357	2100.81767	1560.55011	1	

46	C	77.21225	83.30678	73.67925	-352.41524	704.96076	49.21465	1
47	H	77.13528	84.31620	73.20710	1714.76886	-2070.42778	443.35792	1
48	H	76.97476	83.38764	74.76831	1224.15040	1801.50881	1636.97633	1
49	C	78.99928	81.83040	71.37130	566.85117	537.05831	117.62814	1
50	O	78.38628	82.66091	70.74746	-550.26779	-406.08867	4.21666	1
51	N	79.80821	80.87878	70.93534	566.34832	-425.77725	180.18749	1
52	H	80.22989	80.25240	71.61914	644.44502	2646.80550	-52.73430	1
53	C	80.12056	80.84140	69.54439	612.34801	-281.48662	411.56221	1
54	H	80.11508	81.90524	69.21483	1667.23498	-1490.75142	1556.16753	1
55	C	81.52882	80.10172	69.41588	-714.45746	-175.43074	286.98927	1
56	H	81.43279	79.07384	69.86170	-787.09484	1763.03619	-1922.46060	1
57	O	82.61955	80.73918	70.11022	-429.46514	516.51932	-128.40526	1
58	H	82.85532	80.05548	70.76643	1981.82785	436.16847	-1818.18182	1
59	C	81.70953	79.96854	67.85991	630.79189	-468.94448	76.03230	1
60	H	82.63984	79.40900	67.60601	-1775.71861	2062.30353	131.89849	1
61	H	80.85704	79.42593	67.38562	-1855.14608	88.94118	1993.53760	1
62	H	81.77957	80.96818	67.37136	-1504.82350	-780.94249	-2132.90992	1
63	C	78.94952	79.98761	68.78259	288.57638	618.62814	-397.00270	1
64	O	78.71566	80.19113	67.61350	321.70495	-185.26452	574.37218	1
65	N	78.40956	79.07123	69.58530	-447.05792	-446.53431	367.76425	1
66	H	78.80893	78.99398	70.51896	350.31316	1975.63644	-1843.31522	1
67	C	77.68916	78.00005	68.95732	-511.23061	374.03917	-471.51480	1
68	H	76.92895	78.53436	68.34478	2234.79579	-898.70890	-1273.45190	1
69	C	78.72883	77.17623	68.07429	529.53781	-159.34528	563.72604	1
70	H	78.12057	76.48124	67.43396	654.59388	2347.94251	1217.51488	1
71	H	79.24335	77.87088	67.35929	-1526.55661	2103.42026	817.87394	1
72	O	79.69023	76.41416	68.82388	-554.84278	14.12789	399.58769	1
73	H	79.05759	76.02240	69.53468	1297.06236	2061.84854	1220.68812	1
74	C	77.10498	77.04516	70.13037	-662.15484	-412.13544	123.62687	1
75	O	77.68101	76.00179	70.44839	-540.01537	-317.05804	274.91456	1
76	N	76.01920	77.57553	70.64371	-202.76299	-690.00100	-131.49145	1
77	H	75.69751	78.47712	70.29275	-702.62132	-2617.37191	281.70413	1
78	C	75.35753	76.86429	71.68437	-491.73914	576.34187	222.73509	1
79	H	75.66626	75.80784	71.50702	1977.17978	-1823.58850	-434.68928	1
80	C	75.91786	77.40574	73.07329	-649.50797	-328.66843	306.11224	1
81	H	75.72367	78.49029	73.21378	2075.07803	1452.16490	-1004.45904	1
82	C	75.19231	76.56443	74.17546	-615.18735	-489.99689	-70.96352	1
83	H	75.68817	76.66702	75.17473	-1226.32661	-1724.38906	-1716.47170	1
84	H	74.12255	76.88415	74.28963	2381.64273	-969.84735	900.46860	1
85	H	75.18902	75.47867	73.91960	2122.74991	1702.23946	-141.36228	1
86	C	77.45760	77.12224	73.13000	-501.86074	-479.61276	-376.42482	1
87	H	77.85722	77.18706	74.16911	993.79261	-2246.95401	-1177.81305	1
88	H	77.69791	76.10575	72.73052	42.71279	-626.15391	-2651.37258	1
89	H	78.02522	77.85162	72.50595	-2026.39012	-1590.33709	-887.82922	1
90	C	73.74464	77.13853	71.52088	-672.89153	382.57394	-156.34072	1
91	O	73.04654	76.24041	71.11029	410.04627	221.86223	500.35950	1
92	N	73.41581	78.39765	71.78244	-378.11782	-443.79414	-441.10984	1
93	H	74.15841	79.00788	72.11889	2404.15973	-568.14894	1149.30085	1
94	C	72.03472	78.73385	71.97486	-544.54484	466.16019	331.29119	1
95	H	72.08644	79.84540	71.99236	-1409.80988	-170.17955	2325.32679	1
96	C	71.32007	78.17346	70.66932	-184.48284	116.78282	-758.89137	1
97	H	72.09477	77.86758	69.92767	1893.78641	1861.14652	611.04528	1
98	H	70.72869	77.25407	70.89124	-2170.79665	-974.19311	1327.50117	1
99	C	70.43710	79.29344	70.03497	389.51668	672.81878	-138.49152	1
100	H	69.55824	79.52951	70.67143	510.64577	1933.03327	1851.02484	1
101	H	71.00373	80.24986	70.00113	-2302.30869	-1105.72939	-948.89774	1
102	C	69.94545	78.94130	68.58072	-559.93427	-126.34590	542.30857	1
103	O	69.26089	79.73102	67.98244	-670.36003	-111.83166	76.36448	1
104	N	70.36861	77.74361	68.12133	-216.06729	-537.07037	446.51379	1
105	H	70.92724	77.01714	68.58451	-1251.96487	1074.12894	-2168.52500	1
106	H	70.13382	77.37328	67.19374	-2451.83023	-720.73851	944.84612	1
107	C	71.63211	78.16959	73.43640	546.24052	-563.88337	-85.11809	1

108	O	72.46909	78.24237	74.30538	71.70702	-307.40463	606.69673	1
109	N	70.34028	77.83075	73.58595	479.90863	-504.50129	222.86849	1
110	C	69.90549	77.34125	74.85760	75.51268	-600.91904	506.73700	1
111	H	70.68623	77.63309	75.59987	-2033.61562	1795.30103	254.89480	1
112	C	68.49297	78.06006	74.99772	523.79067	517.99274	284.45581	1
113	H	67.83188	77.57139	75.74762	1599.61665	-1127.00911	1895.98173	1
114	H	68.60099	79.12280	75.30875	-1881.83093	1275.82488	-1501.55016	1
115	C	67.95741	77.94680	73.53807	-600.05639	-404.05026	316.64485	1
116	H	67.61707	76.90763	73.31792	-2597.05260	496.36221	657.73249	1
117	H	67.09994	78.62224	73.31724	-1666.24518	1294.38985	-1723.90591	1
118	C	69.26901	78.30456	72.71720	493.57570	-129.95376	-602.56394	1
119	H	69.35569	77.77489	71.73923	-1469.08415	-637.84797	2204.22581	1
120	H	69.45436	79.39542	72.57716	-1038.97840	1068.88701	-2280.71789	1
121	C	69.58524	75.73394	74.82130	188.88100	241.05089	-727.87821	1
122	O	69.00787	75.19290	73.91080	531.88613	-49.19943	427.07960	1
123	N	69.82375	75.20601	76.06513	708.14833	26.93417	-179.73509	1
124	H	70.36058	75.95184	76.51994	-2232.69501	-1179.09831	1023.94816	1
125	C	70.34204	73.81792	76.15543	-738.32412	259.92548	104.42456	1
126	H	70.56861	73.79716	77.24494	2028.89123	1260.02983	1311.33324	1
127	C	69.28568	72.81905	75.75435	-258.65678	-345.52513	661.28459	1
128	H	69.30133	72.76060	74.64085	-1826.06090	-1801.46097	-918.64554	1
129	C	69.54063	71.42961	76.31407	-541.23400	531.92970	-218.41428	1
130	H	69.03733	70.63585	75.69844	1311.73218	-2219.18200	882.19023	1
131	H	70.63776	71.17857	76.35271	-1048.71298	1223.58118	-2196.97971	1
132	H	69.14720	71.30951	77.36249	419.06414	1903.92898	1903.44670	1
133	C	67.88750	73.26354	76.15467	-423.86431	152.66566	-648.55262	1
134	H	67.10295	72.53255	75.81972	105.68386	-2342.50080	1387.51238	1
135	H	67.79046	73.37346	77.26805	-1695.63603	-1484.73621	-1531.02793	1
136	H	67.63980	74.26091	75.69708	-1853.57121	-487.39031	1936.59343	1
137	C	71.72897	73.82390	75.26960	539.71428	-510.58232	267.58633	1
138	O	72.45075	74.80743	75.30926	-15.93758	-278.34085	-624.49402	1
139	N	71.96002	72.66520	74.70720	-676.81886	12.05292	276.17960	1
140	H	71.22285	71.97396	74.79859	-1694.44250	-373.84189	-2100.66098	1
141	C	73.07130	72.38768	73.83903	412.33078	-664.70360	108.35451	1
142	H	72.60699	72.33503	72.82975	1765.77476	1294.44366	1621.76594	1
143	C	74.17952	73.49644	73.95868	-179.66635	-721.95667	-264.73915	1
144	H	73.80132	74.47434	73.57023	-607.34922	2587.87032	-598.10018	1
145	H	74.41681	73.67192	75.03276	-359.69332	-1479.13954	-2259.74260	1
146	C	75.44407	73.02419	73.16023	-240.01076	616.02425	431.85322	1
147	H	75.48763	71.91294	73.11204	-1359.17131	782.54425	2227.99181	1
148	H	75.40467	73.37574	72.10504	-820.36667	85.81767	-2596.78715	1
149	C	76.72026	73.58039	73.90806	-513.07015	236.18570	-551.87280	1
150	H	76.67566	74.68893	74.01823	1816.11944	-1183.11722	-1650.94321	1
151	H	76.77617	73.17605	74.94535	-1800.04429	-1361.53473	1526.34643	1
152	C	77.96231	73.16729	73.08407	726.08972	-253.19732	-179.64713	1
153	H	78.11916	72.07299	73.00190	1224.27271	-456.51798	-2390.90304	1
154	H	78.03004	73.63822	72.08224	1206.40339	-1150.93514	-2154.90344	1
155	N	79.21945	73.69378	73.85298	329.70796	-633.68968	-155.67358	1
156	H	80.15223	73.46829	73.40143	1348.31305	1938.76845	1359.00643	1
157	H	79.30164	74.74394	73.98398	2096.92035	1446.54551	-966.48890	1
158	H	79.37171	73.33299	74.83991	-1197.07217	-2303.53719	827.28733	1
159	C	73.62785	70.92650	74.33803	-378.01186	-556.17301	-413.96481	1
160	O	74.28813	70.75602	75.36643	-409.44433	-307.55053	-453.30833	1
161	N	73.22270	70.08964	73.42334	-429.02477	524.70884	274.08502	1
162	H	72.67242	70.50791	72.67339	1706.34263	-1425.96036	1574.38926	1
163	C	73.35279	68.67491	73.45650	-45.25864	-626.22952	478.93267	1
164	H	72.50642	68.36269	72.80513	1988.63164	570.90773	1772.87287	1
165	C	74.73555	68.31055	72.77727	551.77128	-20.49526	-564.54996	1
166	H	74.83620	68.81915	71.79263	1434.61535	-1753.10253	1513.99471	1
167	H	75.59235	68.67794	73.38274	-714.67738	1819.09770	1898.36494	1
168	C	74.77070	66.75447	72.60963	446.99263	-555.77305	338.97221	1
169	H	74.68324	66.24737	73.59804	1953.68466	1892.25957	-161.67766	1

170	H	73.90053	66.39990	72.01348	-403.03785	2688.07032	-188.43591	1
171	C	76.12783	66.37041	71.89474	567.86262	335.74681	434.04421	1
172	H	76.16656	66.79178	70.86394	-1080.02275	1568.26081	-1948.78900	1
173	H	76.99616	66.81185	72.43229	-919.54108	2111.34692	1456.13463	1
174	C	76.23059	64.82763	71.86437	195.81897	173.33862	-745.11536	1
175	H	76.31883	64.35147	72.86114	1405.67949	-2301.21089	-390.08113	1
176	H	75.43947	64.32385	71.27394	-940.37328	-1118.32446	2299.72133	1
177	N	77.56439	64.45605	71.13191	319.26422	656.36007	-42.02424	1
178	H	77.76578	63.41785	71.04904	1961.03633	619.91968	1787.09422	1
179	H	77.66334	64.76642	70.12159	854.14343	-2156.80752	1429.08711	1
180	H	78.46921	64.80900	71.56032	1237.02905	-1378.50857	-1998.28500	1
181	C	73.16211	68.15289	75.00195	532.53319	-268.57236	517.55729	1
182	O	72.07977	68.21150	75.53703	266.16714	-290.73804	-558.88002	1
183	N	74.30857	67.69709	75.48591	-226.25352	640.49678	-270.32839	1
184	H	75.15462	67.74431	74.92136	2007.69063	-1035.27229	1523.50231	1
185	C	74.32818	67.10910	76.77934	-540.76542	-573.33303	49.50000	1
186	H	73.27143	67.20225	77.12866	-2374.20950	-1036.76023	843.75774	1
187	C	74.80328	65.58162	76.59901	-77.09082	666.87422	-415.84136	1
188	H	75.91300	65.56845	76.41877	-985.81834	617.19825	2463.91927	1
189	O	74.21139	64.86396	75.50620	293.29899	-391.65602	-477.80926	1
190	H	75.01003	64.58198	75.01345	2528.72714	-681.76262	-751.27122	1
191	C	74.50473	64.99530	78.02609	252.47363	-605.14473	440.05134	1
192	H	74.79495	63.92089	78.09259	-2052.65063	1456.49051	-1043.51830	1
193	H	75.07051	65.54472	78.82472	-2152.98800	-1661.97574	-161.70652	1
194	H	73.41966	65.05934	78.27586	-473.12726	-1584.27339	2165.61725	1
195	C	75.40680	67.94361	77.66441	360.36307	488.46713	505.10056	1
196	O	75.95744	67.39519	78.59826	-200.08817	-528.03552	-385.82850	1
197	N	75.49659	69.22005	77.30362	-597.54095	-226.44775	355.20479	1
198	H	74.97735	69.60935	76.47579	2179.23655	-1300.70981	-991.33835	1
199	C	76.51506	69.95627	77.96721	-687.68921	297.39807	-249.45179	1
200	H	76.97342	69.24027	78.69543	-349.16256	-2467.37713	-1101.72831	1
201	C	77.54631	70.50229	76.85980	672.47345	361.54328	-201.62880	1
202	H	77.00755	71.01823	76.03264	1541.41502	582.18425	2169.97026	1
203	H	78.23902	71.24288	77.32115	-2534.67717	60.25153	997.72295	1
204	C	78.31445	69.27822	76.35020	574.26774	-389.43119	-377.02542	1
205	C	79.28652	68.66394	77.19769	688.82679	-287.33580	-257.96133	1
206	H	79.51881	69.08810	78.19154	331.14182	1470.38163	2269.80013	1
207	C	78.00974	68.72241	75.07105	-383.52382	-675.04808	144.24917	1
208	H	77.25732	69.19851	74.41787	4.09847	1517.59662	2262.86397	1
209	C	79.92159	67.50610	76.75255	-134.76730	428.45285	-649.50303	1
210	H	80.66740	67.02569	77.41009	-903.23433	1600.49020	2011.53387	1
211	C	78.67700	67.56294	74.67032	-335.53281	-615.00040	-364.39058	1
212	H	78.44135	67.13791	73.68041	1596.45398	-1369.33862	1732.02659	1
213	C	79.64652	66.91112	75.48671	585.48547	-340.24194	-406.23938	1
214	O	80.32094	65.72908	75.08521	-419.15649	-173.04408	-511.94141	1
215	H	79.91608	65.60172	74.19446	-1071.84350	1559.71507	-1960.13012	1
216	C	75.89225	71.28227	78.68442	291.41878	-183.13091	710.72246	1
217	O	76.38600	71.66885	79.72047	379.87695	523.47396	-222.23622	1
218	N	74.93235	71.86498	77.97166	564.30591	373.09380	277.24371	1
219	H	74.59785	71.47694	77.06944	-120.59931	-2436.07824	-1214.35098	1
220	C	74.29685	72.96623	78.62720	404.07514	-299.37480	608.84009	1
221	H	74.83960	73.12175	79.59370	-1071.07882	-841.69025	2359.66467	1
222	C	74.41799	74.17061	77.59954	-683.12807	68.71770	-390.13096	1
223	H	75.45816	74.24432	77.20876	2068.88918	1596.58590	770.89603	1
224	H	73.77405	73.95649	76.71277	1379.86429	2342.49779	-179.85638	1
225	C	73.98656	75.50930	78.26797	-176.39967	537.49466	550.97268	1
226	H	72.96939	75.43072	78.71161	-396.28051	1942.22168	1869.33314	1
227	H	74.66402	75.79128	79.10417	-94.44700	586.00678	-2659.20016	1
228	C	74.03286	76.58605	77.08137	-291.69381	-718.18079	-150.72929	1
229	H	75.04622	76.77045	76.63463	-2303.38776	1089.76242	964.62032	1
230	H	73.29444	76.33585	76.25789	884.16729	2568.80533	-207.74283	1
231	N	73.58801	77.75546	77.69812	-594.49522	-252.81478	342.29276	1

232	H	72.83529	77.64045	78.36085	-1735.17426	2084.05705	-263.71605	1
233	C	74.01365	78.93281	77.46521	595.23177	-271.52487	442.22352	1
234	N	75.03809	79.12443	76.53356	585.53813	-424.79750	-105.81303	1
235	H	75.49041	78.45267	75.91685	959.88797	1327.56823	-2177.11905	1
236	H	75.41033	80.03263	76.25373	1578.48647	16.27378	-2220.76233	1
237	N	73.31987	79.86289	78.24938	-452.17763	-390.33541	-421.51853	1
238	H	72.56955	79.74117	78.92791	470.26107	1974.25629	-1817.92087	1
239	H	73.50105	80.86664	78.21020	1856.67307	-1573.97321	-1224.35416	1
240	C	72.71367	72.58733	78.77642	-531.47271	-581.45780	-55.06206	1
241	O	72.06955	72.18305	77.80914	-243.00837	192.73507	609.52485	1
242	N	72.29173	72.85902	79.98879	343.49288	-644.25607	38.09164	1
243	H	73.02704	73.19638	80.61100	-1691.16043	-1535.97525	-1484.73099	1
244	C	71.02373	72.41751	80.54307	542.66492	350.14337	454.42563	1
245	H	70.98265	72.90171	81.54801	1209.57979	-2396.95920	463.86744	1
246	C	69.88595	72.82841	79.61819	-737.14309	145.93010	242.71942	1
247	H	70.14407	72.45743	78.59598	-1050.18303	159.36419	-2509.06125	1
248	C	68.57194	72.19693	80.03531	-706.77696	-252.88343	-245.16230	1
249	H	67.73477	72.46930	79.33521	-1624.64039	-1665.49085	1417.86935	1
250	H	68.63993	71.07080	80.04921	2566.10521	598.51109	693.22305	1
251	H	68.26366	72.52257	81.06736	-1972.69758	107.10018	-1876.34312	1
252	C	69.73917	74.33589	79.53503	412.85148	672.58832	-27.69222	1
253	H	68.97229	74.63953	78.76960	1447.02277	1762.76533	-1490.78944	1
254	H	69.41994	74.77533	80.52007	1320.77379	-145.20455	2378.68491	1
255	H	70.71000	74.82726	79.24976	-1512.10848	1470.52031	1724.75147	1
256	C	71.04104	70.74923	80.67798	-607.11113	499.56689	73.73769	1
257	O	70.79403	70.27401	81.75406	357.97126	460.81534	356.68785	1
258	N	71.34482	70.17146	79.53685	536.55407	-368.62270	332.76306	1
259	H	71.50709	70.76779	78.69738	524.38866	2297.69985	1367.20941	1
260	C	71.23183	68.76800	79.34721	46.50277	-774.29190	-147.97904	1
261	H	71.91664	68.58614	78.48891	1676.51875	1883.29066	1032.55549	1
262	C	71.64522	67.95373	80.67654	-559.41456	-34.19198	-556.30433	1
263	H	70.84040	68.08628	81.44335	-64.66664	395.18769	2695.05373	1
264	H	71.69432	66.85735	80.47173	-2703.44278	-60.40056	333.79418	1
265	C	72.95464	68.45560	81.22235	-519.76435	377.31045	459.42366	1
266	H	72.91026	69.56947	81.25683	-1746.74323	1667.50644	-1261.73691	1
267	C	73.17482	67.94679	82.64153	570.95554	16.46261	-545.27700	1
268	H	74.14568	68.31266	83.06548	2391.58273	28.05277	-1305.07271	1
269	H	72.36078	68.29151	83.33084	175.75588	917.63458	2559.43867	1
270	H	73.19560	66.82732	82.68242	-1063.97851	-2155.34650	1283.00462	1
271	C	74.13216	68.04088	80.34834	193.76014	2.62946	-765.53141	1
272	H	75.10945	68.40420	80.76245	507.39394	-846.55087	2539.60089	1
273	H	74.21205	66.92629	80.25593	1337.57841	1818.19054	1526.01994	1
274	H	74.05476	68.45068	79.30430	1100.88635	-1172.91350	-2199.08909	1
275	C	69.70718	68.49469	78.92506	-549.21115	475.64486	-309.38218	1
276	O	68.95015	69.36025	78.56378	556.06106	-390.37755	-78.24250	1
277	O	69.29789	67.13848	78.90698	-572.27940	-310.19032	-209.75862	1
278	H	70.17100	66.71169	79.12145	-1380.08193	2212.14486	790.85944	1

Listing 53: C00053.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	1.4410	5764
		0.2500	300.00	0.00	0.00	0.00	-1293.6730	0.0000	300.0000
3	H	80.89357	79.22160	85.63356	-2043.14101	-1757.64893	399.89339		1
4	N	81.43146	79.31452	84.77479	426.75047	490.45733	-334.42467		1
5	H	80.71450	79.60539	84.11376	442.25559	-1110.30854	-2448.52907		1
6	C	82.53701	80.19070	84.86681	415.32972	-666.39213	83.73172		1
7	H	82.93187	80.03662	85.89339	879.32219	2491.00447	667.35213		1
8	C	83.58697	79.77982	83.71308	31.35357	477.41777	628.23362		1
9	H	83.07093	79.73479	82.72427	1168.38489	2240.25337	-1019.71136		1
10	H	84.38357	80.55599	83.61411	-360.43770	2534.90498	931.67112		1
11	C	84.18105	78.43766	84.05211	463.18208	512.70242	-382.34388		1

12	H	83.35283	77.75753	84.35494	1725.29117	1863.52247	-987.07854	1
13	C	84.87359	77.84177	82.83267	710.42801	-144.27427	-313.15367	1
14	H	85.31309	76.83556	83.05647	364.20195	-1033.13725	2494.72524	1
15	H	84.16330	77.71110	81.97569	2567.61904	335.80679	847.48802	1
16	H	85.70960	78.49585	82.47355	-2587.99029	680.92867	-512.16411	1
17	C	85.17651	78.54373	85.19929	268.17616	741.64379	-40.42634	1
18	H	85.63507	77.55024	85.44142	1283.54314	-1945.37420	-1411.27812	1
19	H	86.01575	79.24412	84.95213	-1258.57796	1317.15249	-2026.02085	1
20	H	84.69451	78.92306	86.13669	-2502.84526	909.80597	575.92391	1
21	C	81.97767	81.69878	84.64661	619.36578	-458.64843	-172.09273	1
22	O	81.89481	82.47794	85.59268	-81.40433	433.87611	522.34594	1
23	N	81.65100	81.89942	83.39484	175.23996	-622.20190	341.55523	1
24	H	81.76290	81.19518	82.64732	-876.57256	-303.22879	-2561.90213	1
25	C	80.96381	83.10073	83.01343	-571.88214	-534.10783	-106.15033	1
26	H	80.23308	83.36010	83.81364	-2713.20841	-16.25800	-248.80809	1
27	C	82.11209	84.20371	82.87169	166.60354	288.16399	-716.09568	1
28	H	82.92610	83.80399	82.19942	-2097.85574	1636.78449	-586.18044	1
29	O	82.86880	84.49931	84.06470	-317.80580	-363.38227	484.43082	1
30	H	82.49434	83.80251	84.69441	1863.74748	-1451.84923	1357.29467	1
31	C	81.42370	85.42062	82.16916	503.80731	517.99032	318.51606	1
32	H	82.17472	86.19025	81.86313	640.61020	-2157.10410	-1536.29104	1
33	H	80.86443	85.11278	81.24991	1687.88455	465.60692	2087.56452	1
34	H	80.70083	85.92879	82.85005	-1293.07895	-1899.88581	-1463.57452	1
35	C	80.34160	82.59985	81.60670	-153.07550	-733.68902	248.70981	1
36	O	80.94238	81.70444	81.03489	186.15459	-480.78787	-449.34387	1
37	N	79.23811	83.24285	81.24262	-487.53139	543.18517	42.03850	1
38	C	78.53538	82.92160	80.02516	-699.35871	69.34393	360.10701	1
39	H	78.55330	81.80868	79.96935	2.81126	-221.99807	-2715.58072	1
40	C	77.10249	83.56628	80.23699	-507.46439	-592.59194	122.07761	1
41	H	76.63977	83.88262	79.27326	-1975.08116	525.87560	-1801.71556	1
42	H	76.39553	82.84825	80.70963	1588.27743	-1913.22100	1113.83566	1
43	C	77.41682	84.76281	81.18895	-613.62442	-457.55993	-194.14490	1
44	H	77.85911	85.61660	80.62871	1707.54637	-721.27992	1996.92523	1
45	H	76.52366	85.15734	81.72366	758.23357	2100.81767	1560.55011	1
46	C	78.48283	84.09091	82.15758	-352.41524	704.96076	49.21465	1
47	H	79.17455	84.79785	82.66728	1714.76886	-2070.42778	443.35792	1
48	H	78.04467	83.40085	82.91720	1224.15040	1801.50881	1636.97633	1
49	C	79.21360	83.59922	78.71565	566.85117	537.05831	117.62814	1
50	O	78.49166	83.97750	77.79413	-550.26779	-406.08867	4.21666	1
51	N	80.52566	83.58913	78.77830	566.34832	-425.77725	180.18749	1
52	H	80.95655	83.17709	79.61266	644.44502	2646.80550	-52.73430	1
53	C	81.25301	84.39215	77.84348	612.34801	-281.48662	411.56221	1
54	H	80.55482	85.24401	77.68042	1667.23498	-1490.75142	1556.16753	1
55	C	82.65677	84.77932	78.48076	-714.45746	-175.43074	286.98927	1
56	H	83.28674	83.85223	78.56436	-787.09484	1763.03619	-1922.46060	1
57	O	82.61278	85.34640	79.81127	-429.46514	516.51932	-128.40526	1
58	H	83.21666	84.74297	80.28631	1981.82785	436.16847	-1818.18182	1
59	C	83.26287	85.71710	77.37264	630.79189	-468.94448	76.03230	1
60	H	84.29916	86.03481	77.63320	-1775.71861	2062.30353	131.89849	1
61	H	83.31296	85.21025	76.37901	-1855.14608	88.94118	1993.53760	1
62	H	82.65659	86.64354	77.24426	-1504.82350	-780.94249	-2132.90992	1
63	C	81.44621	83.50561	76.47655	288.57638	618.62814	-397.00270	1
64	O	82.52440	83.09164	76.13015	321.70495	-185.26452	574.37218	1
65	N	80.26666	83.39787	75.87550	-447.05792	-446.53431	367.76425	1
66	H	79.40996	83.78810	76.34022	350.31316	1975.63644	-1843.31522	1
67	C	80.18879	82.48781	74.77511	-511.23061	374.03917	-471.51480	1
68	H	80.99454	82.82318	74.08654	2234.79579	-898.70890	-1273.45190	1
69	C	80.50857	81.02519	75.34498	529.53781	-159.34528	563.72604	1
70	H	80.58878	80.34462	74.45391	654.59388	2347.94251	1217.51488	1
71	H	81.52848	81.06996	75.81558	-1526.55661	2103.42026	817.87394	1
72	O	79.54427	80.45249	76.26457	-554.84278	14.12789	399.58769	1
73	H	79.83986	80.88045	77.09134	1297.06236	2061.84854	1220.68812	1

74	C	78.69666	82.53218	74.13163	-662.15484	-412.13544	123.62687	1
75	O	78.59694	82.41567	72.93083	-540.01537	-317.05804	274.91456	1
76	N	77.72949	82.56029	75.04868	-202.76299	-690.00100	-131.49145	1
77	H	78.08047	82.61009	76.00921	-702.62132	-2617.37191	281.70413	1
78	C	76.33442	82.91240	74.79567	-491.73914	576.34187	222.73509	1
79	H	76.18789	83.82969	75.41287	1977.17978	-1823.58850	-434.68928	1
80	C	76.01719	83.11293	73.33238	-649.50797	-328.66843	306.11224	1
81	H	76.52111	82.30532	72.74291	2075.07803	1452.16490	-1004.45904	1
82	C	74.52340	83.02239	73.07213	-615.18735	-489.99689	-70.96352	1
83	H	74.28156	83.15156	71.98188	-1226.32661	-1724.38906	-1716.47170	1
84	H	74.10419	82.02597	73.39195	2381.64273	-969.84735	900.46860	1
85	H	73.95690	83.81312	73.63594	2122.74991	1702.23946	-141.36228	1
86	C	76.54287	84.44437	72.82386	-501.86074	-479.61276	-376.42482	1
87	H	76.30288	84.59953	71.73654	993.79261	-2246.95401	-1177.81305	1
88	H	76.10422	85.31068	73.39084	42.71279	-626.15391	-2651.37258	1
89	H	77.66288	84.50237	72.93031	-2026.39012	-1590.33709	-887.82922	1
90	C	75.44100	81.65359	75.45045	-672.89153	382.57394	-156.34072	1
91	O	74.70617	81.92147	76.37620	410.04627	221.86223	500.35950	1
92	N	75.64419	80.51222	74.82705	-378.11782	-443.79414	-441.10984	1
93	H	76.38140	80.58765	74.12928	2404.15973	-568.14894	1149.30085	1
94	C	75.00029	79.27729	75.13198	-544.54484	466.16019	331.29119	1
95	H	75.79809	78.51558	75.00119	-1409.80988	-170.17955	2325.32679	1
96	C	74.45545	79.40909	76.60749	-184.48284	116.78282	-758.89137	1
97	H	75.24834	79.87525	77.23940	1893.78641	1861.14652	611.04528	1
98	H	73.59706	80.12889	76.61546	-2170.79665	-974.19311	1327.50117	1
99	C	74.00003	78.05249	77.24089	389.51668	672.81878	-138.49152	1
100	H	73.17411	77.59638	76.64799	510.64577	1933.03327	1851.02484	1
101	H	74.81350	77.29423	77.19265	-2302.30869	-1105.72939	-948.89774	1
102	C	73.55575	78.27327	78.72399	-559.93427	-126.34590	542.30857	1
103	O	73.23237	77.31666	79.40775	-670.36003	-111.83166	76.36448	1
104	N	73.61433	79.55345	79.11750	-216.06729	-537.07037	446.51379	1
105	H	73.87470	80.40404	78.60156	-1251.96487	1074.12894	-2168.52500	1
106	H	73.36439	79.86713	80.06283	-2451.83023	-720.73851	944.84612	1
107	C	73.74165	79.05842	74.10827	546.24052	-563.88337	-85.11809	1
108	O	72.90389	79.91476	73.98898	71.70702	-307.40463	606.69673	1
109	N	73.79508	77.84954	73.52274	479.90863	-504.50129	222.86849	1
110	C	72.74651	77.39778	72.66200	75.51268	-600.91904	506.73700	1
111	H	72.20102	78.30607	72.31240	-2033.61562	1795.30103	254.89480	1
112	C	73.58269	76.61175	71.55255	523.79067	517.99274	284.45581	1
113	H	72.96041	75.91021	70.95375	1599.61665	-1127.00911	1895.98173	1
114	H	74.06427	77.30957	70.83228	-1881.83093	1275.82488	-1501.55016	1
115	C	74.63899	75.89113	72.44185	-600.05639	-404.05026	316.64485	1
116	H	74.19276	75.00834	72.95193	-2597.05260	496.36221	657.73249	1
117	H	75.52040	75.51958	71.87232	-1666.24518	1294.38985	-1723.90591	1
118	C	75.00256	77.03637	73.48374	493.57570	-129.95376	-602.56394	1
119	H	75.20700	76.67341	74.51872	-1469.08415	-637.84797	2204.22581	1
120	H	75.82318	77.71927	73.15852	-1038.97840	1068.88701	-2280.71789	1
121	C	71.79026	76.31500	73.41175	188.88100	241.05089	-727.87821	1
122	O	72.04391	75.85130	74.50905	531.88613	-49.19943	427.07960	1
123	N	70.79173	75.91112	72.57596	708.14833	26.93417	-179.73509	1
124	H	70.88837	76.59739	71.81498	-2232.69501	-1179.09831	1023.94816	1
125	C	69.45704	75.61954	73.15297	-738.32412	259.92548	104.42456	1
126	H	69.28067	76.43266	73.89290	2028.89123	1260.02983	1311.33324	1
127	C	68.45812	75.59557	72.02615	-258.65678	-345.52513	661.28459	1
128	H	68.87407	74.94768	71.22096	-1826.06090	-1801.46097	-918.64554	1
129	C	67.12806	75.00426	72.46409	-541.23400	531.92970	-218.41428	1
130	H	66.41513	74.89402	71.60183	1311.73218	-2219.18200	882.19023	1
131	H	67.25891	73.98485	72.92541	-1048.71298	1223.58118	-2196.97971	1
132	H	66.62446	75.64884	73.23519	419.06414	1903.92898	1903.44670	1
133	C	68.21557	76.97346	71.43258	-423.86431	152.66566	-648.55262	1
134	H	67.47901	76.93497	70.58397	105.68386	-2342.50080	1387.51238	1
135	H	67.80165	77.68469	72.19870	-1695.63603	-1484.73621	-1531.02793	1

136	H	69.16073	77.43087	71.03258	-1853.57121	-487.39031	1936.59343	1
137	C	69.49158	74.12850	73.86142	539.71428	-510.58232	267.58633	1
138	O	68.67276	73.87117	74.71836	-15.93758	-278.34085	-624.49402	1
139	N	70.34787	73.30837	73.26839	-676.81886	12.05292	276.17960	1
140	H	70.92567	73.78554	72.57758	-1694.44250	-373.84189	-2100.66098	1
141	C	70.72628	72.06419	73.84632	412.33078	-664.70360	108.35451	1
142	H	71.78598	71.93408	73.52409	1765.77476	1294.44366	1621.76594	1
143	C	70.52759	72.14277	75.41588	-179.66635	-721.95667	-264.73915	1
144	H	70.98142	73.07336	75.82414	-607.34922	2587.87032	-598.10018	1
145	H	69.43996	72.20214	75.68229	-359.69332	-1479.13954	-2259.74260	1
146	C	71.17888	70.86493	76.04390	-240.01076	616.02425	431.85322	1
147	H	70.56957	69.95819	75.82232	-1359.17131	782.54425	2227.99181	1
148	H	72.18291	70.66748	75.60345	-820.36667	85.81767	-2596.78715	1
149	C	71.28601	71.11225	77.60111	-513.07015	236.18570	-551.87280	1
150	H	71.89153	72.02232	77.82323	1816.11944	-1183.11722	-1650.94321	1
151	H	70.28170	71.30133	78.04534	-1800.04429	-1361.53473	1526.34643	1
152	C	71.93484	69.84520	78.20698	726.08972	-253.19732	-179.64713	1
153	H	71.34393	68.91682	78.07407	1224.27271	-456.51798	-2390.90304	1
154	H	72.98507	69.67180	77.89803	1206.40339	-1150.93514	-2154.90344	1
155	N	71.99769	70.05584	79.75543	329.70796	-633.68968	-155.67358	1
156	H	72.41712	69.25968	80.31746	1348.31305	1938.76845	1359.00643	1
157	H	72.55943	70.88456	80.10851	2096.92035	1446.54551	-966.48890	1
158	H	71.06935	70.19463	80.24944	-1197.07217	-2303.53719	827.28733	1
159	C	69.78558	70.82878	73.33847	-378.01186	-556.17301	-413.96481	1
160	O	70.09271	69.68899	73.61480	-409.44433	-307.55053	-453.30833	1
161	N	68.66466	71.24551	72.74409	-429.02477	524.70884	274.08502	1
162	H	68.61317	72.24287	72.54079	1706.34263	-1425.96036	1574.38926	1
163	C	67.93763	70.24073	72.03165	-45.25864	-626.22952	478.93267	1
164	H	68.07046	69.31236	72.63454	1988.63164	570.90773	1772.87287	1
165	C	66.44646	70.74748	71.93177	551.77128	-20.49526	-564.54996	1
166	H	66.10143	71.12276	72.92182	1434.61535	-1753.10253	1513.99471	1
167	H	66.35998	71.61311	71.23725	-714.67738	1819.09770	1898.36494	1
168	C	65.56070	69.54703	71.45558	446.99263	-555.77305	338.97221	1
169	H	65.80260	69.27080	70.40456	1953.68466	1892.25957	-161.67766	1
170	H	65.76644	68.63946	72.06602	-403.03785	2688.07032	-188.43591	1
171	C	64.04421	69.97239	71.60033	567.86262	335.74681	434.04421	1
172	H	63.81212	70.25243	72.65370	-1080.02275	1568.26081	-1948.78900	1
173	H	63.82779	70.88012	70.99179	-919.54108	2111.34692	1456.13463	1
174	C	63.16116	68.78636	71.14809	195.81897	173.33862	-745.11536	1
175	H	63.24395	68.53338	70.07232	1405.67949	-2301.21089	-390.08113	1
176	H	63.26825	67.86960	71.76167	-940.37328	-1118.32446	2299.72133	1
177	N	61.66474	69.20972	71.33914	319.26422	656.36007	-42.02424	1
178	H	60.94451	68.48580	71.05200	1961.03633	619.91968	1787.09422	1
179	H	61.34714	69.43710	72.32619	854.14343	-2156.80752	1429.08711	1
180	H	61.33027	70.05991	70.79900	1237.02905	-1378.50857	-1998.28500	1
181	C	68.64344	70.12059	70.54590	532.53319	-268.57236	517.55729	1
182	O	68.98395	71.08361	69.89725	266.16714	-290.73804	-558.88002	1
183	N	68.64258	68.83854	70.22812	-226.25352	640.49678	-270.32839	1
184	H	68.27518	68.20240	70.93410	2007.69063	-1035.27229	1523.50231	1
185	C	69.26826	68.29904	69.07410	-540.76542	-573.33303	49.50000	1
186	H	68.75955	67.31741	68.95195	-2374.20950	-1036.76023	843.75774	1
187	C	69.05693	69.28653	67.83962	-77.09082	666.87422	-415.84136	1
188	H	69.62924	70.23988	68.03947	-985.81834	617.19825	2463.91927	1
189	O	67.68887	69.69156	67.60222	293.29899	-391.65602	-477.80926	1
190	H	67.68126	70.54019	68.09860	2528.72714	-681.76262	-751.27122	1
191	C	69.76324	68.49201	66.68184	252.47363	-605.14473	440.05134	1
192	H	69.83279	69.10138	65.75075	-2052.65063	1456.49051	-1043.51830	1
193	H	70.79967	68.18883	66.96234	-2152.98800	-1661.97574	-161.70652	1
194	H	69.20631	67.56079	66.42654	-473.12726	-1584.27339	2165.61725	1
195	C	70.86759	68.07215	69.38792	360.36307	488.46713	505.10056	1
196	O	71.29541	66.95452	69.21746	-200.08817	-528.03552	-385.82850	1
197	N	71.53324	69.16751	69.73439	-597.54095	-226.44775	355.20479	1

198	H	71.02549	70.05012	69.82867	2179.23655	-1300.70981	-991.33835	1
199	C	72.91983	69.00951	69.99652	-687.68921	297.39807	-249.45179	1
200	H	73.07792	67.93578	70.26075	-349.16256	-2467.37713	-1101.72831	1
201	C	73.73855	69.47375	68.68917	672.47345	361.54328	-201.62880	1
202	H	73.45800	70.51678	68.42046	1541.41502	582.18425	2169.97026	1
203	H	74.82380	69.48889	68.94074	-2534.67717	60.25153	997.72295	1
204	C	73.49751	68.54021	67.49993	574.26774	-389.43119	-377.02542	1
205	C	73.92799	67.17965	67.56346	688.82679	-287.33580	-257.96133	1
206	H	74.42374	66.78552	68.46937	331.14182	1470.38163	2269.80013	1
207	C	72.85404	69.04210	66.32712	-383.52382	-675.04808	144.24917	1
208	H	72.52270	70.09469	66.27316	4.09847	1517.59662	2262.86397	1
209	C	73.69013	66.35439	66.46610	-134.76730	428.45285	-649.50303	1
210	H	74.01273	65.29971	66.51971	-903.23433	1600.49020	2011.53387	1
211	C	72.64026	68.17488	65.25414	-335.53281	-615.00040	-364.39058	1
212	H	72.13505	68.57094	64.35596	1596.45398	-1369.33862	1732.02659	1
213	C	73.04239	66.80719	65.27977	585.48547	-340.24194	-406.23938	1
214	O	72.82580	65.91840	64.19549	-419.15649	-173.04408	-511.94141	1
215	H	72.37131	66.52936	63.56805	-1071.84350	1559.71507	-1960.13012	1
216	C	73.46359	70.11692	71.04880	291.41878	-183.13091	710.72246	1
217	O	73.15715	71.28226	70.97937	379.87695	523.47396	-222.23622	1
218	N	74.42862	69.56577	71.81188	564.30591	373.09380	277.24371	1
219	H	74.52929	68.53395	71.91178	-120.59931	-2436.07824	-1214.35098	1
220	C	75.15161	70.53711	72.58896	404.07514	-299.37480	608.84009	1
221	H	75.26846	71.37205	71.85994	-1071.07882	-841.69025	2359.66467	1
222	C	74.18222	70.99173	73.75271	-683.12807	68.71770	-390.13096	1
223	H	73.15482	71.14289	73.33790	2068.88918	1596.58590	770.89603	1
224	H	74.08690	70.19503	74.52487	1379.86429	2342.49779	-179.85638	1
225	C	74.74387	72.31013	74.37707	-176.39967	537.49466	550.97268	1
226	H	75.71376	72.12131	74.89783	-396.28051	1942.22168	1869.33314	1
227	H	74.96465	73.06443	73.58957	-94.44700	586.00678	-2659.20016	1
228	C	73.63250	72.84633	75.37913	-291.69381	-718.18079	-150.72929	1
229	H	72.84208	73.48715	74.91958	-2303.38776	1089.76242	964.62032	1
230	H	73.13351	72.02707	75.94996	884.16729	2568.80533	-207.74283	1
231	N	74.26770	73.60644	76.42940	-594.49522	-252.81478	342.29276	1
232	H	75.23138	73.50979	76.72745	-1735.17426	2084.05705	-263.71605	1
233	C	73.61806	74.41407	77.21464	595.23177	-271.52487	442.22352	1
234	N	72.20524	74.65484	76.97257	585.53813	-424.79750	-105.81303	1
235	H	71.93644	74.93071	76.00170	959.88797	1327.56823	-2177.11905	1
236	H	71.90391	75.41783	77.58051	1578.48647	16.27378	-2220.76233	1
237	N	74.22656	75.05835	78.29287	-452.17763	-390.33541	-421.51853	1
238	H	75.21310	74.98927	78.56538	470.26107	1974.25629	-1817.92087	1
239	H	73.71946	75.74493	78.91111	1856.67307	-1573.97321	-1224.35416	1
240	C	76.55438	69.98445	73.21951	-531.47271	-581.45780	-55.06206	1
241	O	77.09241	70.66371	74.07164	-243.00837	192.73507	609.52485	1
242	N	76.95996	68.85245	72.68293	343.49288	-644.25607	38.09164	1
243	H	76.37695	68.48487	71.93413	-1691.16043	-1535.97525	-1484.73099	1
244	C	78.12224	68.12339	73.10018	542.66492	350.14337	454.42563	1
245	H	78.76982	68.11795	72.19629	1209.57979	-2396.95920	463.86744	1
246	C	78.84701	68.72993	74.37455	-737.14309	145.93010	242.71942	1
247	H	78.11452	69.13387	75.11453	-1050.18303	159.36419	-2509.06125	1
248	C	79.69211	67.57010	75.01192	-706.77696	-252.88343	-245.16230	1
249	H	80.38953	67.94555	75.79809	-1624.64039	-1665.49085	1417.86935	1
250	H	79.03451	66.80118	75.48642	2566.10521	598.51109	693.22305	1
251	H	80.29828	67.03644	74.24069	-1972.69758	107.10018	-1876.34312	1
252	C	79.83450	69.84916	73.89485	412.85148	672.58832	-27.69222	1
253	H	80.40688	70.28567	74.74662	1447.02277	1762.76533	-1490.78944	1
254	H	80.57579	69.45848	73.15888	1320.77379	-145.20455	2378.68491	1
255	H	79.27865	70.68515	73.40437	-1512.10848	1470.52031	1724.75147	1
256	C	77.68964	66.60656	73.47682	-607.11113	499.56689	73.73769	1
257	O	78.52964	65.73195	73.53060	357.97126	460.81534	356.68785	1
258	N	76.40732	66.53874	73.86659	536.55407	-368.62270	332.76306	1
259	H	75.86153	67.39281	73.72590	524.38866	2297.69985	1367.20941	1

260	C	75.75478	65.28632	73.60415	46.50277	-774.29190	-147.97904	1
261	H	76.55735	64.62204	73.20656	1676.51875	1883.29066	1032.55549	1
262	C	75.14977	64.74166	74.99868	-559.41456	-34.19198	-556.30433	1
263	H	74.28227	65.37433	75.30139	-64.66664	395.18769	2695.05373	1
264	H	74.74792	63.70731	74.88190	-2703.44278	-60.40056	333.79418	1
265	C	76.22925	64.79538	76.04583	-519.76435	377.31045	459.42366	1
266	H	76.65877	65.82353	76.04267	-1746.74323	1667.50644	-1261.73691	1
267	C	75.65870	64.52033	77.43130	570.95554	16.46261	-545.27700	1
268	H	76.44988	64.58037	78.22257	2391.58273	28.05277	-1305.07271	1
269	H	74.86090	65.25834	77.70354	175.75588	917.63458	2559.43867	1
270	H	75.20300	63.49918	77.49571	-1063.97851	-2155.34650	1283.00462	1
271	C	77.35380	63.81509	75.74323	193.76014	2.62946	-765.53141	1
272	H	78.10994	63.78527	76.56970	507.39394	-846.55087	2539.60089	1
273	H	76.97053	62.77091	75.60717	1337.57841	1818.19054	1526.01994	1
274	H	77.90383	64.10466	74.80318	1100.88635	-1172.91350	-2199.08909	1
275	C	74.60709	65.63443	72.55236	-549.21115	475.64486	-309.38218	1
276	O	74.40982	66.76778	72.14655	556.06106	-390.37755	-78.24250	1
277	O	73.82293	64.56446	72.09383	-572.27940	-310.19032	-209.75862	1
278	H	74.25177	63.82389	72.61939	-1380.08193	2212.14486	790.85944	1

Listing 54: C00054.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.9262	3705
		0.2500	300.00	0.00	0.00	0.00	-1293.6558	0.0000	300.0000
3	H	72.18135	64.80745	83.08062	-2043.14101	-1757.64893	399.89339		1
4	N	73.10615	64.54146	82.74919	426.75047	490.45733	-334.42467		1
5	H	72.90729	64.25040	81.79388	442.25559	-1110.30854	-2448.52907		1
6	C	74.09936	65.53669	82.86639	415.32972	-666.39213	83.73172		1
7	H	73.84715	66.04987	83.81830	879.32219	2491.00447	667.35213		1
8	C	75.54475	64.83151	82.86168	31.35357	477.41777	628.23362		1
9	H	75.65045	64.22251	81.93143	1168.38489	2240.25337	-1019.71136		1
10	H	76.35715	65.59740	82.82361	-360.43770	2534.90498	931.67112		1
11	C	75.67384	63.96171	84.08845	463.18208	512.70242	-382.34388		1
12	H	74.72476	63.39258	84.21200	1725.29117	1863.52247	-987.07854		1
13	C	76.81406	62.96655	83.91836	710.42801	-144.27427	-313.15367		1
14	H	76.92433	62.30589	84.81705	364.20195	-1033.13725	2494.72524		1
15	H	76.65173	62.29907	83.03263	2567.61904	335.80679	847.48802		1
16	H	77.79537	63.48651	83.76657	-2587.99029	680.92867	-512.16411		1
17	C	75.90952	64.80247	85.33529	268.17616	741.64379	-40.42634		1
18	H	76.00457	64.16476	86.25201	1283.54314	-1945.37420	-1411.27812		1
19	H	76.85069	65.40552	85.25286	-1258.57796	1317.15249	-2026.02085		1
20	H	75.07015	65.52185	85.51749	-2502.84526	909.80597	575.92391		1
21	C	73.98482	66.50533	81.55782	619.36578	-458.64843	-172.09273		1
22	O	74.83596	66.52393	80.69145	-81.40433	433.87611	522.34594		1
23	N	72.86497	67.21470	81.62577	175.23996	-622.20190	341.55523		1
24	H	72.26201	67.10963	82.44039	-876.57256	-303.22879	-2561.90213		1
25	C	72.55476	68.07906	80.53422	-571.88214	-534.10783	-106.15033		1
26	H	73.15294	67.68831	79.67596	-2713.20841	-16.25800	-248.80809		1
27	C	70.95996	68.06765	80.33235	166.60354	288.16399	-716.09568		1
28	H	70.48231	68.32741	81.31710	-2097.85574	1636.78449	-586.18044		1
29	O	70.37142	66.81969	79.94499	-317.80580	-363.38227	484.43082		1
30	H	69.80069	66.62877	80.71936	1863.74748	-1451.84923	1357.29467		1
31	C	70.81731	69.27251	79.33131	503.80731	517.99032	318.51606		1
32	H	69.75293	69.56681	79.18034	640.61020	-2157.10410	-1536.29104		1
33	H	71.37374	70.17308	79.70348	1687.88455	465.60692	2087.56452		1
34	H	71.23400	69.02145	78.32832	-1293.07895	-1899.88581	-1463.57452		1
35	C	72.94649	69.59448	80.97657	-153.07550	-733.68902	248.70981		1
36	O	72.26774	70.18881	81.80454	186.15459	-480.78787	-449.34387		1
37	N	73.98672	70.02301	80.26916	-487.53139	543.18517	42.03850		1
38	C	74.48390	71.36054	80.41235	-699.35871	69.34393	360.10701		1
39	H	74.44905	71.61109	81.49602	2.81126	-221.99807	-2715.58072		1

40	C	75.92561	71.24192	79.77154	-507.46439	-592.59194	122.07761	1
41	H	76.33619	72.22388	79.44401	-1975.08116	525.87560	-1801.71556	1
42	H	76.65964	70.81207	80.48988	1588.27743	-1913.22100	1113.83566	1
43	C	75.64913	70.26231	78.58708	-613.62442	-457.55993	-194.14490	1
44	H	75.13249	70.79347	77.75358	1707.54637	-721.27992	1996.92523	1
45	H	76.56800	69.80286	78.15742	758.23357	2100.81767	1560.55011	1
46	C	74.68170	69.21050	79.27445	-352.41524	704.96076	49.21465	1
47	H	73.91707	68.75749	78.59746	1714.76886	-2070.42778	443.35792	1
48	H	75.19377	68.39334	79.85217	1224.15040	1801.50881	1636.97633	1
49	C	73.50723	72.32463	79.50187	566.85117	537.05831	117.62814	1
50	O	73.36228	72.12472	78.32060	-550.26779	-406.08867	4.21666	1
51	N	73.05346	73.30493	80.26874	566.34832	-425.77725	180.18749	1
52	H	73.34482	73.30799	81.24631	644.44502	2646.80550	-52.73430	1
53	C	71.99766	74.16274	79.86765	612.34801	-281.48662	411.56221	1
54	H	71.94095	74.86948	80.72575	1667.23498	-1490.75142	1556.16753	1
55	C	72.37223	74.85905	78.48086	-714.45746	-175.43074	286.98927	1
56	H	72.35272	74.06737	77.67913	-787.09484	1763.03619	-1922.46060	1
57	O	73.66330	75.49043	78.41592	-429.46514	516.51932	-128.40526	1
58	H	74.09817	74.95812	77.71934	1981.82785	436.16847	-1818.18182	1
59	C	71.15068	75.83571	78.30952	630.79189	-468.94448	76.03230	1
60	H	71.14207	76.32365	77.29200	-1775.71861	2062.30353	131.89849	1
61	H	70.16940	75.30918	78.42039	-1855.14608	88.94118	1993.53760	1
62	H	71.17779	76.65700	79.06207	-1504.82350	-780.94249	-2132.90992	1
63	C	70.64253	73.24075	79.71123	288.57638	618.62814	-397.00270	1
64	O	70.10282	73.05586	78.64577	321.70495	-185.26452	574.37218	1
65	N	70.28791	72.79096	80.90591	-447.05792	-446.53431	367.76425	1
66	H	70.84838	73.03118	81.72227	350.31316	1975.63644	-1843.31522	1
67	C	69.05324	72.10827	81.04317	-511.23061	374.03917	-471.51480	1
68	H	68.75951	71.80692	80.01004	2234.79579	-898.70890	-1273.45190	1
69	C	69.37724	70.89292	82.03747	529.53781	-159.34528	563.72604	1
70	H	68.37775	70.48777	82.34910	654.59388	2347.94251	1217.51488	1
71	H	69.86742	70.09724	81.41453	-1526.55661	2103.42026	817.87394	1
72	O	70.20659	71.14317	83.17328	-554.84278	14.12789	399.58769	1
73	H	71.11276	70.82490	82.79725	1297.06236	2061.84854	1220.68812	1
74	C	67.98391	73.13774	81.72735	-662.15484	-412.13544	123.62687	1
75	O	68.20484	73.73516	82.77767	-540.01537	-317.05804	274.91456	1
76	N	66.91826	73.20444	80.96173	-202.76299	-690.00100	-131.49145	1
77	H	66.95828	72.61063	80.13395	-702.62132	-2617.37191	281.70413	1
78	C	65.69089	73.88467	81.32622	-491.73914	576.34187	222.73509	1
79	H	65.00464	73.61532	80.48728	1977.17978	-1823.58850	-434.68928	1
80	C	65.22991	73.35936	82.67773	-649.50797	-328.66843	306.11224	1
81	H	66.01635	73.62732	83.42231	2075.07803	1452.16490	-1004.45904	1
82	C	63.91913	73.98757	83.10976	-615.18735	-489.99689	-70.96352	1
83	H	63.57844	73.60202	84.10995	-1226.32661	-1724.38906	-1716.47170	1
84	H	64.01134	75.11189	83.19598	2381.64273	-969.84735	900.46860	1
85	H	63.09514	73.77577	82.37337	2122.74991	1702.23946	-141.36228	1
86	C	65.09966	71.84669	82.66817	-501.86074	-479.61276	-376.42482	1
87	H	64.79486	71.44482	83.67302	993.79261	-2246.95401	-1177.81305	1
88	H	64.33059	71.50328	81.92240	42.71279	-626.15391	-2651.37258	1
89	H	66.07314	71.35580	82.39200	-2026.39012	-1590.33709	-887.82922	1
90	C	65.98547	75.52835	81.39244	-672.89153	382.57394	-156.34072	1
91	O	65.54988	76.22876	82.27792	410.04627	221.86223	500.35950	1
92	N	66.60374	75.94661	80.26617	-378.11782	-443.79414	-441.10984	1
93	H	66.83571	75.07296	79.78553	2404.15973	-568.14894	1149.30085	1
94	C	67.63090	76.94694	80.45221	-544.54484	466.16019	331.29119	1
95	H	67.17087	77.76085	81.05188	-1409.80988	-170.17955	2325.32679	1
96	C	68.75341	76.16696	81.24494	-184.48284	116.78282	-758.89137	1
97	H	68.30736	75.76483	82.18835	1893.78641	1861.14652	611.04528	1
98	H	69.08571	75.27422	80.66639	-2170.79665	-974.19311	1327.50117	1
99	C	69.97129	77.07476	81.59740	389.51668	672.81878	-138.49152	1
100	H	70.41867	77.51210	80.67810	510.64577	1933.03327	1851.02484	1
101	H	69.63078	77.95736	82.18132	-2302.30869	-1105.72939	-948.89774	1

102	C	71.06945	76.29612	82.42078	-559.93427	-126.34590	542.30857	1
103	O	72.13845	76.82073	82.60400	-670.36003	-111.83166	76.36448	1
104	N	70.69466	75.08543	82.88553	-216.06729	-537.07037	446.51379	1
105	H	69.77399	74.58460	82.84357	-1251.96487	1074.12894	-2168.52500	1
106	H	71.30766	74.55805	83.52339	-2451.83023	-720.73851	944.84612	1
107	C	68.06201	77.36003	78.94588	546.24052	-563.88337	-85.11809	1
108	O	68.22929	76.48227	78.13842	71.70702	-307.40463	606.69673	1
109	N	68.24547	78.68190	78.80296	479.90863	-504.50129	222.86849	1
110	C	68.32157	79.28349	77.50725	75.51268	-600.91904	506.73700	1
111	H	67.66479	78.69290	76.82803	-2033.61562	1795.30103	254.89480	1
112	C	67.85606	80.77201	77.82086	523.79067	517.99274	284.45581	1
113	H	68.17447	81.49869	77.04015	1599.61665	-1127.00911	1895.98173	1
114	H	66.74950	80.85151	77.90285	-1881.83093	1275.82488	-1501.55016	1
115	C	68.54902	81.00015	79.19766	-600.05639	-404.05026	316.64485	1
116	H	69.64957	81.12337	79.07419	-2597.05260	496.36221	657.73249	1
117	H	68.17822	81.89376	79.74864	-1666.24518	1294.38985	-1723.90591	1
118	C	68.19875	79.62391	79.91287	493.57570	-129.95376	-602.56394	1
119	H	68.92375	79.29190	80.69162	-1469.08415	-637.84797	2204.22581	1
120	H	67.16269	79.57246	80.32417	-1038.97840	1068.88701	-2280.71789	1
121	C	69.86760	79.38479	76.97659	188.88100	241.05089	-727.87821	1
122	O	70.80688	79.45871	77.73415	531.88613	-49.19943	427.07960	1
123	N	69.85156	79.64521	75.64577	708.14833	26.93417	-179.73509	1
124	H	68.87658	79.49586	75.37425	-2232.69501	-1179.09831	1023.94816	1
125	C	70.92897	79.19775	74.74074	-738.32412	259.92548	104.42456	1
126	H	70.68694	79.68379	73.76700	2028.89123	1260.02983	1311.33324	1
127	C	72.25410	79.64637	75.31200	-258.65678	-345.52513	661.28459	1
128	H	72.32762	79.26086	76.36378	-1826.06090	-1801.46097	-918.64554	1
129	C	73.43241	79.10771	74.52224	-541.23400	531.92970	-218.41428	1
130	H	74.41181	79.46425	74.94411	1311.73218	-2219.18200	882.19023	1
131	H	73.46152	77.97377	74.52739	-1048.71298	1223.58118	-2196.97971	1
132	H	73.39585	79.43479	73.44678	419.06414	1903.92898	1903.44670	1
133	C	72.34366	81.16197	75.38027	-423.86431	152.66566	-648.55262	1
134	H	73.30742	81.50170	75.84869	105.68386	-2342.50080	1387.51238	1
135	H	72.28485	81.62873	74.35907	-1695.63603	-1484.73621	-1531.02793	1
136	H	71.50299	81.58907	75.99303	-1853.57121	-487.39031	1936.59343	1
137	C	70.83156	77.55907	74.63326	539.71428	-510.58232	267.58633	1
138	O	70.40045	76.87708	75.54275	-15.93758	-278.34085	-624.49402	1
139	N	71.29804	77.14053	73.46666	-676.81886	12.05292	276.17960	1
140	H	71.64966	77.84923	72.82645	-1694.44250	-373.84189	-2100.66098	1
141	C	71.70267	75.76880	73.39740	412.33078	-664.70360	108.35451	1
142	H	71.38469	75.35522	74.38583	1765.77476	1294.44366	1621.76594	1
143	C	70.91611	75.13124	72.18376	-179.66635	-721.95667	-264.73915	1
144	H	69.82428	75.31153	72.30379	-607.34922	2587.87032	-598.10018	1
145	H	71.18655	75.61852	71.22094	-359.69332	-1479.13954	-2259.74260	1
146	C	71.21856	73.59571	72.15507	-240.01076	616.02425	431.85322	1
147	H	72.29882	73.40044	71.97030	-1359.17131	782.54425	2227.99181	1
148	H	70.98458	73.12810	73.13770	-820.36667	85.81767	-2596.78715	1
149	C	70.32081	72.97472	71.01042	-513.07015	236.18570	-551.87280	1
150	H	69.24974	73.23929	71.16611	1816.11944	-1183.11722	-1650.94321	1
151	H	70.59611	73.40061	70.01834	-1800.04429	-1361.53473	1526.34643	1
152	C	70.50261	71.43942	71.01945	726.08972	-253.19732	-179.64713	1
153	H	71.51924	71.09174	70.74836	1224.27271	-456.51798	-2390.90304	1
154	H	70.16680	70.94008	71.95021	1206.40339	-1150.93514	-2154.90344	1
155	N	69.56926	70.85730	69.90381	329.70796	-633.68968	-155.67358	1
156	H	69.58582	69.80267	69.79115	1348.31305	1938.76845	1359.00643	1
157	H	68.52813	71.03852	70.00412	2096.92035	1446.54551	-966.48890	1
158	H	69.75135	71.17678	68.90808	-1197.07217	-2303.53719	827.28733	1
159	C	73.33360	75.80164	73.22325	-378.01186	-556.17301	-413.96481	1
160	O	74.02183	76.01719	74.19805	-409.44433	-307.55053	-453.30833	1
161	N	73.72601	75.61410	71.97583	-429.02477	524.70884	274.08502	1
162	H	73.06486	75.42964	71.22357	1706.34263	-1425.96036	1574.38926	1
163	C	75.10318	75.83914	71.66790	-45.25864	-626.22952	478.93267	1

164	H	75.46638	76.62334	72.37064	1988.63164	570.90773	1772.87287	1
165	C	75.82049	74.44864	71.92452	551.77128	-20.49526	-564.54996	1
166	H	75.70163	74.14903	72.99027	1434.61535	-1753.10253	1513.99471	1
167	H	75.34525	73.63772	71.32878	-714.67738	1819.09770	1898.36494	1
168	C	77.33022	74.61227	71.55357	446.99263	-555.77305	338.97221	1
169	H	77.45577	74.76484	70.45732	1953.68466	1892.25957	-161.67766	1
170	H	77.76497	75.51236	72.04469	-403.03785	2688.07032	-188.43591	1
171	C	78.08008	73.30469	72.03054	567.86262	335.74681	434.04421	1
172	H	77.89817	73.11065	73.11270	-1080.02275	1568.26081	-1948.78900	1
173	H	77.70268	72.40528	71.49054	-919.54108	2111.34692	1456.13463	1
174	C	79.58580	73.52795	71.75714	195.81897	173.33862	-745.11536	1
175	H	79.84642	73.61684	70.68400	1405.67949	-2301.21089	-390.08113	1
176	H	80.04779	74.35808	72.33093	-940.37328	-1118.32446	2299.72133	1
177	N	80.31881	72.23552	72.24297	319.26422	656.36007	-42.02424	1
178	H	81.36036	72.18104	72.04957	1961.03633	619.91968	1787.09422	1
179	H	80.28343	72.02283	73.28243	854.14343	-2156.80752	1429.08711	1
180	H	79.97625	71.32360	71.82324	1237.02905	-1378.50857	-1998.28500	1
181	C	75.16527	76.21207	70.07559	532.53319	-268.57236	517.55729	1
182	O	74.45658	75.66150	69.26403	266.16714	-290.73804	-558.88002	1
183	N	76.12571	77.10852	69.86370	-226.25352	640.49678	-270.32839	1
184	H	76.65479	77.47902	70.65262	2007.69063	-1035.27229	1523.50231	1
185	C	76.38744	77.45141	68.50640	-540.76542	-573.33303	49.50000	1
186	H	75.41093	77.30235	67.98910	-2374.20950	-1036.76023	843.75774	1
187	C	76.98510	78.93373	68.46046	-77.09082	666.87422	-415.84136	1
188	H	77.95951	78.94564	69.02327	-985.81834	617.19825	2463.91927	1
189	O	76.17000	79.95744	69.05619	293.29899	-391.65602	-477.80926	1
190	H	76.76501	80.28721	69.75999	2528.72714	-681.76262	-751.27122	1
191	C	77.28678	79.09278	66.92466	252.47363	-605.14473	440.05134	1
192	H	77.80049	80.05876	66.71010	-2052.65063	1456.49051	-1043.51830	1
193	H	77.95103	78.27258	66.54718	-2152.98800	-1661.97574	-161.70652	1
194	H	76.35117	79.07009	66.31845	-473.12726	-1584.27339	2165.61725	1
195	C	77.54747	76.43159	67.94346	360.36307	488.46713	505.10056	1
196	O	77.48824	76.04961	66.79591	-200.08817	-528.03552	-385.82850	1
197	N	78.44836	76.18843	68.88394	-597.54095	-226.44775	355.20479	1
198	H	78.26184	76.62418	69.78693	2179.23655	-1300.70981	-991.33835	1
199	C	79.76556	75.75385	68.60519	-687.68921	297.39807	-249.45179	1
200	H	80.19306	75.47755	69.59347	-349.16256	-2467.37713	-1101.72831	1
201	C	79.72908	74.55570	67.54602	672.47345	361.54328	-201.62880	1
202	H	79.14650	74.87881	66.63984	1541.41502	582.18425	2169.97026	1
203	H	80.76304	74.31419	67.20737	-2534.67717	60.25153	997.72295	1
204	C	79.07147	73.32431	68.18510	574.26774	-389.43119	-377.02542	1
205	C	79.87331	72.28270	68.74094	688.82679	-287.33580	-257.96133	1
206	H	80.97664	72.34558	68.72305	331.14182	1470.38163	2269.80013	1
207	C	77.64735	73.23097	68.21261	-383.52382	-675.04808	144.24917	1
208	H	77.02640	74.03761	67.77700	4.09847	1517.59662	2262.86397	1
209	C	79.23265	71.18293	69.31043	-134.76730	428.45285	-649.50303	1
210	H	79.85232	70.37452	69.73580	-903.23433	1600.49020	2011.53387	1
211	C	77.05231	72.11126	68.79748	-335.53281	-615.00040	-364.39058	1
212	H	75.94965	72.05406	68.80999	1596.45398	-1369.33862	1732.02659	1
213	C	77.81488	71.05162	69.36950	585.48547	-340.24194	-406.23938	1
214	O	77.21999	69.91690	69.98001	-419.15649	-173.04408	-511.94141	1
215	H	76.27155	70.09807	69.77674	-1071.84350	1559.71507	-1960.13012	1
216	C	80.59169	76.98081	67.89435	291.41878	-183.13091	710.72246	1
217	O	80.07394	77.85971	67.24114	379.87695	523.47396	-222.23622	1
218	N	81.87450	76.70090	68.06418	564.30591	373.09380	277.24371	1
219	H	82.08808	75.87057	68.61455	-120.59931	-2436.07824	-1214.35098	1
220	C	82.92566	77.56379	67.64905	404.07514	-299.37480	608.84009	1
221	H	83.81694	76.90060	67.58177	-1071.07882	-841.69025	2359.66467	1
222	C	82.48785	78.22155	66.27583	-683.12807	68.71770	-390.13096	1
223	H	81.99606	77.46105	65.62783	2068.88918	1596.58590	770.89603	1
224	H	81.70980	79.00415	66.45877	1379.86429	2342.49779	-179.85638	1
225	C	83.73338	78.83561	65.56406	-176.39967	537.49466	550.97268	1

226	H	84.20994	79.62694	66.18474	-396.28051	1942.22168	1869.33314	1
227	H	84.52264	78.07136	65.38693	-94.44700	586.00678	-2659.20016	1
228	C	83.16250	79.42107	64.19158	-291.69381	-718.18079	-150.72929	1
229	H	82.71275	78.66654	63.49693	-2303.38776	1089.76242	964.62032	1
230	H	82.42639	80.25740	64.30239	884.16729	2568.80533	-207.74283	1
231	N	84.30203	79.94291	63.56549	-594.49522	-252.81478	342.29276	1
232	H	85.16096	79.91750	64.09146	-1735.17426	2084.05705	-263.71605	1
233	C	84.31472	80.44195	62.39606	595.23177	-271.52487	442.22352	1
234	N	83.10899	80.46989	61.68556	585.53813	-424.79750	-105.81303	1
235	H	82.18456	80.14598	61.96531	959.88797	1327.56823	-2177.11905	1
236	H	82.99627	80.84523	60.74350	1578.48647	16.27378	-2220.76233	1
237	N	85.59954	80.88183	62.04721	-452.17763	-390.33541	-421.51853	1
238	H	86.47897	80.85691	62.56030	470.26107	1974.25629	-1817.92087	1
239	H	85.81423	81.30802	61.14488	1856.67307	-1573.97321	-1224.35416	1
240	C	83.11197	78.75998	68.75487	-531.47271	-581.45780	-55.06206	1
241	O	82.20609	79.48739	69.15069	-243.00837	192.73507	609.52485	1
242	N	84.39711	78.84333	69.01951	343.49288	-644.25607	38.09164	1
243	H	84.96555	78.13898	68.55042	-1691.16043	-1535.97525	-1484.73099	1
244	C	84.95371	79.62584	70.11150	542.66492	350.14337	454.42563	1
245	H	86.05681	79.51432	69.98241	1209.57979	-2396.95920	463.86744	1
246	C	84.47349	81.06701	69.99153	-737.14309	145.93010	242.71942	1
247	H	83.35713	81.06099	70.04286	-1050.18303	159.36419	-2509.06125	1
248	C	85.00096	81.92890	71.12128	-706.77696	-252.88343	-245.16230	1
249	H	84.64026	82.99131	71.03728	-1624.64039	-1665.49085	1417.86935	1
250	H	84.67174	81.53974	72.13332	2566.10521	598.51109	693.22305	1
251	H	86.12546	81.96049	71.12557	-1972.69758	107.10018	-1876.34312	1
252	C	84.85766	81.67378	68.65452	412.85148	672.58832	-27.69222	1
253	H	84.47884	82.72770	68.54851	1447.02277	1762.76533	-1490.78944	1
254	H	85.97386	81.70402	68.51862	1320.77379	-145.20455	2378.68491	1
255	H	84.43304	81.07744	67.80089	-1512.10848	1470.52031	1724.75147	1
256	C	84.44185	78.92499	71.53646	-607.11113	499.56689	73.73769	1
257	O	85.28555	78.53663	72.30253	357.97126	460.81534	356.68785	1
258	N	83.12787	78.90982	71.66170	536.55407	-368.62270	332.76306	1
259	H	82.50831	79.27586	70.90787	524.38866	2297.69985	1367.20941	1
260	C	82.61442	78.39715	72.88106	46.50277	-774.29190	-147.97904	1
261	H	83.43790	77.76904	73.29162	1676.51875	1883.29066	1032.55549	1
262	C	82.27323	79.64357	73.85422	-559.41456	-34.19198	-556.30433	1
263	H	81.54397	80.31367	73.34113	-64.66664	395.18769	2695.05373	1
264	H	81.76382	79.28485	74.78001	-2703.44278	-60.40056	333.79418	1
265	C	83.52329	80.40342	74.19843	-519.76435	377.31045	459.42366	1
266	H	84.06040	80.64823	73.24410	-1746.74323	1667.50644	-1261.73691	1
267	C	83.18093	81.70518	74.91308	570.95554	16.46261	-545.27700	1
268	H	84.10023	82.30008	75.15117	2391.58273	28.05277	-1305.07271	1
269	H	82.51480	82.35748	74.29196	175.75588	917.63458	2559.43867	1
270	H	82.65076	81.51508	75.88141	-1063.97851	-2155.34650	1283.00462	1
271	C	84.45934	79.58599	75.07843	193.76014	2.62946	-765.53141	1
272	H	85.34928	80.18580	75.40140	507.39394	-846.55087	2539.60089	1
273	H	83.94697	79.22479	76.00710	1337.57841	1818.19054	1526.01994	1
274	H	84.85192	78.68558	74.53477	1100.88635	-1172.91350	-2199.08909	1
275	C	81.24151	77.60119	72.58473	-549.21115	475.64486	-309.38218	1
276	O	80.52288	77.81639	71.64449	556.06106	-390.37755	-78.24250	1
277	O	80.84952	76.67412	73.58267	-572.27940	-310.19032	-209.75862	1
278	H	81.61820	76.79284	74.20711	-1380.08193	2212.14486	790.85944	1

Listing 55: C00055.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.6534	0.0000	300.0000
3	H	71.37730	64.98872	62.03234	-2043.14101	-1757.64893	399.89339		1
4	N	71.39791	65.91270	62.46494	426.75047	490.45733	-334.42467		1
5	H	71.53437	65.70940	63.46823	442.25559	-1110.30854	-2448.52907		1

6	C	72.41840	66.75283	61.96331	415.32972	-666.39213	83.73172	1
7	H	72.92220	66.16850	61.16353	879.32219	2491.00447	667.35213	1
8	C	71.77798	68.12007	61.39828	31.35357	477.41777	628.23362	1
9	H	71.17617	68.60529	62.20364	1168.38489	2240.25337	-1019.71136	1
10	H	72.58014	68.84889	61.13162	-360.43770	2534.90498	931.67112	1
11	C	70.91693	67.82211	60.19997	463.18208	512.70242	-382.34388	1
12	H	70.15777	67.06334	60.49615	1725.29117	1863.52247	-987.07854	1
13	C	70.19564	69.08501	59.74359	710.42801	-144.27427	-313.15367	1
14	H	69.52819	68.88664	58.86568	364.20195	-1033.13725	2494.72524	1
15	H	69.55688	69.51516	60.55739	2567.61904	335.80679	847.48802	1
16	H	70.91949	69.88259	59.43453	-2587.99029	680.92867	-512.16411	1
17	C	71.73247	67.26808	59.03924	268.17616	741.64379	-40.42634	1
18	H	71.09995	67.11480	58.12702	1283.54314	-1945.37420	-1411.27812	1
19	H	72.56473	67.96107	58.75203	-1258.57796	1317.15249	-2026.02085	1
20	H	72.19468	66.27870	59.28789	-2502.84526	909.80597	575.92391	1
21	C	73.33603	66.98586	63.27851	619.36578	-458.64843	-172.09273	1
22	O	73.13617	66.33332	64.29105	-81.40433	433.87611	522.34594	1
23	N	74.28845	67.87474	63.03146	175.23996	-622.20190	341.55523	1
24	H	74.29180	68.34498	62.12785	-876.57256	-303.22879	-2561.90213	1
25	C	75.14052	68.30156	64.09471	-571.88214	-534.10783	-106.15033	1
26	H	75.38711	67.36739	64.64390	-2713.20841	-16.25800	-248.80809	1
27	C	76.37712	69.03912	63.40357	166.60354	288.16399	-716.09568	1
28	H	75.97440	69.90885	62.81565	-2097.85574	1636.78449	-586.18044	1
29	O	77.11922	68.23774	62.46185	-317.80580	-363.38227	484.43082	1
30	H	76.97688	68.73845	61.63550	1863.74748	-1451.84923	1357.29467	1
31	C	77.21272	69.59313	64.61510	503.80731	517.99032	318.51606	1
32	H	78.04151	70.25131	64.26453	640.61020	-2157.10410	-1536.29104	1
33	H	76.59220	70.19977	65.33550	1687.88455	465.60692	2087.56452	1
34	H	77.68382	68.76630	65.19508	-1293.07895	-1899.88581	-1463.57452	1
35	C	74.30527	69.37200	64.99883	-153.07550	-733.68902	248.70981	1
36	O	73.63415	70.21016	64.45892	186.15459	-480.78787	-449.34387	1
37	N	74.59982	69.22195	66.29752	-487.53139	543.18517	42.03850	1
38	C	74.09621	70.12664	67.28737	-699.35871	69.34393	360.10701	1
39	H	73.04388	70.35729	67.00194	2.81126	-221.99807	-2715.58072	1
40	C	74.28127	69.30409	68.63374	-507.46439	-592.59194	122.07761	1
41	H	74.35152	69.95574	69.53366	-1975.08116	525.87560	-1801.71556	1
42	H	73.43245	68.60630	68.80963	1588.27743	-1913.22100	1113.83566	1
43	C	75.59999	68.52725	68.33679	-613.62442	-457.55993	-194.14490	1
44	H	76.48589	69.19822	68.41236	1707.54637	-721.27992	1996.92523	1
45	H	75.78403	67.67145	69.02466	758.23357	2100.81767	1560.55011	1
46	C	75.33215	68.08279	66.83347	-352.41524	704.96076	49.21465	1
47	H	76.24922	67.90913	66.22589	1714.76886	-2070.42778	443.35792	1
48	H	74.64604	67.20882	66.72218	1224.15040	1801.50881	1636.97633	1
49	C	75.02936	71.46647	67.35422	566.85117	537.05831	117.62814	1
50	O	76.10007	71.56720	66.79898	-550.26779	-406.08867	4.21666	1
51	N	74.48082	72.33647	68.26172	566.34832	-425.77725	180.18749	1
52	H	73.54415	71.93600	68.39161	644.44502	2646.80550	-52.73430	1
53	C	74.56213	73.73275	67.88085	612.34801	-281.48662	411.56221	1
54	H	74.61343	73.74924	66.77072	1667.23498	-1490.75142	1556.16753	1
55	C	73.24793	74.38621	68.47868	-714.45746	-175.43074	286.98927	1
56	H	73.29357	74.33128	69.60139	-787.09484	1763.03619	-1922.46060	1
57	O	72.01000	73.72894	68.11613	-429.46514	516.51932	-128.40526	1
58	H	71.64308	73.51667	68.99492	1981.82785	436.16847	-1818.18182	1
59	C	73.38237	75.88817	68.03020	630.79189	-468.94448	76.03230	1
60	H	72.54735	76.50807	68.43185	-1775.71861	2062.30353	131.89849	1
61	H	74.33589	76.34775	68.38515	-1855.14608	88.94118	1993.53760	1
62	H	73.36125	75.98423	66.91975	-1504.82350	-780.94249	-2132.90992	1
63	C	75.86542	74.38937	68.58789	288.57638	618.62814	-397.00270	1
64	O	76.37957	75.38454	68.12472	321.70495	-185.26452	574.37218	1
65	N	76.13160	73.80065	69.75404	-447.05792	-446.53431	367.76425	1
66	H	75.60626	72.96490	70.00701	350.31316	1975.63644	-1843.31522	1
67	C	77.23373	74.31546	70.51249	-511.23061	374.03917	-471.51480	1

68	H	77.90908	74.72500	69.72375	2234.79579	-898.70890	-1273.45190	1
69	C	76.62773	75.46531	71.42205	529.53781	-159.34528	563.72604	1
70	H	77.45995	75.93412	72.00464	654.59388	2347.94251	1217.51488	1
71	H	76.21245	76.26297	70.75810	-1526.55661	2103.42026	817.87394	1
72	O	75.58831	75.02559	72.41483	-554.84278	14.12789	399.58769	1
73	H	74.84125	74.96035	71.80495	1297.06236	2061.84854	1220.68812	1
74	C	77.84999	73.05562	71.34164	-662.15484	-412.13544	123.62687	1
75	O	78.82623	72.48762	70.92720	-540.01537	-317.05804	274.91456	1
76	N	77.13034	72.77283	72.43458	-202.76299	-690.00100	-131.49145	1
77	H	76.31958	73.37289	72.67643	-702.62132	-2617.37191	281.70413	1
78	C	77.52801	71.62148	73.24746	-491.73914	576.34187	222.73509	1
79	H	78.11974	71.01027	72.52297	1977.17978	-1823.58850	-434.68928	1
80	C	78.35244	72.11493	74.42572	-649.50797	-328.66843	306.11224	1
81	H	77.73698	72.84529	74.99621	2075.07803	1452.16490	-1004.45904	1
82	C	78.71226	70.97198	75.35674	-615.18735	-489.99689	-70.96352	1
83	H	79.28392	71.33015	76.25687	-1226.32661	-1724.38906	-1716.47170	1
84	H	77.79376	70.43982	75.73101	2381.64273	-969.84735	900.46860	1
85	H	79.35056	70.20366	74.83883	2122.74991	1702.23946	-141.36228	1
86	C	79.60716	72.83743	73.97197	-501.86074	-479.61276	-376.42482	1
87	H	80.21186	73.21711	74.84134	993.79261	-2246.95401	-1177.81305	1
88	H	80.27377	72.16306	73.36571	42.71279	-626.15391	-2651.37258	1
89	H	79.35785	73.72116	73.32128	-2026.39012	-1590.33709	-887.82922	1
90	C	76.15023	70.87256	73.79900	-672.89153	382.57394	-156.34072	1
91	O	75.99410	69.69853	73.56564	410.04627	221.86223	500.35950	1
92	N	75.36808	71.68368	74.49106	-378.11782	-443.79414	-441.10984	1
93	H	75.63853	72.66001	74.58909	2404.15973	-568.14894	1149.30085	1
94	C	74.26444	71.11750	75.19327	-544.54484	466.16019	331.29119	1
95	H	74.17468	70.07281	74.81042	-1409.80988	-170.17955	2325.32679	1
96	C	74.62714	71.20494	76.74641	-184.48284	116.78282	-758.89137	1
97	H	75.70276	70.97194	76.91008	1893.78641	1861.14652	611.04528	1
98	H	74.47644	72.23867	77.13613	-2170.79665	-974.19311	1327.50117	1
99	C	73.72204	70.17959	77.49370	389.51668	672.81878	-138.49152	1
100	H	72.65697	70.49507	77.41509	510.64577	1933.03327	1851.02484	1
101	H	73.76413	69.18976	76.98819	-2302.30869	-1105.72939	-948.89774	1
102	C	74.11771	69.97072	79.00509	-559.93427	-126.34590	542.30857	1
103	O	73.78377	68.96323	79.58671	-670.36003	-111.83166	76.36448	1
104	N	74.80514	71.00727	79.52975	-216.06729	-537.07037	446.51379	1
105	H	74.88084	71.96945	79.11515	-1251.96487	1074.12894	-2168.52500	1
106	H	74.99699	71.06559	80.53921	-2451.83023	-720.73851	944.84612	1
107	C	72.97797	72.08097	74.96730	546.24052	-563.88337	-85.11809	1
108	O	73.09594	73.29496	75.05280	71.70702	-307.40463	606.69673	1
109	N	71.87763	71.36373	74.76008	479.90863	-504.50129	222.86849	1
110	C	70.61649	72.00918	74.50043	75.51268	-600.91904	506.73700	1
111	H	70.87180	72.85764	73.82416	-2033.61562	1795.30103	254.89480	1
112	C	69.75417	70.84804	73.84844	523.79067	517.99274	284.45581	1
113	H	68.65943	70.99782	73.98414	1599.61665	-1127.00911	1895.98173	1
114	H	69.93280	70.77214	72.75248	-1881.83093	1275.82488	-1501.55016	1
115	C	70.29868	69.59245	74.59827	-600.05639	-404.05026	316.64485	1
116	H	69.87321	69.53013	75.62506	-2597.05260	496.36221	657.73249	1
117	H	70.06045	68.62927	74.09302	-1666.24518	1294.38985	-1723.90591	1
118	C	71.85475	69.91255	74.63593	493.57570	-129.95376	-602.56394	1
119	H	72.40434	69.46462	75.49459	-1469.08415	-637.84797	2204.22581	1
120	H	72.39851	69.67855	73.68975	-1038.97840	1068.88701	-2280.71789	1
121	C	69.99552	72.53602	75.91108	188.88100	241.05089	-727.87821	1
122	O	69.04989	71.99181	76.40925	531.88613	-49.19943	427.07960	1
123	N	70.72828	73.56313	76.36020	708.14833	26.93417	-179.73509	1
124	H	71.58783	73.80355	75.80293	-2232.69501	-1179.09831	1023.94816	1
125	C	70.14898	74.65208	77.16613	-738.32412	259.92548	104.42456	1
126	H	70.37780	75.57172	76.57673	2028.89123	1260.02983	1311.33324	1
127	C	68.67594	74.48048	77.46500	-258.65678	-345.52513	661.28459	1
128	H	68.52545	73.45253	77.87917	-1826.06090	-1801.46097	-918.64554	1
129	C	68.21750	75.48468	78.50904	-541.23400	531.92970	-218.41428	1

130	H	67.15941	75.29475	78.83788	1311.73218	-2219.18200	882.19023	1
131	H	68.87124	75.44851	79.42693	-1048.71298	1223.58118	-2196.97971	1
132	H	68.26333	76.53719	78.11707	419.06414	1903.92898	1903.44670	1
133	C	67.80965	74.60775	76.22525	-423.86431	152.66566	-648.55262	1
134	H	66.71742	74.48500	76.46363	105.68386	-2342.50080	1387.51238	1
135	H	67.93695	75.61357	75.73410	-1695.63603	-1484.73621	-1531.02793	1
136	H	68.07508	73.82690	75.45772	-1853.57121	-487.39031	1936.59343	1
137	C	70.97529	74.62989	78.59354	539.71428	-510.58232	267.58633	1
138	O	71.13892	75.66825	79.22520	-15.93758	-278.34085	-624.49402	1
139	N	71.28193	73.40793	78.96002	-676.81886	12.05292	276.17960	1
140	H	71.08243	72.67964	78.27895	-1694.44250	-373.84189	-2100.66098	1
141	C	71.91064	73.23736	80.24027	412.33078	-664.70360	108.35451	1
142	H	71.29741	73.84575	80.94376	1765.77476	1294.44366	1621.76594	1
143	C	71.96731	71.69792	80.58916	-179.66635	-721.95667	-264.73915	1
144	H	70.95382	71.23769	80.58112	-607.34922	2587.87032	-598.10018	1
145	H	72.56100	71.13766	79.82733	-359.69332	-1479.13954	-2259.74260	1
146	C	72.63371	71.59378	82.00351	-240.01076	616.02425	431.85322	1
147	H	73.58780	72.16721	82.01333	-1359.17131	782.54425	2227.99181	1
148	H	71.99491	72.05245	82.79079	-820.36667	85.81767	-2596.78715	1
149	C	72.90998	70.06858	82.30602	-513.07015	236.18570	-551.87280	1
150	H	71.97414	69.54408	82.60972	1816.11944	-1183.11722	-1650.94321	1
151	H	73.26822	69.53860	81.36961	-1800.04429	-1361.53473	1526.34643	1
152	C	73.98265	69.99048	83.41816	726.08972	-253.19732	-179.64713	1
153	H	74.92296	70.53140	83.19008	1224.27271	-456.51798	-2390.90304	1
154	H	73.62655	70.25984	84.43287	1206.40339	-1150.93514	-2154.90344	1
155	N	74.41894	68.49149	83.51237	329.70796	-633.68968	-155.67358	1
156	H	75.19017	68.26827	84.20602	1348.31305	1938.76845	1359.00643	1
157	H	73.67611	67.78351	83.78327	2096.92035	1446.54551	-966.48890	1
158	H	74.80720	68.06761	82.62062	-1197.07217	-2303.53719	827.28733	1
159	C	73.42280	73.84022	80.08525	-378.01186	-556.17301	-413.96481	1
160	O	74.17698	73.58614	79.14521	-409.44433	-307.55053	-453.30833	1
161	N	73.67130	74.49836	81.19119	-429.02477	524.70884	274.08502	1
162	H	72.91042	74.53739	81.86748	1706.34263	-1425.96036	1574.38926	1
163	C	74.81648	75.33322	81.34623	-45.25864	-626.22952	478.93267	1
164	H	74.91586	75.45431	82.44882	1988.63164	570.90773	1772.87287	1
165	C	76.05495	74.59881	80.68099	551.77128	-20.49526	-564.54996	1
166	H	76.09204	73.53828	81.01971	1434.61535	-1753.10253	1513.99471	1
167	H	75.93200	74.55413	79.56625	-714.67738	1819.09770	1898.36494	1
168	C	77.38376	75.34441	81.02846	446.99263	-555.77305	338.97221	1
169	H	77.38286	76.37316	80.59592	1953.68466	1892.25957	-161.67766	1
170	H	77.51678	75.46728	82.12683	-403.03785	2688.07032	-188.43591	1
171	C	78.52444	74.44201	80.40399	567.86262	335.74681	434.04421	1
172	H	78.59375	73.46908	80.94259	-1080.02275	1568.26081	-1948.78900	1
173	H	78.28366	74.18482	79.34689	-919.54108	2111.34692	1456.13463	1
174	C	79.86681	75.20396	80.47056	195.81897	173.33862	-745.11536	1
175	H	79.93193	76.07286	79.78698	1405.67949	-2301.21089	-390.08113	1
176	H	80.18759	75.49150	81.49181	-940.37328	-1118.32446	2299.72133	1
177	N	80.98586	74.23445	79.95833	319.26422	656.36007	-42.02424	1
178	H	81.96758	74.63551	79.94379	1961.03633	619.91968	1787.09422	1
179	H	81.13550	73.33580	80.50274	854.14343	-2156.80752	1429.08711	1
180	H	80.89243	73.87761	78.96315	1237.02905	-1378.50857	-1998.28500	1
181	C	74.54972	76.77237	80.62432	532.53319	-268.57236	517.55729	1
182	O	75.44302	77.57991	80.67402	266.16714	-290.73804	-558.88002	1
183	N	73.35521	76.87305	80.05764	-226.25352	640.49678	-270.32839	1
184	H	72.66432	76.09003	80.07055	2007.69063	-1035.27229	1523.50231	1
185	C	72.87030	78.13617	79.60667	-540.76542	-573.33303	49.50000	1
186	H	71.80733	77.88808	79.37497	-2374.20950	-1036.76023	843.75774	1
187	C	73.00904	79.17374	80.82097	-77.09082	666.87422	-415.84136	1
188	H	74.10458	79.40905	80.94172	-985.81834	617.19825	2463.91927	1
189	O	72.54297	78.69709	82.09679	293.29899	-391.65602	-477.80926	1
190	H	73.38136	78.68058	82.60059	2528.72714	-681.76262	-751.27122	1
191	C	72.25712	80.45505	80.30816	252.47363	-605.14473	440.05134	1

192	H	72.33439	81.28959	81.04407	-2052.65063	1456.49051	-1043.51830	1
193	H	72.67583	80.83039	79.33043	-2152.98800	-1661.97574	-161.70652	1
194	H	71.17107	80.25458	80.15326	-473.12726	-1584.27339	2165.61725	1
195	C	73.69789	78.61834	78.29637	360.36307	488.46713	505.10056	1
196	O	73.66032	79.80518	77.96171	-200.08817	-528.03552	-385.82850	1
197	N	74.26239	77.60528	77.68046	-597.54095	-226.44775	355.20479	1
198	H	74.12915	76.70681	78.14510	2179.23655	-1300.70981	-991.33835	1
199	C	75.03384	77.69690	76.50178	-687.68921	297.39807	-249.45179	1
200	H	75.17726	76.63476	76.20423	-349.16256	-2467.37713	-1101.72831	1
201	C	74.25558	78.57670	75.41715	672.47345	361.54328	-201.62880	1
202	H	74.15718	79.62713	75.78152	1541.41502	582.18425	2169.97026	1
203	H	74.85740	78.61684	74.47999	-2534.67717	60.25153	997.72295	1
204	C	72.86185	77.99668	75.13310	574.26774	-389.43119	-377.02542	1
205	C	72.70985	76.77235	74.41469	688.82679	-287.33580	-257.96133	1
206	H	73.59309	76.18362	74.10435	331.14182	1470.38163	2269.80013	1
207	C	71.71404	78.72493	75.57090	-383.52382	-675.04808	144.24917	1
208	H	71.83103	79.65092	76.16332	4.09847	1517.59662	2262.86397	1
209	C	71.41983	76.34324	74.09750	-134.76730	428.45285	-649.50303	1
210	H	71.30276	75.40252	73.53204	-903.23433	1600.49020	2011.53387	1
211	C	70.44394	78.25904	75.22049	-335.53281	-615.00040	-364.39058	1
212	H	69.56409	78.84274	75.54399	1596.45398	-1369.33862	1732.02659	1
213	C	70.24853	77.07051	74.45862	585.48547	-340.24194	-406.23938	1
214	O	68.95737	76.60399	74.08038	-419.15649	-173.04408	-511.94141	1
215	H	68.41296	77.36584	74.39292	-1071.84350	1559.71507	-1960.13012	1
216	C	76.46002	78.45916	76.77222	291.41878	-183.13091	710.72246	1
217	O	77.48311	77.92931	76.40916	379.87695	523.47396	-222.23622	1
218	N	76.29178	79.67272	77.28632	564.30591	373.09380	277.24371	1
219	H	75.33516	80.00610	77.55635	-120.59931	-2436.07824	-1214.35098	1
220	C	77.45828	80.37806	77.67903	404.07514	-299.37480	608.84009	1
221	H	78.32911	79.80804	77.27602	-1071.07882	-841.69025	2359.66467	1
222	C	77.31065	81.85737	77.12090	-683.12807	68.71770	-390.13096	1
223	H	77.06748	81.84298	76.03493	2068.88918	1596.58590	770.89603	1
224	H	76.45845	82.37798	77.61271	1379.86429	2342.49779	-179.85638	1
225	C	78.65167	82.60916	77.38143	-176.39967	537.49466	550.97268	1
226	H	78.88752	82.63717	78.46893	-396.28051	1942.22168	1869.33314	1
227	H	79.50299	82.07758	76.90105	-94.44700	586.00678	-2659.20016	1
228	C	78.49203	84.08773	76.79807	-291.69381	-718.18079	-150.72929	1
229	H	78.22168	84.14165	75.71257	-2303.38776	1089.76242	964.62032	1
230	H	77.79362	84.76078	77.35693	884.16729	2568.80533	-207.74283	1
231	N	79.79450	84.59490	76.92214	-594.49522	-252.81478	342.29276	1
232	H	80.50988	83.94776	77.21476	-1735.17426	2084.05705	-263.71605	1
233	C	80.13030	85.79397	76.66874	595.23177	-271.52487	442.22352	1
234	N	79.12443	86.67820	76.26307	585.53813	-424.79750	-105.81303	1
235	H	78.13223	86.50380	76.10869	959.88797	1327.56823	-2177.11905	1
236	H	79.27482	87.65624	76.01400	1578.48647	16.27378	-2220.76233	1
237	N	81.50626	85.98806	76.86121	-452.17763	-390.33541	-421.51853	1
238	H	82.24763	85.33354	77.10660	470.26107	1974.25629	-1817.92087	1
239	H	81.97133	86.87752	76.67676	1856.67307	-1573.97321	-1224.35416	1
240	C	77.44039	80.53935	79.31883	-531.47271	-581.45780	-55.06206	1
241	O	76.42442	80.69047	79.95390	-243.00837	192.73507	609.52485	1
242	N	78.70057	80.59958	79.73253	343.49288	-644.25607	38.09164	1
243	H	79.44603	80.48671	79.04755	-1691.16043	-1535.97525	-1484.73099	1
244	C	78.94289	80.55920	81.13637	542.66492	350.14337	454.42563	1
245	H	77.98978	80.12875	81.52339	1209.57979	-2396.95920	463.86744	1
246	C	80.23843	79.67529	81.37218	-737.14309	145.93010	242.71942	1
247	H	81.13599	80.16671	80.93449	-1050.18303	159.36419	-2509.06125	1
248	C	80.40920	79.44730	82.91299	-706.77696	-252.88343	-245.16230	1
249	H	81.34137	78.87930	83.14338	-1624.64039	-1665.49085	1417.86935	1
250	H	80.45879	80.42692	83.47929	2566.10521	598.51109	693.22305	1
251	H	79.55536	78.86661	83.33501	-1972.69758	107.10018	-1876.34312	1
252	C	80.04354	78.26330	80.72039	412.85148	672.58832	-27.69222	1
253	H	80.93566	77.61365	80.88235	1447.02277	1762.76533	-1490.78944	1

254	H	79.15917	77.73679	81.14899	1320.77379	-145.20455	2378.68491	1
255	H	79.88051	78.33971	79.61964	-1512.10848	1470.52031	1724.75147	1
256	C	79.13589	82.10981	81.64844	-607.11113	499.56689	73.73769	1
257	O	78.15399	82.80362	81.77826	357.97126	460.81534	356.68785	1
258	N	80.41230	82.43992	81.78869	536.55407	-368.62270	332.76306	1
259	H	81.11771	81.72460	81.61411	524.38866	2297.69985	1367.20941	1
260	C	80.76442	83.58572	82.56113	46.50277	-774.29190	-147.97904	1
261	H	81.85255	83.70141	82.36104	1676.51875	1883.29066	1032.55549	1
262	C	79.89599	84.85544	82.07170	-559.41456	-34.19198	-556.30433	1
263	H	78.82197	84.70442	82.36330	-64.66664	395.18769	2695.05373	1
264	H	80.22631	85.79330	82.57883	-2703.44278	-60.40056	333.79418	1
265	C	80.01479	84.98116	80.57692	-519.76435	377.31045	459.42366	1
266	H	79.87330	83.96999	80.13145	-1746.74323	1667.50644	-1261.73691	1
267	C	78.92772	85.89319	80.02228	570.95554	16.46261	-545.27700	1
268	H	79.00406	85.99337	78.90837	2391.58273	28.05277	-1305.07271	1
269	H	77.90433	85.49778	80.25251	175.75588	917.63458	2559.43867	1
270	H	78.99281	86.92480	80.45425	-1063.97851	-2155.34650	1283.00462	1
271	C	81.38553	85.50861	80.17456	193.76014	2.62946	-765.53141	1
272	H	81.46018	85.64338	79.06562	507.39394	-846.55087	2539.60089	1
273	H	81.59950	86.50339	80.64332	1337.57841	1818.19054	1526.01994	1
274	H	82.20629	84.81112	80.48272	1100.88635	-1172.91350	-2199.08909	1
275	C	80.49244	83.23835	84.10117	-549.21115	475.64486	-309.38218	1
276	O	80.46308	82.10416	84.52213	556.06106	-390.37755	-78.24250	1
277	O	80.43217	84.32628	85.00047	-572.27940	-310.19032	-209.75862	1
278	H	80.53748	85.07178	84.34841	-1380.08193	2212.14486	790.85944	1

Listing 56: C00056.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.6502	0.0000	300.0000
3	H	72.77505	69.33813	69.64068	-2043.14101	-1757.64893	399.89339		1
4	N	73.53534	68.77266	69.26137	426.75047	490.45733	-334.42467		1
5	H	73.07585	68.19540	68.53833	442.25559	-1110.30854	-2448.52907		1
6	C	74.59368	69.53908	68.72342	415.32972	-666.39213	83.73172		1
7	H	74.38038	70.59958	68.98400	879.32219	2491.00447	667.35213		1
8	C	76.00682	69.03949	69.31837	31.35357	477.41777	628.23362		1
9	H	76.20649	68.00141	68.96012	1168.38489	2240.25337	-1019.71136		1
10	H	76.84049	69.66558	68.91913	-360.43770	2534.90498	931.67112		1
11	C	75.98591	69.07711	70.82308	463.18208	512.70242	-382.34388		1
12	H	75.11799	68.47237	71.17112	1725.29117	1863.52247	-987.07854		1
13	C	77.26698	68.46467	71.37726	710.42801	-144.27427	-313.15367		1
14	H	77.26164	68.43402	72.49709	364.20195	-1033.13725	2494.72524		1
15	H	77.41448	67.41439	71.01586	2567.61904	335.80679	847.48802		1
16	H	78.17015	69.05090	71.06702	-2587.99029	680.92867	-512.16411		1
17	C	75.83354	70.49652	71.35268	268.17616	741.64379	-40.42634		1
18	H	75.84612	70.52219	72.47286	1283.54314	-1945.37420	-1411.27812		1
19	H	76.66266	71.16148	70.99770	-1258.57796	1317.15249	-2026.02085		1
20	H	74.86948	70.96181	71.02246	-2502.84526	909.80597	575.92391		1
21	C	74.47449	69.20022	67.14226	619.36578	-458.64843	-172.09273		1
22	O	73.58612	68.45713	66.73136	-81.40433	433.87611	522.34594		1
23	N	75.46704	69.77693	66.49669	175.23996	-622.20190	341.55523		1
24	H	76.09087	70.34876	67.06598	-876.57256	-303.22879	-2561.90213		1
25	C	75.52612	69.90893	65.07413	-571.88214	-534.10783	-106.15033		1
26	H	76.54844	70.32975	64.94886	-2713.20841	-16.25800	-248.80809		1
27	C	75.44648	68.44785	64.42575	166.60354	288.16399	-716.09568		1
28	H	74.45290	67.97917	64.67733	-2097.85574	1636.78449	-586.18044		1
29	O	76.40843	67.48839	64.90507	-317.80580	-363.38227	484.43082		1
30	H	75.82228	66.86681	65.38203	1863.74748	-1451.84923	1357.29467		1
31	C	75.54789	68.78491	62.89253	503.80731	517.99032	318.51606		1
32	H	75.34448	67.88756	62.26270	640.61020	-2157.10410	-1536.29104		1
33	H	74.83127	69.58464	62.58458	1687.88455	465.60692	2087.56452		1

34	H	76.56947	69.14469	62.62915	-1293.07895	-1899.88581	-1463.57452	1
35	C	74.46182	71.08040	64.72264	-153.07550	-733.68902	248.70981	1
36	O	74.81607	72.19881	65.08459	186.15459	-480.78787	-449.34387	1
37	N	73.33636	70.74783	64.10037	-487.53139	543.18517	42.03850	1
38	C	72.41696	71.76106	63.66083	-699.35871	69.34393	360.10701	1
39	H	73.01636	72.61868	63.27842	2.81126	-221.99807	-2715.58072	1
40	C	71.56965	70.96160	62.58359	-507.46439	-592.59194	122.07761	1
41	H	70.61514	71.46706	62.31502	-1975.08116	525.87560	-1801.71556	1
42	H	72.13744	70.81643	61.63739	1588.27743	-1913.22100	1113.83566	1
43	C	71.36160	69.61305	63.34185	-613.62442	-457.55993	-194.14490	1
44	H	70.58117	69.71257	64.12883	1707.54637	-721.27992	1996.92523	1
45	H	71.04290	68.77525	62.68129	758.23357	2100.81767	1560.55011	1
46	C	72.79918	69.39632	63.97591	-352.41524	704.96076	49.21465	1
47	H	72.82101	68.94869	65.01660	1714.76886	-2070.42778	443.35792	1
48	H	73.49526	68.83391	63.30881	1224.15040	1801.50881	1636.97633	1
49	C	71.43198	72.17057	64.90730	566.85117	537.05831	117.62814	1
50	O	71.47913	71.62451	65.98324	-550.26779	-406.08867	4.21666	1
51	N	70.62006	73.13183	64.48506	566.34832	-425.77725	180.18749	1
52	H	70.71654	73.43448	63.51755	644.44502	2646.80550	-52.73430	1
53	C	69.63911	73.69889	65.34045	612.34801	-281.48662	411.56221	1
54	H	69.10526	74.41697	64.67894	1667.23498	-1490.75142	1556.16753	1
55	C	68.68573	72.50232	65.81182	-714.45746	-175.43074	286.98927	1
56	H	69.29083	71.81499	66.46745	-787.09484	1763.03619	-1922.46060	1
57	O	68.15625	71.68477	64.74858	-429.46514	516.51932	-128.40526	1
58	H	68.58495	70.82919	64.94605	1981.82785	436.16847	-1818.18182	1
59	C	67.59041	73.21360	66.68534	630.79189	-468.94448	76.03230	1
60	H	66.91643	72.47180	67.17497	-1775.71861	2062.30353	131.89849	1
61	H	68.04952	73.84314	67.50081	-1855.14608	88.94118	1993.53760	1
62	H	66.94689	73.88197	66.06680	-1504.82350	-780.94249	-2132.90992	1
63	C	70.41449	74.44928	66.56426	288.57638	618.62814	-397.00270	1
64	O	69.88041	74.59697	67.64499	321.70495	-185.26452	574.37218	1
65	N	71.57536	74.94746	66.15678	-447.05792	-446.53431	367.76425	1
66	H	71.87311	74.76238	65.20032	350.31316	1975.63644	-1843.31522	1
67	C	72.47823	75.46084	67.11894	-511.23061	374.03917	-471.51480	1
68	H	71.97927	75.30067	68.10278	2234.79579	-898.70890	-1273.45190	1
69	C	73.83667	74.63328	66.93689	529.53781	-159.34528	563.72604	1
70	H	74.50102	74.94615	67.78903	654.59388	2347.94251	1217.51488	1
71	H	73.60535	73.54556	67.10501	-1526.55661	2103.42026	817.87394	1
72	O	74.56571	74.77975	65.71440	-554.84278	14.12789	399.58769	1
73	H	74.65305	73.79662	65.42892	1297.06236	2061.84854	1220.68812	1
74	C	72.69413	77.04287	66.75004	-662.15484	-412.13544	123.62687	1
75	O	72.91183	77.48686	65.64986	-540.01537	-317.05804	274.91456	1
76	N	72.65311	77.70984	67.91744	-202.76299	-690.00100	-131.49145	1
77	H	72.33088	77.13489	68.69387	-702.62132	-2617.37191	281.70413	1
78	C	72.54472	79.16830	67.92065	-491.73914	576.34187	222.73509	1
79	H	73.19281	79.45686	67.05992	1977.17978	-1823.58850	-434.68928	1
80	C	71.09312	79.56163	67.72137	-649.50797	-328.66843	306.11224	1
81	H	70.50427	79.18790	68.58806	2075.07803	1452.16490	-1004.45904	1
82	C	70.94752	81.07253	67.67302	-615.18735	-489.99689	-70.96352	1
83	H	69.87340	81.38517	67.56013	-1226.32661	-1724.38906	-1716.47170	1
84	H	71.34176	81.55461	68.60988	2381.64273	-969.84735	900.46860	1
85	H	71.51606	81.51390	66.80891	2122.74991	1702.23946	-141.36228	1
86	C	70.49481	78.93863	66.47319	-501.86074	-479.61276	-376.42482	1
87	H	69.45617	79.31769	66.26866	993.79261	-2246.95401	-1177.81305	1
88	H	71.12282	79.15772	65.56501	42.71279	-626.15391	-2651.37258	1
89	H	70.43340	77.81839	66.56052	-2026.39012	-1590.33709	-887.82922	1
90	C	73.11339	79.69357	69.39562	-672.89153	382.57394	-156.34072	1
91	O	74.06595	80.43542	69.43078	410.04627	221.86223	500.35950	1
92	N	72.40084	79.22711	70.40686	-378.11782	-443.79414	-441.10984	1
93	H	71.62367	78.61579	70.16950	2404.15973	-568.14894	1149.30085	1
94	C	72.77977	79.56897	71.74203	-544.54484	466.16019	331.29119	1
95	H	73.30633	80.54064	71.58571	-1409.80988	-170.17955	2325.32679	1

96	C	71.40592	79.68839	72.53347	-184.48284	116.78282	-758.89137	1
97	H	70.68675	80.30126	71.94676	1893.78641	1861.14652	611.04528	1
98	H	70.92629	78.68995	72.64186	-2170.79665	-974.19311	1327.50117	1
99	C	71.67083	80.31969	73.93773	389.51668	672.81878	-138.49152	1
100	H	72.37357	79.67839	74.51800	510.64577	1933.03327	1851.02484	1
101	H	72.21669	81.28169	73.81251	-2302.30869	-1105.72939	-948.89774	1
102	C	70.37525	80.55808	74.78698	-559.93427	-126.34590	542.30857	1
103	O	70.46972	80.65636	75.99642	-670.36003	-111.83166	76.36448	1
104	N	69.26225	80.67066	74.05043	-216.06729	-537.07037	446.51379	1
105	H	69.14617	80.61704	73.03135	-1251.96487	1074.12894	-2168.52500	1
106	H	68.32870	80.85847	74.43641	-2451.83023	-720.73851	944.84612	1
107	C	73.75961	78.52626	72.50767	546.24052	-563.88337	-85.11809	1
108	O	74.30056	78.98425	73.50971	71.70702	-307.40463	606.69673	1
109	N	73.85925	77.28711	72.03160	479.90863	-504.50129	222.86849	1
110	C	74.43179	76.22632	72.81628	75.51268	-600.91904	506.73700	1
111	H	74.00914	76.36378	73.83752	-2033.61562	1795.30103	254.89480	1
112	C	73.98647	74.91901	72.04189	523.79067	517.99274	284.45581	1
113	H	74.66485	74.05704	72.23424	1599.61665	-1127.00911	1895.98173	1
114	H	72.96256	74.59566	72.33475	-1881.83093	1275.82488	-1501.55016	1
115	C	74.02518	75.40430	70.55828	-600.05639	-404.05026	316.64485	1
116	H	75.07008	75.44403	70.17694	-2597.05260	496.36221	657.73249	1
117	H	73.45095	74.75618	69.85876	-1666.24518	1294.38985	-1723.90591	1
118	C	73.41046	76.86192	70.71251	493.57570	-129.95376	-602.56394	1
119	H	73.77840	77.61558	69.97703	-1469.08415	-637.84797	2204.22581	1
120	H	72.29557	76.88669	70.75854	-1038.97840	1068.88701	-2280.71789	1
121	C	76.06463	76.33190	72.80931	188.88100	241.05089	-727.87821	1
122	O	76.72410	75.46943	72.28496	531.88613	-49.19943	427.07960	1
123	N	76.46600	77.40368	73.48810	708.14833	26.93417	-179.73509	1
124	H	75.77590	78.10971	73.84485	-2232.69501	-1179.09831	1023.94816	1
125	C	77.85283	77.70132	73.43751	-738.32412	259.92548	104.42456	1
126	H	78.37054	76.76926	73.11056	2028.89123	1260.02983	1311.33324	1
127	C	78.01643	78.90374	72.40425	-258.65678	-345.52513	661.28459	1
128	H	77.37671	79.76116	72.70611	-1826.06090	-1801.46097	-918.64554	1
129	C	79.52573	79.31717	72.35308	-541.23400	531.92970	-218.41428	1
130	H	79.70430	80.13478	71.61568	1311.73218	-2219.18200	882.19023	1
131	H	79.88167	79.68129	73.34599	-1048.71298	1223.58118	-2196.97971	1
132	H	80.17669	78.45926	72.06275	419.06414	1903.92898	1903.44670	1
133	C	77.61670	78.40861	70.97325	-423.86431	152.66566	-648.55262	1
134	H	77.75713	79.20558	70.20509	105.68386	-2342.50080	1387.51238	1
135	H	78.22747	77.52928	70.65922	-1695.63603	-1484.73621	-1531.02793	1
136	H	76.54537	78.09638	70.93766	-1853.57121	-487.39031	1936.59343	1
137	C	78.29336	78.27787	74.91503	539.71428	-510.58232	267.58633	1
138	O	77.57244	78.99824	75.56599	-15.93758	-278.34085	-624.49402	1
139	N	79.54796	77.91548	75.13185	-676.81886	12.05292	276.17960	1
140	H	79.97960	77.31308	74.43319	-1694.44250	-373.84189	-2100.66098	1
141	C	80.23059	78.21660	76.34314	412.33078	-664.70360	108.35451	1
142	H	81.26727	77.87514	76.12582	1765.77476	1294.44366	1621.76594	1
143	C	80.12814	79.77888	76.57120	-179.66635	-721.95667	-264.73915	1
144	H	80.55669	80.33079	75.70455	-607.34922	2587.87032	-598.10018	1
145	H	79.05800	80.10086	76.61701	-359.69332	-1479.13954	-2259.74260	1
146	C	80.88923	80.13762	77.89053	-240.01076	616.02425	431.85322	1
147	H	80.53854	79.50423	78.73640	-1359.17131	782.54425	2227.99181	1
148	H	81.97939	79.93670	77.79238	-820.36667	85.81767	-2596.78715	1
149	C	80.61450	81.66689	78.18631	-513.07015	236.18570	-551.87280	1
150	H	81.03567	82.31074	77.38025	1816.11944	-1183.11722	-1650.94321	1
151	H	79.52032	81.87771	78.20064	-1800.04429	-1361.53473	1526.34643	1
152	C	81.25193	82.00120	79.55481	726.08972	-253.19732	-179.64713	1
153	H	80.78603	81.48480	80.41776	1224.27271	-456.51798	-2390.90304	1
154	H	82.35305	81.88239	79.59324	1206.40339	-1150.93514	-2154.90344	1
155	N	81.00851	83.52432	79.82604	329.70796	-633.68968	-155.67358	1
156	H	81.37657	83.88936	80.75146	1348.31305	1938.76845	1359.00643	1
157	H	81.44350	84.21165	79.14408	2096.92035	1446.54551	-966.48890	1

158	H	80.00055	83.85556	79.85756	-1197.07217	-2303.53719	827.28733	1
159	C	79.56506	77.29471	77.52816	-378.01186	-556.17301	-413.96481	1
160	O	79.92271	76.12173	77.59764	-409.44433	-307.55053	-453.30833	1
161	N	78.73418	77.96051	78.29663	-429.02477	524.70884	274.08502	1
162	H	78.59210	78.92886	78.01456	1706.34263	-1425.96036	1574.38926	1
163	C	77.74503	77.33699	79.11116	-45.25864	-626.22952	478.93267	1
164	H	77.02775	78.16067	79.32670	1988.63164	570.90773	1772.87287	1
165	C	77.11797	76.16391	78.24650	551.77128	-20.49526	-564.54996	1
166	H	76.71123	76.55016	77.28431	1434.61535	-1753.10253	1513.99471	1
167	H	77.89779	75.41837	77.96114	-714.67738	1819.09770	1898.36494	1
168	C	76.00719	75.48987	79.11424	446.99263	-555.77305	338.97221	1
169	H	76.39462	75.26408	80.13386	1953.68466	1892.25957	-161.67766	1
170	H	75.14489	76.18112	79.24931	-403.03785	2688.07032	-188.43591	1
171	C	75.55730	74.15600	78.39630	567.86262	335.74681	434.04421	1
172	H	75.18033	74.35828	77.36763	-1080.02275	1568.26081	-1948.78900	1
173	H	76.41358	73.45324	78.27752	-919.54108	2111.34692	1456.13463	1
174	C	74.45027	73.54724	79.29489	195.81897	173.33862	-745.11536	1
175	H	74.78555	73.25287	80.31078	1405.67949	-2301.21089	-390.08113	1
176	H	73.53489	74.16990	79.37241	-940.37328	-1118.32446	2299.72133	1
177	N	73.95182	72.23477	78.64496	319.26422	656.36007	-42.02424	1
178	H	73.00101	71.86644	79.12954	1961.03633	619.91968	1787.09422	1
179	H	73.71464	72.28130	77.61377	854.14343	-2156.80752	1429.08711	1
180	H	74.60753	71.40338	78.66392	1237.02905	-1378.50857	-1998.28500	1
181	C	78.37506	76.71453	80.48647	532.53319	-268.57236	517.55729	1
182	O	77.91965	77.10103	81.55320	266.16714	-290.73804	-558.88002	1
183	N	79.27319	75.80313	80.22457	-226.25352	640.49678	-270.32839	1
184	H	79.54800	75.64118	79.22402	2007.69063	-1035.27229	1523.50231	1
185	C	80.05786	75.18690	81.23426	-540.76542	-573.33303	49.50000	1
186	H	80.79175	74.59431	80.64291	-2374.20950	-1036.76023	843.75774	1
187	C	80.75634	76.33922	82.10164	-77.09082	666.87422	-415.84136	1
188	H	79.94901	76.95605	82.58661	-985.81834	617.19825	2463.91927	1
189	O	81.58439	77.26184	81.37345	293.29899	-391.65602	-477.80926	1
190	H	81.07184	78.08953	81.47095	2528.72714	-681.76262	-751.27122	1
191	C	81.49771	75.47314	83.18454	252.47363	-605.14473	440.05134	1
192	H	81.97845	76.11157	83.96111	-2052.65063	1456.49051	-1043.51830	1
193	H	80.80176	74.77738	83.71052	-2152.98800	-1661.97574	-161.70652	1
194	H	82.30143	74.85023	82.72752	-473.12726	-1584.27339	2165.61725	1
195	C	79.13956	74.22781	82.19520	360.36307	488.46713	505.10056	1
196	O	79.36290	73.03676	82.17018	-200.08817	-528.03552	-385.82850	1
197	N	78.26552	74.89463	82.93010	-597.54095	-226.44775	355.20479	1
198	H	78.13393	75.92954	82.80826	2179.23655	-1300.70981	-991.33835	1
199	C	77.63814	74.18523	83.97748	-687.68921	297.39807	-249.45179	1
200	H	78.01949	73.13931	83.90083	-349.16256	-2467.37713	-1101.72831	1
201	C	77.98175	74.88975	85.37914	672.47345	361.54328	-201.62880	1
202	H	77.91374	75.99788	85.29561	1541.41502	582.18425	2169.97026	1
203	H	77.22188	74.57145	86.13090	-2534.67717	60.25153	997.72295	1
204	C	79.38100	74.46003	85.83725	574.26774	-389.43119	-377.02542	1
205	C	79.62264	73.08361	86.13119	688.82679	-287.33580	-257.96133	1
206	H	78.81298	72.33766	86.04222	331.14182	1470.38163	2269.80013	1
207	C	80.42985	75.41839	85.98073	-383.52382	-675.04808	144.24917	1
208	H	80.24917	76.48650	85.76390	4.09847	1517.59662	2262.86397	1
209	C	80.89994	72.69669	86.53286	-134.76730	428.45285	-649.50303	1
210	H	81.08429	71.63052	86.75275	-903.23433	1600.49020	2011.53387	1
211	C	81.69267	74.98225	86.38996	-335.53281	-615.00040	-364.39058	1
212	H	82.49637	75.73222	86.49215	1596.45398	-1369.33862	1732.02659	1
213	C	81.98008	73.61557	86.67562	585.48547	-340.24194	-406.23938	1
214	O	83.25979	73.15978	87.08612	-419.15649	-173.04408	-511.94141	1
215	H	83.74674	74.01711	87.09777	-1071.84350	1559.71507	-1960.13012	1
216	C	76.00778	74.30580	83.92592	291.41878	-183.13091	710.72246	1
217	O	75.32824	73.83348	84.81011	379.87695	523.47396	-222.23622	1
218	N	75.53937	74.90017	82.77748	564.30591	373.09380	277.24371	1
219	H	76.42287	75.17253	82.32751	-120.59931	-2436.07824	-1214.35098	1

220	C	74.59501	75.97758	83.04551	404.07514	-299.37480	608.84009	1
221	H	74.96563	76.50363	83.95079	-1071.07882	-841.69025	2359.66467	1
222	C	74.66807	76.81360	81.72108	-683.12807	68.71770	-390.13096	1
223	H	75.64932	77.34036	81.63850	2068.88918	1596.58590	770.89603	1
224	H	74.63649	76.10301	80.86474	1379.86429	2342.49779	-179.85638	1
225	C	73.47541	77.81565	81.58652	-176.39967	537.49466	550.97268	1
226	H	72.50083	77.32171	81.79896	-396.28051	1942.22168	1869.33314	1
227	H	73.55299	78.66611	82.29895	-94.44700	586.00678	-2659.20016	1
228	C	73.58073	78.27852	80.06106	-291.69381	-718.18079	-150.72929	1
229	H	74.48796	78.88255	79.80651	-2303.38776	1089.76242	964.62032	1
230	H	73.51696	77.44740	79.31636	884.16729	2568.80533	-207.74283	1
231	N	72.45154	79.06083	79.79145	-594.49522	-252.81478	342.29276	1
232	H	71.77066	79.16632	80.52645	-1735.17426	2084.05705	-263.71605	1
233	C	72.24010	79.61580	78.66639	595.23177	-271.52487	442.22352	1
234	N	73.20284	79.44815	77.65939	585.53813	-424.79750	-105.81303	1
235	H	74.09354	78.95359	77.66843	959.88797	1327.56823	-2177.11905	1
236	H	73.12812	79.86577	76.73180	1578.48647	16.27378	-2220.76233	1
237	N	71.03212	80.32011	78.62147	-452.17763	-390.33541	-421.51853	1
238	H	70.30493	80.40934	79.33653	470.26107	1974.25629	-1817.92087	1
239	H	70.69275	80.74084	77.72106	1856.67307	-1573.97321	-1224.35416	1
240	C	73.08624	75.40054	83.22947	-531.47271	-581.45780	-55.06206	1
241	O	72.33918	75.87340	84.05440	-243.00837	192.73507	609.52485	1
242	N	72.78152	74.57905	82.20517	343.49288	-644.25607	38.09164	1
243	H	73.62189	74.32841	81.68204	-1691.16043	-1535.97525	-1484.73099	1
244	C	71.76155	73.58266	82.41755	542.66492	350.14337	454.42563	1
245	H	71.64392	73.48682	83.51967	1209.57979	-2396.95920	463.86744	1
246	C	70.46014	74.08482	81.66414	-737.14309	145.93010	242.71942	1
247	H	70.72430	74.39760	80.63063	-1050.18303	159.36419	-2509.06125	1
248	C	69.43010	72.90344	81.64314	-706.77696	-252.88343	-245.16230	1
249	H	68.49841	73.17722	81.09442	-1624.64039	-1665.49085	1417.86935	1
250	H	69.86394	72.00517	81.13848	2566.10521	598.51109	693.22305	1
251	H	69.13303	72.59610	82.67330	-1972.69758	107.10018	-1876.34312	1
252	C	69.82797	75.28184	82.45411	412.85148	672.58832	-27.69222	1
253	H	68.96045	75.72496	81.91077	1447.02277	1762.76533	-1490.78944	1
254	H	69.46724	74.96398	83.46030	1320.77379	-145.20455	2378.68491	1
255	H	70.57610	76.09555	82.61789	-1512.10848	1470.52031	1724.75147	1
256	C	72.34081	72.28483	81.64624	-607.11113	499.56689	73.73769	1
257	O	72.13033	72.12626	80.42893	357.97126	460.81534	356.68785	1
258	N	73.05292	71.53916	82.44964	536.55407	-368.62270	332.76306	1
259	H	73.13617	71.78669	83.43693	524.38866	2297.69985	1367.20941	1
260	C	73.81002	70.48366	81.86096	46.50277	-774.29190	-147.97904	1
261	H	74.17811	70.92219	80.90778	1676.51875	1883.29066	1032.55549	1
262	C	74.95924	70.01208	82.88372	-559.41456	-34.19198	-556.30433	1
263	H	74.48826	69.70249	83.84776	-64.66664	395.18769	2695.05373	1
264	H	75.47576	69.10358	82.48910	-2703.44278	-60.40056	333.79418	1
265	C	75.94976	71.12649	83.11392	-519.76435	377.31045	459.42366	1
266	H	75.39278	72.05722	83.37488	-1746.74323	1667.50644	-1261.73691	1
267	C	76.86559	70.77032	84.27835	570.95554	16.46261	-545.27700	1
268	H	77.65706	71.54830	84.43577	2391.58273	28.05277	-1305.07271	1
269	H	76.29493	70.67767	85.23875	175.75588	917.63458	2559.43867	1
270	H	77.39026	69.79501	84.10733	-1063.97851	-2155.34650	1283.00462	1
271	C	76.77751	71.38396	81.86472	193.76014	2.62946	-765.53141	1
272	H	77.60428	72.14100	82.05104	507.39394	-846.55087	2539.60089	1
273	H	77.27426	70.44709	81.50216	1337.57841	1818.19054	1526.01994	1
274	H	76.15023	71.77478	81.02265	1100.88635	-1172.91350	-2199.08909	1
275	C	72.82589	69.23288	81.58650	-549.21115	475.64486	-309.38218	1
276	O	71.89186	68.94056	82.28497	556.06106	-390.37755	-78.24250	1
277	O	73.24510	68.37250	80.54269	-572.27940	-310.19032	-209.75862	1
278	H	74.02261	68.90032	80.20973	-1380.08193	2212.14486	790.85944	1

Listing 57: C00057.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.6500	0.0000	300.0000
3	H	72.99638	72.88041	69.49698	-2043.14101	-1757.64893	399.89339		1
4	N	73.08255	73.87711	69.31273	426.75047	490.45733	-334.42467		1
5	H	72.67322	74.27735	70.15403	442.25559	-1110.30854	-2448.52907		1
6	C	74.37967	74.32038	68.98704	415.32972	-666.39213	83.73172		1
7	H	74.92774	73.40416	68.68160	879.32219	2491.00447	667.35213		1
8	C	74.30040	75.46107	67.84977	31.35357	477.41777	628.23362		1
9	H	73.70777	76.32292	68.24073	1168.38489	2240.25337	-1019.71136		1
10	H	75.31825	75.87210	67.64045	-360.43770	2534.90498	931.67112		1
11	C	73.66897	74.91033	66.59380	463.18208	512.70242	-382.34388		1
12	H	72.83091	74.23939	66.88853	1725.29117	1863.52247	-987.07854		1
13	C	73.10251	76.04018	65.74442	710.42801	-144.27427	-313.15367		1
14	H	72.63175	75.65500	64.80300	364.20195	-1033.13725	2494.72524		1
15	H	72.31719	76.61964	66.29595	2567.61904	335.80679	847.48802		1
16	H	73.89982	76.76789	65.44265	-2587.99029	680.92867	-512.16411		1
17	C	74.68177	74.11349	65.78403	268.17616	741.64379	-40.42634		1
18	H	74.22509	73.68719	64.85342	1283.54314	-1945.37420	-1411.27812		1
19	H	75.54621	74.75251	65.46553	-1258.57796	1317.15249	-2026.02085		1
20	H	75.10195	73.25737	66.37251	-2502.84526	909.80597	575.92391		1
21	C	74.98968	75.08688	70.28250	619.36578	-458.64843	-172.09273		1
22	O	75.03399	76.31434	70.22811	-81.40433	433.87611	522.34594		1
23	N	75.36273	74.28218	71.25178	175.23996	-622.20190	341.55523		1
24	H	75.19525	73.28294	71.13537	-876.57256	-303.22879	-2561.90213		1
25	C	75.82285	74.82645	72.48833	-571.88214	-534.10783	-106.15033		1
26	H	75.09072	75.61973	72.77556	-2713.20841	-16.25800	-248.80809		1
27	C	75.96830	73.63589	73.52693	166.60354	288.16399	-716.09568		1
28	H	76.50947	72.78342	73.02160	-2097.85574	1636.78449	-586.18044		1
29	O	74.72335	72.93600	73.87880	-317.80580	-363.38227	484.43082		1
30	H	74.66398	73.13342	74.83141	1863.74748	-1451.84923	1357.29467		1
31	C	76.83586	74.24588	74.67582	503.80731	517.99032	318.51606		1
32	H	77.06649	73.49047	75.46389	640.61020	-2157.10410	-1536.29104		1
33	H	77.80830	74.63760	74.29220	1687.88455	465.60692	2087.56452		1
34	H	76.31790	75.09998	75.17310	-1293.07895	-1899.88581	-1463.57452		1
35	C	77.04728	75.91377	72.30897	-153.07550	-733.68902	248.70981		1
36	O	76.99177	76.85362	73.05792	186.15459	-480.78787	-449.34387		1
37	N	78.01220	75.58668	71.44355	-487.53139	543.18517	42.03850		1
38	C	79.00919	76.54750	71.07023	-699.35871	69.34393	360.10701		1
39	H	79.25465	77.09527	72.00939	2.81126	-221.99807	-2715.58072		1
40	C	80.15399	75.65144	70.44352	-507.46439	-592.59194	122.07761		1
41	H	80.75674	76.20809	69.68861	-1975.08116	525.87560	-1801.71556		1
42	H	80.86357	75.28641	71.21976	1588.27743	-1913.22100	1113.83566		1
43	C	79.33770	74.47456	69.81820	-613.62442	-457.55993	-194.14490		1
44	H	78.88585	74.78218	68.84849	1707.54637	-721.27992	1996.92523		1
45	H	79.94768	73.56638	69.61186	758.23357	2100.81767	1560.55011		1
46	C	78.22099	74.24195	70.92214	-352.41524	704.96076	49.21465		1
47	H	77.24921	73.85758	70.53803	1714.76886	-2070.42778	443.35792		1
48	H	78.54227	73.62228	71.79263	1224.15040	1801.50881	1636.97633		1
49	C	78.45670	77.54322	69.89020	566.85117	537.05831	117.62814		1
50	O	79.03128	77.52988	68.82463	-550.26779	-406.08867	4.21666		1
51	N	77.45574	78.32968	70.27062	566.34832	-425.77725	180.18749		1
52	H	77.11260	78.22100	71.22695	644.44502	2646.80550	-52.73430		1
53	C	77.10363	79.40504	69.37764	612.34801	-281.48662	411.56221		1
54	H	77.34770	78.96655	68.37917	1667.23498	-1490.75142	1556.16753		1
55	C	75.63927	79.86521	69.55529	-714.45746	-175.43074	286.98927		1
56	H	75.46174	80.39421	70.52452	-787.09484	1763.03619	-1922.46060		1
57	O	74.36752	78.80285	69.89674	-429.46514	516.51932	-128.40526		1
58	H	74.96388	78.00233	69.96208	1981.82785	436.16847	-1818.18182		1
59	C	75.25059	80.69898	68.31937	630.79189	-468.94448	76.03230		1
60	H	74.22492	81.12937	68.43672	-1775.71861	2062.30353	131.89849		1

61	H	75.95318	81.55996	68.13652	-1855.14608	88.94118	1993.53760	1
62	H	75.24846	80.07304	67.39231	-1504.82350	-780.94249	-2132.90992	1
63	C	77.99712	80.77298	69.69974	288.57638	618.62814	-397.00270	1
64	O	77.38712	81.84711	69.58708	321.70495	-185.26452	574.37218	1
65	N	79.24608	80.54781	69.98704	-447.05792	-446.53431	367.76425	1
66	H	79.35413	79.52767	69.99369	350.31316	1975.63644	-1843.31522	1
67	C	80.36026	81.40685	70.13566	-511.23061	374.03917	-471.51480	1
68	H	81.16031	80.68116	70.40531	2234.79579	-898.70890	-1273.45190	1
69	C	80.63341	82.08080	68.70603	529.53781	-159.34528	563.72604	1
70	H	81.65388	82.55252	68.70790	654.59388	2347.94251	1217.51488	1
71	H	80.67251	81.23808	67.96682	-1526.55661	2103.42026	817.87394	1
72	O	79.70581	83.10541	68.26060	-554.84278	14.12789	399.58769	1
73	H	78.86542	82.60980	68.34756	1297.06236	2061.84854	1220.68812	1
74	C	80.22180	82.56810	71.26413	-662.15484	-412.13544	123.62687	1
75	O	81.17094	82.81196	71.98295	-540.01537	-317.05804	274.91456	1
76	N	79.07590	83.20764	71.16599	-202.76299	-690.00100	-131.49145	1
77	H	78.37126	82.87569	70.45028	-702.62132	-2617.37191	281.70413	1
78	C	78.62854	84.19753	72.14608	-491.73914	576.34187	222.73509	1
79	H	79.51102	84.87072	72.26330	1977.17978	-1823.58850	-434.68928	1
80	C	77.39594	84.83742	71.53762	-649.50797	-328.66843	306.11224	1
81	H	76.65831	84.01992	71.36181	2075.07803	1452.16490	-1004.45904	1
82	C	76.74791	85.85573	72.45688	-615.18735	-489.99689	-70.96352	1
83	H	75.81716	86.29163	71.99893	-1226.32661	-1724.38906	-1716.47170	1
84	H	76.44894	85.39257	73.44002	2381.64273	-969.84735	900.46860	1
85	H	77.44047	86.71177	72.68528	2122.74991	1702.23946	-141.36228	1
86	C	77.69088	85.47567	70.19151	-501.86074	-479.61276	-376.42482	1
87	H	76.75184	85.82925	69.68363	993.79261	-2246.95401	-1177.81305	1
88	H	78.36970	86.36572	70.29574	42.71279	-626.15391	-2651.37258	1
89	H	78.19953	84.75513	69.49177	-2026.39012	-1590.33709	-887.82922	1
90	C	78.28084	83.37800	73.55396	-672.89153	382.57394	-156.34072	1
91	O	77.13886	83.30691	73.93192	410.04627	221.86223	500.35950	1
92	N	79.38468	82.90363	74.07742	-378.11782	-443.79414	-441.10984	1
93	H	80.27452	83.02995	73.55561	2404.15973	-568.14894	1149.30085	1
94	C	79.44832	82.33341	75.39576	-544.54484	466.16019	331.29119	1
95	H	79.98469	83.09332	76.00364	-1409.80988	-170.17955	2325.32679	1
96	C	78.00407	82.01098	75.93849	-184.48284	116.78282	-758.89137	1
97	H	77.40740	82.94520	76.07882	1893.78641	1861.14652	611.04528	1
98	H	77.44602	81.41481	75.17823	-2170.79665	-974.19311	1327.50117	1
99	C	78.14337	81.25549	77.30212	389.51668	672.81878	-138.49152	1
100	H	78.76386	80.34094	77.14808	510.64577	1933.03327	1851.02484	1
101	H	78.70670	81.87578	78.03740	-2302.30869	-1105.72939	-948.89774	1
102	C	76.74332	80.85010	77.92337	-559.93427	-126.34590	542.30857	1
103	O	76.54250	80.85267	79.11202	-670.36003	-111.83166	76.36448	1
104	N	75.87745	80.42869	76.96275	-216.06729	-537.07037	446.51379	1
105	H	76.22958	80.22063	76.02026	-1251.96487	1074.12894	-2168.52500	1
106	H	75.05946	79.78377	77.15802	-2451.83023	-720.73851	944.84612	1
107	C	80.32961	80.97175	75.21704	546.24052	-563.88337	-85.11809	1
108	O	79.98668	80.14724	74.41032	71.70702	-307.40463	606.69673	1
109	N	81.30387	80.90234	76.13232	479.90863	-504.50129	222.86849	1
110	C	82.48550	80.11390	75.90610	75.51268	-600.91904	506.73700	1
111	H	82.86762	80.44010	74.91210	-2033.61562	1795.30103	254.89480	1
112	C	83.42092	80.50100	77.12620	523.79067	517.99274	284.45581	1
113	H	84.05134	79.64870	77.46590	1599.61665	-1127.00911	1895.98173	1
114	H	84.12647	81.31490	76.84664	-1881.83093	1275.82488	-1501.55016	1
115	C	82.41681	80.98450	78.21878	-600.05639	-404.05026	316.64485	1
116	H	81.95117	80.12668	78.75357	-2597.05260	496.36221	657.73249	1
117	H	82.87865	81.63262	78.99700	-1666.24518	1294.38985	-1723.90591	1
118	C	81.35901	81.75210	77.31086	493.57570	-129.95376	-602.56394	1
119	H	80.33354	81.84940	77.74290	-1469.08415	-637.84797	2204.22581	1
120	H	81.71103	82.75072	76.95688	-1038.97840	1068.88701	-2280.71789	1
121	C	82.13910	78.52159	75.87656	188.88100	241.05089	-727.87821	1
122	O	82.79713	77.80174	75.16196	531.88613	-49.19943	427.07960	1

123	N	81.24655	78.20072	76.80280	708.14833	26.93417	-179.73509	1
124	H	80.81169	78.94554	77.38576	-2232.69501	-1179.09831	1023.94816	1
125	C	80.36849	77.08622	76.55438	-738.32412	259.92548	104.42456	1
126	H	80.22302	76.98646	75.45606	2028.89123	1260.02983	1311.33324	1
127	C	81.05920	75.80702	77.19905	-258.65678	-345.52513	661.28459	1
128	H	81.66559	76.11818	78.07677	-1826.06090	-1801.46097	-918.64554	1
129	C	79.99902	74.72693	77.60447	-541.23400	531.92970	-218.41428	1
130	H	80.48382	73.81803	78.03200	1311.73218	-2219.18200	882.19023	1
131	H	79.29195	75.11817	78.37296	-1048.71298	1223.58118	-2196.97971	1
132	H	79.39073	74.39796	76.72958	419.06414	1903.92898	1903.44670	1
133	C	81.95804	75.12726	76.11101	-423.86431	152.66566	-648.55262	1
134	H	82.62785	74.35094	76.55131	105.68386	-2342.50080	1387.51238	1
135	H	81.34439	74.62929	75.32356	-1695.63603	-1484.73621	-1531.02793	1
136	H	82.60884	75.89437	75.59219	-1853.57121	-487.39031	1936.59343	1
137	C	79.07225	77.57421	77.39299	539.71428	-510.58232	267.58633	1
138	O	79.22506	78.48794	78.19881	-15.93758	-278.34085	-624.49402	1
139	N	77.95788	76.95203	77.02333	-676.81886	12.05292	276.17960	1
140	H	78.12509	76.24152	76.30698	-1694.44250	-373.84189	-2100.66098	1
141	C	76.92635	76.64273	77.98709	412.33078	-664.70360	108.35451	1
142	H	77.05840	75.55705	78.19394	1765.77476	1294.44366	1621.76594	1
143	C	77.05112	77.55974	79.25893	-179.66635	-721.95667	-264.73915	1
144	H	78.01746	77.38290	79.78731	-607.34922	2587.87032	-598.10018	1
145	H	77.07235	78.63567	78.95178	-359.69332	-1479.13954	-2259.74260	1
146	C	75.84028	77.26467	80.21007	-240.01076	616.02425	431.85322	1
147	H	74.87396	77.34537	79.66282	-1359.17131	782.54425	2227.99181	1
148	H	75.88450	76.22702	80.61023	-820.36667	85.81767	-2596.78715	1
149	C	75.91864	78.33513	81.36968	-513.07015	236.18570	-551.87280	1
150	H	76.91485	78.31030	81.86854	1816.11944	-1183.11722	-1650.94321	1
151	H	75.81188	79.36775	80.95865	-1800.04429	-1361.53473	1526.34643	1
152	C	74.79190	78.01141	82.37967	726.08972	-253.19732	-179.64713	1
153	H	73.76120	78.12386	81.98151	1224.27271	-456.51798	-2390.90304	1
154	H	74.89621	77.03223	82.88798	1206.40339	-1150.93514	-2154.90344	1
155	N	74.87112	79.06400	83.53196	329.70796	-633.68968	-155.67358	1
156	H	74.10874	78.97695	84.26440	1348.31305	1938.76845	1359.00643	1
157	H	75.74730	79.08505	84.13149	2096.92035	1446.54551	-966.48890	1
158	H	74.76872	80.08026	83.24693	-1197.07217	-2303.53719	827.28733	1
159	C	75.50739	76.95290	77.25596	-378.01186	-556.17301	-413.96481	1
160	O	75.05947	78.08892	77.11351	-409.44433	-307.55053	-453.30833	1
161	N	74.95342	75.81351	76.92473	-429.02477	524.70884	274.08502	1
162	H	75.38260	74.90120	77.09528	1706.34263	-1425.96036	1574.38926	1
163	C	73.64003	75.84975	76.35905	-45.25864	-626.22952	478.93267	1
164	H	73.11758	76.73949	76.78156	1988.63164	570.90773	1772.87287	1
165	C	73.85865	75.95781	74.79093	551.77128	-20.49526	-564.54996	1
166	H	74.60936	76.75170	74.57257	1434.61535	-1753.10253	1513.99471	1
167	H	74.29479	75.00752	74.40535	-714.67738	1819.09770	1898.36494	1
168	C	72.50857	76.25623	74.06108	446.99263	-555.77305	338.97221	1
169	H	71.79439	75.40294	74.16737	1953.68466	1892.25957	-161.67766	1
170	H	72.00621	77.15208	74.49071	-403.03785	2688.07032	-188.43591	1
171	C	72.91357	76.49307	72.55432	567.86262	335.74681	434.04421	1
172	H	73.77161	77.20119	72.48534	-1080.02275	1568.26081	-1948.78900	1
173	H	73.27605	75.54234	72.10074	-919.54108	2111.34692	1456.13463	1
174	C	71.72315	77.05537	71.72541	195.81897	173.33862	-745.11536	1
175	H	70.86695	76.35582	71.61696	1405.67949	-2301.21089	-390.08113	1
176	H	71.35955	78.05418	72.04808	-940.37328	-1118.32446	2299.72133	1
177	N	72.28606	77.25295	70.31883	319.26422	656.36007	-42.02424	1
178	H	71.58438	77.46341	69.56423	1961.03633	619.91968	1787.09422	1
179	H	73.12886	78.08203	70.17588	854.14343	-2156.80752	1429.08711	1
180	H	72.73669	76.38568	69.92870	1237.02905	-1378.50857	-1998.28500	1
181	C	73.05675	74.37980	76.76504	532.53319	-268.57236	517.55729	1
182	O	73.81971	73.42046	76.87753	266.16714	-290.73804	-558.88002	1
183	N	71.75215	74.45266	76.93327	-226.25352	640.49678	-270.32839	1
184	H	71.36816	75.38512	76.77545	2007.69063	-1035.27229	1523.50231	1

185	C	70.88279	73.33225	76.85550	-540.76542	-573.33303	49.50000	1
186	H	69.88536	73.79322	76.68191	-2374.20950	-1036.76023	843.75774	1
187	C	71.36265	72.44577	75.61358	-77.09082	666.87422	-415.84136	1
188	H	72.36866	71.99387	75.84688	-985.81834	617.19825	2463.91927	1
189	O	71.52586	73.14271	74.36408	293.29899	-391.65602	-477.80926	1
190	H	72.48972	73.01676	74.20387	2528.72714	-681.76262	-751.27122	1
191	C	70.26573	71.32136	75.63843	252.47363	-605.14473	440.05134	1
192	H	70.47507	70.54299	74.87030	-2052.65063	1456.49051	-1043.51830	1
193	H	70.21564	70.80906	76.63118	-2152.98800	-1661.97574	-161.70652	1
194	H	69.25155	71.73341	75.42689	-473.12726	-1584.27339	2165.61725	1
195	C	70.90362	72.48454	78.26172	360.36307	488.46713	505.10056	1
196	O	69.88488	71.93169	78.59479	-200.08817	-528.03552	-385.82850	1
197	N	72.10499	72.46479	78.81290	-597.54095	-226.44775	355.20479	1
198	H	72.88079	72.95291	78.31863	2179.23655	-1300.70981	-991.33835	1
199	C	72.37283	71.85276	80.05694	-687.68921	297.39807	-249.45179	1
200	H	73.36506	72.26206	80.34913	-349.16256	-2467.37713	-1101.72831	1
201	C	71.22226	72.16640	81.12505	672.47345	361.54328	-201.62880	1
202	H	70.21680	71.92346	80.69563	1541.41502	582.18425	2169.97026	1
203	H	71.36597	71.51679	82.02019	-2534.67717	60.25153	997.72295	1
204	C	71.31401	73.64858	81.51390	574.26774	-389.43119	-377.02542	1
205	C	72.37319	74.08370	82.36589	688.82679	-287.33580	-257.96133	1
206	H	73.12193	73.36581	82.74709	331.14182	1470.38163	2269.80013	1
207	C	70.35223	74.57963	81.01929	-383.52382	-675.04808	144.24917	1
208	H	69.53743	74.24341	80.35226	4.09847	1517.59662	2262.86397	1
209	C	72.43854	75.43331	82.71154	-134.76730	428.45285	-649.50303	1
210	H	73.25055	75.76597	83.38041	-903.23433	1600.49020	2011.53387	1
211	C	70.45947	75.92073	81.39751	-335.53281	-615.00040	-364.39058	1
212	H	69.70477	76.63162	81.01820	1596.45398	-1369.33862	1732.02659	1
213	C	71.49718	76.39852	82.24971	585.48547	-340.24194	-406.23938	1
214	O	71.61645	77.76252	82.63275	-419.15649	-173.04408	-511.94141	1
215	H	70.80818	78.12517	82.19956	-1071.84350	1559.71507	-1960.13012	1
216	C	72.40104	70.22172	79.94112	291.41878	-183.13091	710.72246	1
217	O	72.52236	69.55823	80.95132	379.87695	523.47396	-222.23622	1
218	N	72.27639	69.82269	78.69149	564.30591	373.09380	277.24371	1
219	H	72.21982	70.55169	77.98321	-120.59931	-2436.07824	-1214.35098	1
220	C	72.40380	68.44919	78.28363	404.07514	-299.37480	608.84009	1
221	H	73.48729	68.26440	78.45181	-1071.07882	-841.69025	2359.66467	1
222	C	71.51681	67.54564	79.22646	-683.12807	68.71770	-390.13096	1
223	H	71.66781	67.85489	80.29751	2068.88918	1596.58590	770.89603	1
224	H	70.43382	67.70938	79.02012	1379.86429	2342.49779	-179.85638	1
225	C	71.90272	66.04377	79.04351	-176.39967	537.49466	550.97268	1
226	H	71.78639	65.71143	77.98816	-396.28051	1942.22168	1869.33314	1
227	H	72.97055	65.86437	79.29776	-94.44700	586.00678	-2659.20016	1
228	C	70.92683	65.23507	80.02156	-291.69381	-718.18079	-150.72929	1
229	H	71.01628	65.47293	81.11116	-2303.38776	1089.76242	964.62032	1
230	H	69.85165	65.30146	79.71219	884.16729	2568.80533	-207.74283	1
231	N	71.34407	63.91825	79.80339	-594.49522	-252.81478	342.29276	1
232	H	71.64485	63.70092	78.86455	-1735.17426	2084.05705	-263.71605	1
233	C	71.32950	62.98059	80.66399	595.23177	-271.52487	442.22352	1
234	N	70.88239	63.26270	81.95741	585.53813	-424.79750	-105.81303	1
235	H	70.51956	64.13199	82.34646	959.88797	1327.56823	-2177.11905	1
236	H	70.80942	62.57865	82.71153	1578.48647	16.27378	-2220.76233	1
237	N	71.79011	61.78508	80.09609	-452.17763	-390.33541	-421.51853	1
238	H	72.07474	61.57110	79.14137	470.26107	1974.25629	-1817.92087	1
239	H	71.82207	60.89933	80.60205	1856.67307	-1573.97321	-1224.35416	1
240	C	72.01170	68.51287	76.70698	-531.47271	-581.45780	-55.06206	1
241	O	72.59345	69.28603	75.97814	-243.00837	192.73507	609.52485	1
242	N	71.09572	67.60315	76.41880	343.49288	-644.25607	38.09164	1
243	H	70.62809	67.06017	77.17098	-1691.16043	-1535.97525	-1484.73099	1
244	C	70.36070	67.61906	75.18227	542.66492	350.14337	454.42563	1
245	H	69.99778	68.66481	75.09784	1209.57979	-2396.95920	463.86744	1
246	C	71.35435	67.29314	73.98887	-737.14309	145.93010	242.71942	1

247	H	72.24777	66.77254	74.39510	-1050.18303	159.36419	-2509.06125	1
248	C	70.75783	66.47822	72.78664	-706.77696	-252.88343	-245.16230	1
249	H	71.50565	66.35638	71.96760	-1624.64039	-1665.49085	1417.86935	1
250	H	70.44981	65.45126	73.10189	2566.10521	598.51109	693.22305	1
251	H	69.86869	66.98656	72.34118	-1972.69758	107.10018	-1876.34312	1
252	C	71.74873	68.65417	73.31803	412.85148	672.58832	-27.69222	1
253	H	72.44557	68.50583	72.45969	1447.02277	1762.76533	-1490.78944	1
254	H	70.85608	69.19710	72.92623	1320.77379	-145.20455	2378.68491	1
255	H	72.26653	69.33740	74.05922	-1512.10848	1470.52031	1724.75147	1
256	C	69.19147	66.58597	75.60377	-607.11113	499.56689	73.73769	1
257	O	68.94431	66.44342	76.79809	357.97126	460.81534	356.68785	1
258	N	68.54608	66.05400	74.56885	536.55407	-368.62270	332.76306	1
259	H	68.89442	66.25423	73.63035	524.38866	2297.69985	1367.20941	1
260	C	67.83937	64.83340	74.81300	46.50277	-774.29190	-147.97904	1
261	H	67.10097	65.11264	75.59498	1676.51875	1883.29066	1032.55549	1
262	C	67.20667	64.29742	73.43904	-559.41456	-34.19198	-556.30433	1
263	H	68.03429	63.87306	72.81976	-64.66664	395.18769	2695.05373	1
264	H	66.51826	63.44181	73.64317	-2703.44278	-60.40056	333.79418	1
265	C	66.50017	65.38486	72.66304	-519.76435	377.31045	459.42366	1
266	H	67.14128	66.29398	72.65625	-1746.74323	1667.50644	-1261.73691	1
267	C	66.29521	64.93749	71.22144	570.95554	16.46261	-545.27700	1
268	H	65.79770	65.73115	70.60667	2391.58273	28.05277	-1305.07271	1
269	H	67.26868	64.69185	70.72287	175.75588	917.63458	2559.43867	1
270	H	65.65361	64.02068	71.16257	-1063.97851	-2155.34650	1283.00462	1
271	C	65.16529	65.74397	73.29814	193.76014	2.62946	-765.53141	1
272	H	64.63739	66.54760	72.72167	507.39394	-846.55087	2539.60089	1
273	H	64.47734	64.86015	73.34078	1337.57841	1818.19054	1526.01994	1
274	H	65.29543	66.11691	74.34719	1100.88635	-1172.91350	-2199.08909	1
275	C	68.88339	63.72134	75.33104	-549.21115	475.64486	-309.38218	1
276	O	70.02805	63.65530	74.96586	556.06106	-390.37755	-78.24250	1
277	O	68.31859	62.68566	76.11587	-572.27940	-310.19032	-209.75862	1
278	H	67.39595	63.04836	76.21122	-1380.08193	2212.14486	790.85944	1

Listing 58: C00058.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.6480	0.0000	300.0000
3	H	74.65997	81.04377	73.22073	-2043.14101	-1757.64893	399.89339		1
4	N	74.74850	81.53136	72.33032	426.75047	490.45733	-334.42467		1
5	H	73.77435	81.78300	72.16680	442.25559	-1110.30854	-2448.52907		1
6	C	75.58823	82.67195	72.42155	415.32972	-666.39213	83.73172		1
7	H	75.19848	83.24987	73.28718	879.32219	2491.00447	667.35213		1
8	C	77.10207	82.17923	72.67998	31.35357	477.41777	628.23362		1
9	H	77.36797	81.40843	71.92053	1168.38489	2240.25337	-1019.71136		1
10	H	77.80926	83.02867	72.52084	-360.43770	2534.90498	931.67112		1
11	C	77.27797	81.60214	74.06006	463.18208	512.70242	-382.34388		1
12	H	76.40469	80.95371	74.29364	1725.29117	1863.52247	-987.07854		1
13	C	78.53449	80.73999	74.10510	710.42801	-144.27427	-313.15367		1
14	H	78.69892	80.30234	75.12377	364.20195	-1033.13725	2494.72524		1
15	H	78.47739	79.88691	73.38040	2567.61904	335.80679	847.48802		1
16	H	79.44971	81.33258	73.84702	-2587.99029	680.92867	-512.16411		1
17	C	77.37785	82.69395	75.11627	268.17616	741.64379	-40.42634		1
18	H	77.52085	82.26335	76.14200	1283.54314	-1945.37420	-1411.27812		1
19	H	78.24529	83.37619	74.92056	-1258.57796	1317.15249	-2026.02085		1
20	H	76.45676	83.33093	75.14652	-2502.84526	909.80597	575.92391		1
21	C	75.51182	83.52692	71.05056	619.36578	-458.64843	-172.09273		1
22	O	75.90072	84.70183	71.09586	-81.40433	433.87611	522.34594		1
23	N	75.09274	82.83297	70.02403	175.23996	-622.20190	341.55523		1
24	H	74.77158	81.89417	70.25767	-876.57256	-303.22879	-2561.90213		1
25	C	75.09280	83.25959	68.66036	-571.88214	-534.10783	-106.15033		1
26	H	74.02949	83.09631	68.37775	-2713.20841	-16.25800	-248.80809		1

27	C	75.53459	84.78678	68.51340	166.60354	288.16399	-716.09568	1
28	H	76.55228	84.90691	68.98694	-2097.85574	1636.78449	-586.18044	1
29	O	74.68064	85.72009	69.17408	-317.80580	-363.38227	484.43082	1
30	H	75.15105	85.73902	70.09464	1863.74748	-1451.84923	1357.29467	1
31	C	75.68625	84.96217	66.95685	503.80731	517.99032	318.51606	1
32	H	75.76636	86.03852	66.67468	640.61020	-2157.10410	-1536.29104	1
33	H	76.60019	84.45191	66.56807	1687.88455	465.60692	2087.56452	1
34	H	74.81338	84.53288	66.40856	-1293.07895	-1899.88581	-1463.57452	1
35	C	76.00860	82.32826	67.68649	-153.07550	-733.68902	248.70981	1
36	O	75.66920	82.36817	66.52776	186.15459	-480.78787	-449.34387	1
37	N	77.07069	81.70230	68.21003	-487.53139	543.18517	42.03850	1
38	C	78.00836	80.99217	67.38709	-699.35871	69.34393	360.10701	1
39	H	78.07950	81.54750	66.42301	2.81126	-221.99807	-2715.58072	1
40	C	79.32256	81.01683	68.28850	-507.46439	-592.59194	122.07761	1
41	H	80.05163	80.22526	68.00481	-1975.08116	525.87560	-1801.71556	1
42	H	79.85650	81.98939	68.20598	1588.27743	-1913.22100	1113.83566	1
43	C	78.72670	80.82088	69.71561	-613.62442	-457.55993	-194.14490	1
44	H	78.48640	79.75066	69.90559	1707.54637	-721.27992	1996.92523	1
45	H	79.40993	81.14055	70.53483	758.23357	2100.81767	1560.55011	1
46	C	77.40403	81.69973	69.62641	-352.41524	704.96076	49.21465	1
47	H	76.52729	81.27241	70.16622	1714.76886	-2070.42778	443.35792	1
48	H	77.52647	82.77164	69.91266	1224.15040	1801.50881	1636.97633	1
49	C	77.56034	79.44627	67.17268	566.85117	537.05831	117.62814	1
50	O	78.36468	78.65588	66.69176	-550.26779	-406.08867	4.21666	1
51	N	76.35871	79.23653	67.62702	566.34832	-425.77725	180.18749	1
52	H	75.80771	80.02156	68.03494	644.44502	2646.80550	-52.73430	1
53	C	75.56691	78.08300	67.29508	612.34801	-281.48662	411.56221	1
54	H	75.51845	78.05198	66.18350	1667.23498	-1490.75142	1556.16753	1
55	C	76.37115	76.80619	67.82601	-714.45746	-175.43074	286.98927	1
56	H	77.02596	77.19797	68.65452	-787.09484	1763.03619	-1922.46060	1
57	O	77.28763	76.27428	66.86113	-429.46514	516.51932	-128.40526	1
58	H	77.88960	77.10024	66.71234	1981.82785	436.16847	-1818.18182	1
59	C	75.35761	75.77337	68.42367	630.79189	-468.94448	76.03230	1
60	H	75.89140	74.95458	68.96223	-1775.71861	2062.30353	131.89849	1
61	H	74.65762	76.25168	69.14866	-1855.14608	88.94118	1993.53760	1
62	H	74.74351	75.29011	67.62727	-1504.82350	-780.94249	-2132.90992	1
63	C	74.17764	78.52382	67.97772	288.57638	618.62814	-397.00270	1
64	O	74.09061	79.66949	68.46991	321.70495	-185.26452	574.37218	1
65	N	73.25970	77.59699	67.90987	-447.05792	-446.53431	367.76425	1
66	H	73.51046	76.72287	67.45333	350.31316	1975.63644	-1843.31522	1
67	C	71.93477	77.75619	68.41982	-511.23061	374.03917	-471.51480	1
68	H	71.61956	78.73778	68.00012	2234.79579	-898.70890	-1273.45190	1
69	C	71.12755	76.48233	67.88445	529.53781	-159.34528	563.72604	1
70	H	70.04731	76.66344	68.12468	654.59388	2347.94251	1217.51488	1
71	H	71.21249	76.45000	66.76570	-1526.55661	2103.42026	817.87394	1
72	O	71.57072	75.19657	68.40541	-554.84278	14.12789	399.58769	1
73	H	71.22482	75.28068	69.31887	1297.06236	2061.84854	1220.68812	1
74	C	71.84834	77.74248	70.03570	-662.15484	-412.13544	123.62687	1
75	O	70.95154	77.15753	70.58398	-540.01537	-317.05804	274.91456	1
76	N	72.82413	78.47460	70.58742	-202.76299	-690.00100	-131.49145	1
77	H	73.43255	79.04094	69.95178	-702.62132	-2617.37191	281.70413	1
78	C	72.92417	78.68341	72.02948	-491.73914	576.34187	222.73509	1
79	H	73.77891	79.39469	72.11059	1977.17978	-1823.58850	-434.68928	1
80	C	71.61649	79.28273	72.51594	-649.50797	-328.66843	306.11224	1
81	H	70.84210	78.48156	72.44404	2075.07803	1452.16490	-1004.45904	1
82	C	71.72510	79.73459	73.96026	-615.18735	-489.99689	-70.96352	1
83	H	70.73966	80.10003	74.35962	-1226.32661	-1724.38906	-1716.47170	1
84	H	72.07242	78.89018	74.62532	2381.64273	-969.84735	900.46860	1
85	H	72.46323	80.57533	74.07576	2122.74991	1702.23946	-141.36228	1
86	C	71.15442	80.43832	71.64603	-501.86074	-479.61276	-376.42482	1
87	H	70.17735	80.86517	72.00144	993.79261	-2246.95401	-1177.81305	1
88	H	71.90077	81.27773	71.63597	42.71279	-626.15391	-2651.37258	1

89	H	71.01122	80.11498	70.57872	-2026.39012	-1590.33709	-887.82922	1
90	C	73.25240	77.23438	72.77835	-672.89153	382.57394	-156.34072	1
91	O	73.16448	77.14079	73.98829	410.04627	221.86223	500.35950	1
92	N	73.65146	76.32702	71.91545	-378.11782	-443.79414	-441.10984	1
93	H	73.68101	76.65851	70.95564	2404.15973	-568.14894	1149.30085	1
94	C	74.00600	75.00880	72.32936	-544.54484	466.16019	331.29119	1
95	H	73.34008	74.79389	73.19312	-1409.80988	-170.17955	2325.32679	1
96	C	73.78278	74.09173	71.06325	-184.48284	116.78282	-758.89137	1
97	H	72.70829	74.08805	70.76877	1893.78641	1861.14652	611.04528	1
98	H	74.33427	74.49059	70.18521	-2170.79665	-974.19311	1327.50117	1
99	C	74.27338	72.64855	71.41581	389.51668	672.81878	-138.49152	1
100	H	75.35840	72.67642	71.67051	510.64577	1933.03327	1851.02484	1
101	H	73.77707	72.29520	72.37012	-2302.30869	-1105.72939	-948.89774	1
102	C	74.03398	71.62933	70.25616	-559.93427	-126.34590	542.30857	1
103	O	74.25963	70.44477	70.43479	-670.36003	-111.83166	76.36448	1
104	N	73.56436	72.19003	69.13317	-216.06729	-537.07037	446.51379	1
105	H	73.32695	73.17013	68.93082	-1251.96487	1074.12894	-2168.52500	1
106	H	73.33217	71.66721	68.27974	-2451.83023	-720.73851	944.84612	1
107	C	75.59272	75.07179	72.74041	546.24052	-563.88337	-85.11809	1
108	O	76.41266	75.23951	71.87731	71.70702	-307.40463	606.69673	1
109	N	75.76328	74.89076	74.05815	479.90863	-504.50129	222.86849	1
110	C	76.94327	75.38216	74.71091	75.51268	-600.91904	506.73700	1
111	H	77.19440	76.33230	74.18660	-2033.61562	1795.30103	254.89480	1
112	C	76.48781	75.54579	76.21904	523.79067	517.99274	284.45581	1
113	H	77.32535	75.37249	76.93209	1599.61665	-1127.00911	1895.98173	1
114	H	76.11217	76.57480	76.41531	-1881.83093	1275.82488	-1501.55016	1
115	C	75.34075	74.49622	76.36581	-600.05639	-404.05026	316.64485	1
116	H	75.74434	73.46790	76.50866	-2597.05260	496.36221	657.73249	1
117	H	74.65423	74.69179	77.22063	-1666.24518	1294.38985	-1723.90591	1
118	C	74.63778	74.65810	74.95256	493.57570	-129.95376	-602.56394	1
119	H	74.05228	73.74202	74.60260	-1469.08415	-637.84797	2204.22581	1
120	H	73.99791	75.59057	74.83943	-1038.97840	1068.88701	-2280.71789	1
121	C	78.21729	74.35827	74.68283	188.88100	241.05089	-727.87821	1
122	O	79.32925	74.80123	74.85218	531.88613	-49.19943	427.07960	1
123	N	77.85838	73.06685	74.64221	708.14833	26.93417	-179.73509	1
124	H	76.86181	72.95780	74.45610	-2232.69501	-1179.09831	1023.94816	1
125	C	78.87450	72.04446	74.39301	-738.32412	259.92548	104.42456	1
126	H	79.76318	72.62154	74.04176	2028.89123	1260.02983	1311.33324	1
127	C	79.11034	71.29883	75.69377	-258.65678	-345.52513	661.28459	1
128	H	78.11814	71.01839	76.11331	-1826.06090	-1801.46097	-918.64554	1
129	C	79.90142	70.02277	75.47410	-541.23400	531.92970	-218.41428	1
130	H	80.04907	69.45349	76.43339	1311.73218	-2219.18200	882.19023	1
131	H	79.37780	69.33334	74.75413	-1048.71298	1223.58118	-2196.97971	1
132	H	80.92156	70.23398	75.04929	419.06414	1903.92898	1903.44670	1
133	C	79.80093	72.17160	76.72573	-423.86431	152.66566	-648.55262	1
134	H	79.89323	71.65158	77.71956	105.68386	-2342.50080	1387.51238	1
135	H	80.83910	72.45669	76.39855	-1695.63603	-1484.73621	-1531.02793	1
136	H	79.23487	73.12985	76.89747	-1853.57121	-487.39031	1936.59343	1
137	C	78.22973	71.01914	73.24996	539.71428	-510.58232	267.58633	1
138	O	78.85092	70.75753	72.24756	-15.93758	-278.34085	-624.49402	1
139	N	77.09311	70.51429	73.68597	-676.81886	12.05292	276.17960	1
140	H	76.76546	70.86504	74.58313	-1694.44250	-373.84189	-2100.66098	1
141	C	76.18871	69.84119	72.79223	412.33078	-664.70360	108.35451	1
142	H	75.93874	70.56103	71.97989	1765.77476	1294.44366	1621.76594	1
143	C	76.94845	68.57625	72.23352	-179.66635	-721.95667	-264.73915	1
144	H	77.92335	68.87787	71.77497	-607.34922	2587.87032	-598.10018	1
145	H	77.20237	67.86760	73.05442	-359.69332	-1479.13954	-2259.74260	1
146	C	76.00304	67.91560	71.17437	-240.01076	616.02425	431.85322	1
147	H	75.06380	67.55496	71.65120	-1359.17131	782.54425	2227.99181	1
148	H	75.68726	68.66097	70.40610	-820.36667	85.81767	-2596.78715	1
149	C	76.80697	66.72330	70.51732	-513.07015	236.18570	-551.87280	1
150	H	77.75399	67.09108	70.05915	1816.11944	-1183.11722	-1650.94321	1

151	H	77.11365	65.97997	71.28887	-1800.04429	-1361.53473	1526.34643	1
152	C	75.90432	66.06454	69.44853	726.08972	-253.19732	-179.64713	1
153	H	74.99371	65.57647	69.84950	1224.27271	-456.51798	-2390.90304	1
154	H	75.63702	66.72503	68.59963	1206.40339	-1150.93514	-2154.90344	1
155	N	76.72783	64.90083	68.80002	329.70796	-633.68968	-155.67358	1
156	H	76.22900	64.35223	68.04160	1348.31305	1938.76845	1359.00643	1
157	H	77.62888	65.16661	68.30583	2096.92035	1446.54551	-966.48890	1
158	H	77.05227	64.12068	69.44255	-1197.07217	-2303.53719	827.28733	1
159	C	74.93417	69.42455	73.74199	-378.01186	-556.17301	-413.96481	1
160	O	75.09334	68.89299	74.81573	-409.44433	-307.55053	-453.30833	1
161	N	73.80552	69.66295	73.07323	-429.02477	524.70884	274.08502	1
162	H	73.84585	70.07363	72.11337	1706.34263	-1425.96036	1574.38926	1
163	C	72.60385	69.76866	73.84612	-45.25864	-626.22952	478.93267	1
164	H	71.83313	69.83664	73.04603	1988.63164	570.90773	1772.87287	1
165	C	72.50552	68.45209	74.71825	551.77128	-20.49526	-564.54996	1
166	H	72.94302	67.59685	74.15492	1434.61535	-1753.10253	1513.99471	1
167	H	73.14269	68.54734	75.63366	-714.67738	1819.09770	1898.36494	1
168	C	71.02108	68.14100	75.10541	446.99263	-555.77305	338.97221	1
169	H	70.52599	69.01160	75.59033	1953.68466	1892.25957	-161.67766	1
170	H	70.41099	67.90594	74.20485	-403.03785	2688.07032	-188.43591	1
171	C	71.09529	66.90500	76.08974	567.86262	335.74681	434.04421	1
172	H	71.58242	66.03596	75.59041	-1080.02275	1568.26081	-1948.78900	1
173	H	71.73531	67.14158	76.97102	-919.54108	2111.34692	1456.13463	1
174	C	69.66368	66.53840	76.54288	195.81897	173.33862	-745.11536	1
175	H	69.17276	67.29677	77.18459	1405.67949	-2301.21089	-390.08113	1
176	H	68.98187	66.23630	75.72318	-940.37328	-1118.32446	2299.72133	1
177	N	69.78488	65.26223	77.44464	319.26422	656.36007	-42.02424	1
178	H	68.87606	64.89253	77.84736	1961.03633	619.91968	1787.09422	1
179	H	70.17874	64.38869	76.98770	854.14343	-2156.80752	1429.08711	1
180	H	70.38433	65.34068	78.31706	1237.02905	-1378.50857	-1998.28500	1
181	C	72.70055	71.15182	74.70468	532.53319	-268.57236	517.55729	1
182	O	73.09163	72.18886	74.18350	266.16714	-290.73804	-558.88002	1
183	N	72.24595	70.96381	75.92367	-226.25352	640.49678	-270.32839	1
184	H	72.00331	70.01354	76.19298	2007.69063	-1035.27229	1523.50231	1
185	C	72.03325	72.03364	76.82617	-540.76542	-573.33303	49.50000	1
186	H	72.24512	72.96757	76.25705	-2374.20950	-1036.76023	843.75774	1
187	C	70.49073	71.85706	77.23031	-77.09082	666.87422	-415.84136	1
188	H	70.34338	70.80311	77.59318	-985.81834	617.19825	2463.91927	1
189	O	69.57309	72.01306	76.12633	293.29899	-391.65602	-477.80926	1
190	H	69.17355	71.12345	76.08922	2528.72714	-681.76262	-751.27122	1
191	C	70.22903	72.82908	78.43399	252.47363	-605.14473	440.05134	1
192	H	69.16742	72.77385	78.77032	-2052.65063	1456.49051	-1043.51830	1
193	H	70.86299	72.57761	79.31604	-2152.98800	-1661.97574	-161.70652	1
194	H	70.42845	73.89045	78.15597	-473.12726	-1584.27339	2165.61725	1
195	C	73.06995	71.77186	78.06132	360.36307	488.46713	505.10056	1
196	O	73.74809	70.76506	78.11813	-200.08817	-528.03552	-385.82850	1
197	N	73.06681	72.81343	78.89111	-597.54095	-226.44775	355.20479	1
198	H	72.42416	73.55261	78.60844	2179.23655	-1300.70981	-991.33835	1
199	C	73.36777	72.64552	80.27661	-687.68921	297.39807	-249.45179	1
200	H	72.55974	73.22875	80.77026	-349.16256	-2467.37713	-1101.72831	1
201	C	73.48129	71.13145	80.77277	672.47345	361.54328	-201.62880	1
202	H	74.13456	70.52948	80.08048	1541.41502	582.18425	2169.97026	1
203	H	73.97920	71.11504	81.78511	-2534.67717	60.25153	997.72295	1
204	C	72.06760	70.53257	80.87003	574.26774	-389.43119	-377.02542	1
205	C	71.27151	70.87017	82.00411	688.82679	-287.33580	-257.96133	1
206	H	71.66837	71.53794	82.79079	331.14182	1470.38163	2269.80013	1
207	C	71.55495	69.65271	79.87013	-383.52382	-675.04808	144.24917	1
208	H	72.17036	69.37952	78.99211	4.09847	1517.59662	2262.86397	1
209	C	69.99198	70.32474	82.11115	-134.76730	428.45285	-649.50303	1
210	H	69.38195	70.57908	82.99547	-903.23433	1600.49020	2011.53387	1
211	C	70.26726	69.13082	80.01912	-335.53281	-615.00040	-364.39058	1
212	H	69.88676	68.44618	79.24082	1596.45398	-1369.33862	1732.02659	1

213	C	69.44033	69.44309	81.13734	585.48547	-340.24194	-406.23938	1
214	O	68.13040	68.92069	81.30180	-419.15649	-173.04408	-511.94141	1
215	H	68.08321	68.33652	80.50902	-1071.84350	1559.71507	-1960.13012	1
216	C	74.83207	73.26128	80.59304	291.41878	-183.13091	710.72246	1
217	O	75.65096	72.60748	81.22267	379.87695	523.47396	-222.23622	1
218	N	74.88492	74.58236	80.29091	564.30591	373.09380	277.24371	1
219	H	74.02051	74.76058	79.76514	-120.59931	-2436.07824	-1214.35098	1
220	C	76.10221	75.04020	79.63977	404.07514	-299.37480	608.84009	1
221	H	76.13005	74.51094	78.66437	-1071.07882	-841.69025	2359.66467	1
222	C	75.86025	76.58784	79.50604	-683.12807	68.71770	-390.13096	1
223	H	75.01350	76.79453	78.81293	2068.88918	1596.58590	770.89603	1
224	H	75.53884	76.99218	80.49260	1379.86429	2342.49779	-179.85638	1
225	C	77.15319	77.32628	79.03032	-176.39967	537.49466	550.97268	1
226	H	78.03224	77.04021	79.65027	-396.28051	1942.22168	1869.33314	1
227	H	77.42502	77.06162	77.98647	-94.44700	586.00678	-2659.20016	1
228	C	76.81713	78.88110	79.17539	-291.69381	-718.18079	-150.72929	1
229	H	75.92248	79.23330	78.60409	-2303.38776	1089.76242	964.62032	1
230	H	76.71481	79.25381	80.22657	884.16729	2568.80533	-207.74283	1
231	N	77.92626	79.51345	78.59948	-594.49522	-252.81478	342.29276	1
232	H	78.65115	78.91597	78.23366	-1735.17426	2084.05705	-263.71605	1
233	C	78.06874	80.77328	78.50924	595.23177	-271.52487	442.22352	1
234	N	77.04954	81.58347	79.02275	585.53813	-424.79750	-105.81303	1
235	H	76.18879	81.31443	79.49776	959.88797	1327.56823	-2177.11905	1
236	H	77.06097	82.60376	79.03173	1578.48647	16.27378	-2220.76233	1
237	N	79.27585	81.10473	77.87771	-452.17763	-390.33541	-421.51853	1
238	H	80.02896	80.51442	77.52778	470.26107	1974.25629	-1817.92087	1
239	H	79.58651	82.06698	77.73802	1856.67307	-1573.97321	-1224.35416	1
240	C	77.43736	74.75571	80.51088	-531.47271	-581.45780	-55.06206	1
241	O	78.48608	74.56307	79.94223	-243.00837	192.73507	609.52485	1
242	N	77.27878	75.00881	81.86179	343.49288	-644.25607	38.09164	1
243	H	76.24956	74.98863	81.92544	-1691.16043	-1535.97525	-1484.73099	1
244	C	78.05500	74.13551	82.78297	542.66492	350.14337	454.42563	1
245	H	78.12175	73.18585	82.20261	1209.57979	-2396.95920	463.86744	1
246	C	79.38611	74.76008	83.11206	-737.14309	145.93010	242.71942	1
247	H	79.18322	75.72362	83.63428	-1050.18303	159.36419	-2509.06125	1
248	C	80.18681	73.87944	84.05772	-706.77696	-252.88343	-245.16230	1
249	H	81.17160	74.34781	84.33005	-1624.64039	-1665.49085	1417.86935	1
250	H	79.62508	73.69905	85.01752	2566.10521	598.51109	693.22305	1
251	H	80.40786	72.87496	83.60456	-1972.69758	107.10018	-1876.34312	1
252	C	80.22496	75.07878	81.88503	412.85148	672.58832	-27.69222	1
253	H	81.25677	75.43085	82.16103	1447.02277	1762.76533	-1490.78944	1
254	H	80.34204	74.17716	81.21990	1320.77379	-145.20455	2378.68491	1
255	H	79.74978	75.88882	81.26302	-1512.10848	1470.52031	1724.75147	1
256	C	77.17210	74.00867	84.16295	-607.11113	499.56689	73.73769	1
257	O	77.52208	74.58219	85.16822	357.97126	460.81534	356.68785	1
258	N	76.09937	73.24532	83.98635	536.55407	-368.62270	332.76306	1
259	H	75.90350	72.81910	83.06392	524.38866	2297.69985	1367.20941	1
260	C	75.48049	72.78601	85.18590	46.50277	-774.29190	-147.97904	1
261	H	76.29443	72.81651	85.94569	1676.51875	1883.29066	1032.55549	1
262	C	74.25142	73.75365	85.59407	-559.41456	-34.19198	-556.30433	1
263	H	73.54081	73.81356	84.73613	-64.66664	395.18769	2695.05373	1
264	H	73.67638	73.30227	86.43794	-2703.44278	-60.40056	333.79418	1
265	C	74.73829	75.12618	85.96864	-519.76435	377.31045	459.42366	1
266	H	75.42275	75.48640	85.16374	-1746.74323	1667.50644	-1261.73691	1
267	C	73.55641	76.08144	86.08988	570.95554	16.46261	-545.27700	1
268	H	73.88891	77.12474	86.32636	2391.58273	28.05277	-1305.07271	1
269	H	72.96088	76.12800	85.14224	175.75588	917.63458	2559.43867	1
270	H	72.85599	75.76532	86.90544	-1063.97851	-2155.34650	1283.00462	1
271	C	75.51277	75.11951	87.27967	193.76014	2.62946	-765.53141	1
272	H	75.78597	76.15799	87.60079	507.39394	-846.55087	2539.60089	1
273	H	74.92134	74.65823	88.11219	1337.57841	1818.19054	1526.01994	1
274	H	76.47181	74.54377	87.18522	1100.88635	-1172.91350	-2199.08909	1

275	C	74.83189	71.33892	84.91460	-549.21115	475.64486	-309.38218	1
276	O	74.42528	70.98382	83.83629	556.06106	-390.37755	-78.24250	1
277	O	74.59818	70.55200	86.06626	-572.27940	-310.19032	-209.75862	1
278	H	75.00540	71.15421	86.75012	-1380.08193	2212.14486	790.85944	1

Listing 59: C00059.xmolout

1		276						
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	1.5102
		0.2500	300.00	0.00	0.00	0.00	-1293.6332	0.0000
3	H	73.97867	76.67287	82.18158	-2043.14101	-1757.64893	399.89339	1
4	N	74.98291	76.60699	82.33795	426.75047	490.45733	-334.42467	1
5	H	75.18724	75.64694	82.06382	442.25559	-1110.30854	-2448.52907	1
6	C	75.76083	77.54555	81.62857	415.32972	-666.39213	83.73172	1
7	H	75.14980	78.46710	81.51134	879.32219	2491.00447	667.35213	1
8	C	77.13634	77.77437	82.43997	31.35357	477.41777	628.23362	1
9	H	77.71833	76.81865	82.45082	1168.38489	2240.25337	-1019.71136	1
10	H	77.78355	78.51737	81.91474	-360.43770	2534.90498	931.67112	1
11	C	76.82609	78.21652	83.84716	463.18208	512.70242	-382.34388	1
12	H	75.99579	77.58306	84.23422	1725.29117	1863.52247	-987.07854	1
13	C	78.04549	78.01106	84.73699	710.42801	-144.27427	-313.15367	1
14	H	77.83689	78.29666	85.80026	364.20195	-1033.13725	2494.72524	1
15	H	78.37932	76.94083	84.73763	2567.61904	335.80679	847.48802	1
16	H	78.91512	78.62734	84.39093	-2587.99029	680.92867	-512.16411	1
17	C	76.39050	79.67413	83.89072	268.17616	741.64379	-40.42634	1
18	H	76.14979	80.00192	84.93517	1283.54314	-1945.37420	-1411.27812	1
19	H	77.19323	80.35554	83.50688	-1258.57796	1317.15249	-2026.02085	1
20	H	75.47648	79.85274	83.26757	-2502.84526	909.80597	575.92391	1
21	C	76.19044	76.81845	80.23516	619.36578	-458.64843	-172.09273	1
22	O	76.58242	75.67783	80.19115	-81.40433	433.87611	522.34594	1
23	N	76.21610	77.76127	79.27347	175.23996	-622.20190	341.55523	1
24	H	75.75001	78.63052	79.54021	-876.57256	-303.22879	-2561.90213	1
25	C	76.08493	77.29120	77.89560	-571.88214	-534.10783	-106.15033	1
26	H	75.36663	76.44222	77.96666	-2713.20841	-16.25800	-248.80809	1
27	C	75.51177	78.48520	77.07862	166.60354	288.16399	-716.09568	1
28	H	76.05526	79.43135	77.28984	-2097.85574	1636.78449	-586.18044	1
29	O	74.01451	78.84478	77.57482	-317.80580	-363.38227	484.43082	1
30	H	74.16202	79.76824	77.75088	1863.74748	-1451.84923	1357.29467	1
31	C	75.55667	78.13378	75.57596	503.80731	517.99032	318.51606	1
32	H	75.16637	78.97021	74.94332	640.61020	-2157.10410	-1536.29104	1
33	H	76.60335	77.91449	75.24018	1687.88455	465.60692	2087.56452	1
34	H	74.94138	77.22832	75.35323	-1293.07895	-1899.88581	-1463.57452	1
35	C	77.49945	76.77463	77.27872	-153.07550	-733.68902	248.70981	1
36	O	77.37654	76.05032	76.31403	186.15459	-480.78787	-449.34387	1
37	N	78.61545	77.33995	77.74801	-487.53139	543.18517	42.03850	1
38	C	79.89762	76.81981	77.38033	-699.35871	69.34393	360.10701	1
39	H	79.70455	76.31996	76.40307	2.81126	-221.99807	-2715.58072	1
40	C	80.76034	78.14501	77.32018	-507.46439	-592.59194	122.07761	1
41	H	81.85610	77.95844	77.38445	-1975.08116	525.87560	-1801.71556	1
42	H	80.59344	78.68555	76.36196	1588.27743	-1913.22100	1113.83566	1
43	C	80.18979	78.96621	78.52220	-613.62442	-457.55993	-194.14490	1
44	H	80.59883	78.61474	79.49526	1707.54637	-721.27992	1996.92523	1
45	H	80.41566	80.05468	78.46337	758.23357	2100.81767	1560.55011	1
46	C	78.64198	78.64285	78.40782	-352.41524	704.96076	49.21465	1
47	H	78.11719	78.52981	79.38447	1714.76886	-2070.42778	443.35792	1
48	H	78.06197	79.33330	77.75251	1224.15040	1801.50881	1636.97633	1
49	C	80.36746	75.72169	78.51570	566.85117	537.05831	117.62814	1
50	O	79.81506	74.64780	78.51816	-550.26779	-406.08867	4.21666	1
51	N	81.33510	76.16829	79.29567	566.34832	-425.77725	180.18749	1
52	H	81.69206	77.10478	79.12435	644.44502	2646.80550	-52.73430	1
53	C	81.85566	75.41289	80.38341	612.34801	-281.48662	411.56221	1
54	H	82.43844	76.18264	80.93658	1667.23498	-1490.75142	1556.16753	1

55	C	80.63997	74.83241	81.24215	-714.45746	-175.43074	286.98927	1
56	H	80.06431	74.08838	80.61765	-787.09484	1763.03619	-1922.46060	1
57	O	79.65434	75.78601	81.68548	-429.46514	516.51932	-128.40526	1
58	H	78.89171	75.54434	81.11233	1981.82785	436.16847	-1818.18182	1
59	C	81.44021	74.08813	82.37261	630.79189	-468.94448	76.03230	1
60	H	80.76007	73.52142	83.04921	-1775.71861	2062.30353	131.89849	1
61	H	82.17444	73.35922	81.95571	-1855.14608	88.94118	1993.53760	1
62	H	82.01338	74.80513	83.00517	-1504.82350	-780.94249	-2132.90992	1
63	C	82.86685	74.30884	79.71306	288.57638	618.62814	-397.00270	1
64	O	83.95003	74.69143	79.34654	321.70495	-185.26452	574.37218	1
65	N	82.38331	73.07606	79.70358	-447.05792	-446.53431	367.76425	1
66	H	81.41642	72.79358	79.95361	350.31316	1975.63644	-1843.31522	1
67	C	83.12025	72.07893	78.96493	-511.23061	374.03917	-471.51480	1
68	H	83.29800	72.52517	77.95992	2234.79579	-898.70890	-1273.45190	1
69	C	84.49632	71.76948	79.72078	529.53781	-159.34528	563.72604	1
70	H	85.11849	71.13947	79.02899	654.59388	2347.94251	1217.51488	1
71	H	85.03683	72.74538	79.84371	-1526.55661	2103.42026	817.87394	1
72	O	84.39071	71.04583	80.98530	-554.84278	14.12789	399.58769	1
73	H	84.30534	71.80623	81.58822	1297.06236	2061.84854	1220.68812	1
74	C	82.06082	70.87157	79.00037	-662.15484	-412.13544	123.62687	1
75	O	80.94420	71.07464	79.48349	-540.01537	-317.05804	274.91456	1
76	N	82.52395	69.77867	78.40942	-202.76299	-690.00100	-131.49145	1
77	H	83.49186	69.87043	78.09385	-702.62132	-2617.37191	281.70413	1
78	C	81.94466	68.45194	78.56693	-491.73914	576.34187	222.73509	1
79	H	82.77534	67.75743	78.29441	1977.17978	-1823.58850	-434.68928	1
80	C	81.45951	68.25882	79.99770	-649.50797	-328.66843	306.11224	1
81	H	80.72470	69.07309	80.21453	2075.07803	1452.16490	-1004.45904	1
82	C	80.75813	66.92269	80.15236	-615.18735	-489.99689	-70.96352	1
83	H	80.24784	66.82851	81.15054	-1226.32661	-1724.38906	-1716.47170	1
84	H	79.97744	66.77701	79.35043	2381.64273	-969.84735	900.46860	1
85	H	81.48019	66.06457	80.06548	2122.74991	1702.23946	-141.36228	1
86	C	82.58928	68.37937	81.00134	-501.86074	-479.61276	-376.42482	1
87	H	82.21623	68.30821	82.06014	993.79261	-2246.95401	-1177.81305	1
88	H	83.35290	67.56501	80.86383	42.71279	-626.15391	-2651.37258	1
89	H	83.13662	69.36751	80.90131	-2026.39012	-1590.33709	-887.82922	1
90	C	80.66567	68.30664	77.51332	-672.89153	382.57394	-156.34072	1
91	O	80.34764	67.20700	77.13446	410.04627	221.86223	500.35950	1
92	N	80.08250	69.46222	77.25031	-378.11782	-443.79414	-441.10984	1
93	H	80.40194	70.31130	77.73314	2404.15973	-568.14894	1149.30085	1
94	C	79.11615	69.47157	76.19587	-544.54484	466.16019	331.29119	1
95	H	79.34441	68.56377	75.58899	-1409.80988	-170.17955	2325.32679	1
96	C	77.70694	69.38213	76.93427	-184.48284	116.78282	-758.89137	1
97	H	77.71149	68.53683	77.65881	1893.78641	1861.14652	611.04528	1
98	H	77.52662	70.30017	77.53823	-2170.79665	-974.19311	1327.50117	1
99	C	76.59623	69.18345	75.85974	389.51668	672.81878	-138.49152	1
100	H	76.46325	70.12677	75.27872	510.64577	1933.03327	1851.02484	1
101	H	76.91424	68.42774	75.10866	-2302.30869	-1105.72939	-948.89774	1
102	C	75.21721	68.72875	76.48347	-559.93427	-126.34590	542.30857	1
103	O	74.38823	68.18668	75.79667	-670.36003	-111.83166	76.36448	1
104	N	75.09657	69.04023	77.78960	-216.06729	-537.07037	446.51379	1
105	H	75.74843	69.56619	78.38344	-1251.96487	1074.12894	-2168.52500	1
106	H	74.24751	68.89096	78.34520	-2451.83023	-720.73851	944.84612	1
107	C	79.18291	70.90349	75.43337	546.24052	-563.88337	-85.11809	1
108	O	79.05585	71.92606	76.08959	71.70702	-307.40463	606.69673	1
109	N	79.31350	70.77479	74.11606	479.90863	-504.50129	222.86849	1
110	C	79.50069	71.92386	73.26776	75.51268	-600.91904	506.73700	1
111	H	80.17920	72.59613	73.84202	-2033.61562	1795.30103	254.89480	1
112	C	80.10981	71.28715	71.95048	523.79067	517.99274	284.45581	1
113	H	79.92754	71.91327	71.04792	1599.61665	-1127.00911	1895.98173	1
114	H	81.21211	71.15554	72.03141	-1881.83093	1275.82488	-1501.55016	1
115	C	79.37548	69.91026	71.90041	-600.05639	-404.05026	316.64485	1
116	H	78.33416	70.03120	71.52668	-2597.05260	496.36221	657.73249	1

117	H	79.86952	69.16543	71.23667	-1666.24518	1294.38985	-1723.90591	1
118	C	79.39361	69.49105	73.43288	493.57570	-129.95376	-602.56394	1
119	H	78.53657	68.85810	73.76090	-1469.08415	-637.84797	2204.22581	1
120	H	80.34892	69.02514	73.77378	-1038.97840	1068.88701	-2280.71789	1
121	C	78.05520	72.61987	72.98052	188.88100	241.05089	-727.87821	1
122	O	77.61527	72.70680	71.84617	531.88613	-49.19943	427.07960	1
123	N	77.58511	73.10469	74.10726	708.14833	26.93417	-179.73509	1
124	H	78.12886	72.95844	74.99023	-2232.69501	-1179.09831	1023.94816	1
125	C	76.22049	73.49491	74.21583	-738.32412	259.92548	104.42456	1
126	H	76.16067	73.85905	75.26711	2028.89123	1260.02983	1311.33324	1
127	C	75.87144	74.61573	73.13691	-258.65678	-345.52513	661.28459	1
128	H	75.91997	74.21772	72.09965	-1826.06090	-1801.46097	-918.64554	1
129	C	74.43482	75.15459	73.45266	-541.23400	531.92970	-218.41428	1
130	H	74.15979	76.02527	72.80368	1311.73218	-2219.18200	882.19023	1
131	H	73.65572	74.36939	73.29708	-1048.71298	1223.58118	-2196.97971	1
132	H	74.34786	75.49079	74.51210	419.06414	1903.92898	1903.44670	1
133	C	76.90956	75.77603	73.28928	-423.86431	152.66566	-648.55262	1
134	H	76.56698	76.71372	72.78998	105.68386	-2342.50080	1387.51238	1
135	H	77.09698	76.00454	74.38059	-1695.63603	-1484.73621	-1531.02793	1
136	H	77.89262	75.49461	72.84167	-1853.57121	-487.39031	1936.59343	1
137	C	75.29136	72.17217	73.96849	539.71428	-510.58232	267.58633	1
138	O	74.78159	71.63613	74.94059	-15.93758	-278.34085	-624.49402	1
139	N	75.25040	71.86012	72.69926	-676.81886	12.05292	276.17960	1
140	H	75.86892	72.37508	72.03457	-1694.44250	-373.84189	-2100.66098	1
141	C	74.51608	70.75665	72.18834	412.33078	-664.70360	108.35451	1
142	H	74.77550	70.77654	71.10529	1765.77476	1294.44366	1621.76594	1
143	C	75.03378	69.44853	72.92702	-179.66635	-721.95667	-264.73915	1
144	H	76.14592	69.40205	72.93339	-607.34922	2587.87032	-598.10018	1
145	H	74.72235	69.44274	73.99927	-359.69332	-1479.13954	-2259.74260	1
146	C	74.40776	68.24815	72.14708	-240.01076	616.02425	431.85322	1
147	H	73.29896	68.34599	72.11716	-1359.17131	782.54425	2227.99181	1
148	H	74.74355	68.25133	71.08583	-820.36667	85.81767	-2596.78715	1
149	C	74.82202	66.89760	72.85852	-513.07015	236.18570	-551.87280	1
150	H	75.92898	66.76958	72.87153	1816.11944	-1183.11722	-1650.94321	1
151	H	74.50028	66.89424	73.92882	-1800.04429	-1361.53473	1526.34643	1
152	C	74.13440	65.76851	72.05541	726.08972	-253.19732	-179.64713	1
153	H	73.02922	65.75424	72.13750	1224.27271	-456.51798	-2390.90304	1
154	H	74.43294	65.71477	70.98934	1206.40339	-1150.93514	-2154.90344	1
155	N	74.59192	64.39678	72.65390	329.70796	-633.68968	-155.67358	1
156	H	74.17049	63.53700	72.19674	1348.31305	1938.76845	1359.00643	1
157	H	75.62777	64.16894	72.61101	2096.92035	1446.54551	-966.48890	1
158	H	74.36960	64.21985	73.67644	-1197.07217	-2303.53719	827.28733	1
159	C	72.90463	70.90232	72.43291	-378.01186	-556.17301	-413.96481	1
160	O	72.16108	70.94993	71.46639	-409.44433	-307.55053	-453.30833	1
161	N	72.58376	70.88076	73.70619	-429.02477	524.70884	274.08502	1
162	H	73.30339	70.90060	74.47024	1706.34263	-1425.96036	1574.38926	1
163	C	71.18586	70.80772	73.99392	-45.25864	-626.22952	478.93267	1
164	H	70.79544	70.20455	73.14055	1988.63164	570.90773	1772.87287	1
165	C	71.01927	70.16996	75.42947	551.77128	-20.49526	-564.54996	1
166	H	71.49598	69.16469	75.48633	1434.61535	-1753.10253	1513.99471	1
167	H	71.53964	70.79266	76.19213	-714.67738	1819.09770	1898.36494	1
168	C	69.48302	70.09848	75.72289	446.99263	-555.77305	338.97221	1
169	H	69.01926	71.09573	75.53962	1953.68466	1892.25957	-161.67766	1
170	H	68.97257	69.38850	75.03424	-403.03785	2688.07032	-188.43591	1
171	C	69.28296	69.67557	77.23269	567.86262	335.74681	434.04421	1
172	H	69.64968	68.63864	77.41178	-1080.02275	1568.26081	-1948.78900	1
173	H	69.88095	70.33045	77.90719	-919.54108	2111.34692	1456.13463	1
174	C	67.77430	69.80177	77.55222	195.81897	173.33862	-745.11536	1
175	H	67.35374	70.81436	77.38951	1405.67949	-2301.21089	-390.08113	1
176	H	67.13007	69.04281	77.06443	-940.37328	-1118.32446	2299.72133	1
177	N	67.59871	69.55706	79.08767	319.26422	656.36007	-42.02424	1
178	H	66.60651	69.63145	79.45585	1961.03633	619.91968	1787.09422	1

179	H	67.89472	68.61183	79.46943	854.14343	-2156.80752	1429.08711	1
180	H	68.11005	70.22596	79.73302	1237.02905	-1378.50857	-1998.28500	1
181	C	70.56790	72.34117	73.97288	532.53319	-268.57236	517.55729	1
182	O	70.30159	72.90951	74.99976	266.16714	-290.73804	-558.88002	1
183	N	70.43623	72.69331	72.70833	-226.25352	640.49678	-270.32839	1
184	H	70.79913	72.03816	71.98209	2007.69063	-1035.27229	1523.50231	1
185	C	69.66331	73.80355	72.27881	-540.76542	-573.33303	49.50000	1
186	H	69.32226	73.50095	71.26434	-2374.20950	-1036.76023	843.75774	1
187	C	68.46175	74.07180	73.29692	-77.09082	666.87422	-415.84136	1
188	H	68.90104	74.32625	74.30663	-985.81834	617.19825	2463.91927	1
189	O	67.55839	72.96574	73.49569	293.29899	-391.65602	-477.80926	1
190	H	67.78691	72.71660	74.41523	2528.72714	-681.76262	-751.27122	1
191	C	67.81501	75.37251	72.69325	252.47363	-605.14473	440.05134	1
192	H	66.99159	75.75392	73.34059	-2052.65063	1456.49051	-1043.51830	1
193	H	68.56083	76.19468	72.58408	-2152.98800	-1661.97574	-161.70652	1
194	H	67.38036	75.18077	71.68522	-473.12726	-1584.27339	2165.61725	1
195	C	70.63798	75.11930	72.22530	360.36307	488.46713	505.10056	1
196	O	71.19325	75.55919	73.20063	-200.08817	-528.03552	-385.82850	1
197	N	70.53182	75.67886	70.99521	-597.54095	-226.44775	355.20479	1
198	H	70.03501	75.05598	70.35424	2179.23655	-1300.70981	-991.33835	1
199	C	71.78506	76.20625	70.49346	-687.68921	297.39807	-249.45179	1
200	H	72.53114	75.39914	70.65211	-349.16256	-2467.37713	-1101.72831	1
201	C	71.55437	76.58195	68.96905	672.47345	361.54328	-201.62880	1
202	H	70.68662	77.27498	68.87916	1541.41502	582.18425	2169.97026	1
203	H	72.44832	77.13059	68.59206	-2534.67717	60.25153	997.72295	1
204	C	71.31208	75.32882	68.10921	574.26774	-389.43119	-377.02542	1
205	C	72.43246	74.55613	67.68213	688.82679	-287.33580	-257.96133	1
206	H	73.45622	74.82597	67.99885	331.14182	1470.38163	2269.80013	1
207	C	69.99117	74.96408	67.70992	-383.52382	-675.04808	144.24917	1
208	H	69.11825	75.55141	68.04795	4.09847	1517.59662	2262.86397	1
209	C	72.21134	73.46320	66.84316	-134.76730	428.45285	-649.50303	1
210	H	73.08012	72.87252	66.50428	-903.23433	1600.49020	2011.53387	1
211	C	69.82071	73.86072	66.86827	-335.53281	-615.00040	-364.39058	1
212	H	68.79570	73.59487	66.55583	1596.45398	-1369.33862	1732.02659	1
213	C	70.91426	73.07669	66.39769	585.48547	-340.24194	-406.23938	1
214	O	70.75457	71.96180	65.53283	-419.15649	-173.04408	-511.94141	1
215	H	69.77532	71.97618	65.42100	-1071.84350	1559.71507	-1960.13012	1
216	C	72.15293	77.57175	71.29208	291.41878	-183.13091	710.72246	1
217	O	73.29070	77.79011	71.63874	379.87695	523.47396	-222.23622	1
218	N	71.08962	78.40216	71.29951	564.30591	373.09380	277.24371	1
219	H	70.25016	77.91330	70.97980	-120.59931	-2436.07824	-1214.35098	1
220	C	70.96316	79.38047	72.34023	404.07514	-299.37480	608.84009	1
221	H	69.86780	79.57854	72.33212	-1071.07882	-841.69025	2359.66467	1
222	C	71.47559	78.74622	73.69388	-683.12807	68.71770	-390.13096	1
223	H	71.02639	77.73730	73.85815	2068.88918	1596.58590	770.89603	1
224	H	72.58062	78.58496	73.66139	1379.86429	2342.49779	-179.85638	1
225	C	71.05454	79.76135	74.80251	-176.39967	537.49466	550.97268	1
226	H	71.64128	80.70539	74.71444	-396.28051	1942.22168	1869.33314	1
227	H	69.99233	80.06211	74.66234	-94.44700	586.00678	-2659.20016	1
228	C	71.26053	79.09523	76.23933	-291.69381	-718.18079	-150.72929	1
229	H	70.64029	78.17602	76.40249	-2303.38776	1089.76242	964.62032	1
230	H	72.32777	78.89866	76.57025	884.16729	2568.80533	-207.74283	1
231	N	70.73215	80.13402	77.01906	-594.49522	-252.81478	342.29276	1
232	H	70.01542	80.70181	76.59162	-1735.17426	2084.05705	-263.71605	1
233	C	71.05664	80.39860	78.22465	595.23177	-271.52487	442.22352	1
234	N	72.02325	79.61166	78.84277	585.53813	-424.79750	-105.81303	1
235	H	72.55722	78.80789	78.41445	959.88797	1327.56823	-2177.11905	1
236	H	72.34307	79.75735	79.80677	1578.48647	16.27378	-2220.76233	1
237	N	70.32273	81.49198	78.71396	-452.17763	-390.33541	-421.51853	1
238	H	69.62946	82.08073	78.25597	470.26107	1974.25629	-1817.92087	1
239	H	70.43700	81.87295	79.65301	1856.67307	-1573.97321	-1224.35416	1
240	C	71.83741	80.70770	71.97733	-531.47271	-581.45780	-55.06206	1

241	O	72.66855	81.15956	72.72775	-243.00837	192.73507	609.52485	1
242	N	71.37940	81.25960	70.83553	343.49288	-644.25607	38.09164	1
243	H	70.72973	80.63886	70.35155	-1691.16043	-1535.97525	-1484.73099	1
244	C	72.21709	82.24900	70.14569	542.66492	350.14337	454.42563	1
245	H	73.16966	82.24445	70.73013	1209.57979	-2396.95920	463.86744	1
246	C	72.36563	81.81138	68.69935	-737.14309	145.93010	242.71942	1
247	H	71.34748	81.77427	68.25056	-1050.18303	159.36419	-2509.06125	1
248	C	73.19442	82.80004	67.90076	-706.77696	-252.88343	-245.16230	1
249	H	73.25411	82.51547	66.81426	-1624.64039	-1665.49085	1417.86935	1
250	H	72.76109	83.83941	67.95468	2566.10521	598.51109	693.22305	1
251	H	74.24834	82.86325	68.28863	-1972.69758	107.10018	-1876.34312	1
252	C	72.96246	80.41933	68.59699	412.85148	672.58832	-27.69222	1
253	H	72.99370	80.05367	67.53412	1447.02277	1762.76533	-1490.78944	1
254	H	74.01534	80.39415	68.99121	1320.77379	-145.20455	2378.68491	1
255	H	72.37287	79.67059	69.19563	-1512.10848	1470.52031	1724.75147	1
256	C	71.45183	83.71396	70.20613	-607.11113	499.56689	73.73769	1
257	O	72.07217	84.72369	69.94679	357.97126	460.81534	356.68785	1
258	N	70.15460	83.59002	70.44196	536.55407	-368.62270	332.76306	1
259	H	69.82405	82.65442	70.67383	524.38866	2297.69985	1367.20941	1
260	C	69.43718	84.74838	70.85002	46.50277	-774.29190	-147.97904	1
261	H	70.22312	85.51713	71.03228	1676.51875	1883.29066	1032.55549	1
262	C	68.40393	85.19003	69.68961	-559.41456	-34.19198	-556.30433	1
263	H	67.62699	84.39810	69.57080	-64.66664	395.18769	2695.05373	1
264	H	67.85273	86.11072	69.99617	-2703.44278	-60.40056	333.79418	1
265	C	69.12146	85.41090	68.38547	-519.76435	377.31045	459.42366	1
266	H	69.65898	84.47191	68.12003	-1746.74323	1667.50644	-1261.73691	1
267	C	68.12217	85.73009	67.27978	570.95554	16.46261	-545.27700	1
268	H	68.62919	85.86181	66.28944	2391.58273	28.05277	-1305.07271	1
269	H	67.36329	84.91493	67.15881	175.75588	917.63458	2559.43867	1
270	H	67.56109	86.67611	67.49232	-1063.97851	-2155.34650	1283.00462	1
271	C	70.14463	86.53170	68.48708	193.76014	2.62946	-765.53141	1
272	H	70.54929	86.81545	67.48118	507.39394	-846.55087	2539.60089	1
273	H	69.70737	87.45785	68.94198	1337.57841	1818.19054	1526.01994	1
274	H	71.02865	86.21443	69.12436	1100.88635	-1172.91350	-2199.08909	1
275	C	68.57010	84.31987	72.13507	-549.21115	475.64486	-309.38218	1
276	O	68.44392	83.17896	72.49763	556.06106	-390.37755	-78.24250	1
277	O	67.88009	85.36605	72.79514	-572.27940	-310.19032	-209.75862	1
278	H	68.20149	86.13278	72.24582	-1380.08193	2212.14486	790.85944	1

Listing 60: C00060.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.6324	0.0000	300.0000
3	H	61.06076	70.95545	83.37899	-2043.14101	-1757.64893	399.89339		1
4	N	61.65840	70.74764	82.58071	426.75047	490.45733	-334.42467		1
5	H	60.99405	70.72897	81.80654	442.25559	-1110.30854	-2448.52907		1
6	C	62.69569	71.67690	82.35951	415.32972	-666.39213	83.73172		1
7	H	63.00447	72.08448	83.34614	879.32219	2491.00447	667.35213		1
8	C	63.87867	70.92111	81.56693	31.35357	477.41777	628.23362		1
9	H	63.48494	70.58175	80.57862	1168.38489	2240.25337	-1019.71136		1
10	H	64.70975	71.63204	81.34081	-360.43770	2534.90498	931.67112		1
11	C	64.37747	69.73906	82.35945	463.18208	512.70242	-382.34388		1
12	H	63.49555	69.14010	82.68130	1725.29117	1863.52247	-987.07854		1
13	C	65.26712	68.86235	81.48718	710.42801	-144.27427	-313.15367		1
14	H	65.63628	67.96228	82.04333	364.20195	-1033.13725	2494.72524		1
15	H	64.72222	68.49256	80.58020	2567.61904	335.80679	847.48802		1
16	H	66.16866	69.42182	81.12640	-2587.99029	680.92867	-512.16411		1
17	C	65.14601	70.17922	83.59711	268.17616	741.64379	-40.42634		1
18	H	65.54655	69.30167	84.16812	1283.54314	-1945.37420	-1411.27812		1
19	H	66.02016	70.82807	83.33034	-1258.57796	1317.15249	-2026.02085		1
20	H	64.49906	70.76502	84.29995	-2502.84526	909.80597	575.92391		1

21	C	62.09099	72.77975	81.31821	619.36578	-458.64843	-172.09273	1
22	O	61.39462	72.46521	80.37772	-81.40433	433.87611	522.34594	1
23	N	62.58402	73.97637	81.62648	175.23996	-622.20190	341.55523	1
24	H	63.19902	74.07683	82.43359	-876.57256	-303.22879	-2561.90213	1
25	C	62.29899	75.06668	80.76987	-571.88214	-534.10783	-106.15033	1
26	H	61.68675	74.65077	79.93602	-2713.20841	-16.25800	-248.80809	1
27	C	61.55564	76.20089	81.63572	166.60354	288.16399	-716.09568	1
28	H	62.18516	76.42224	82.54086	-2097.85574	1636.78449	-586.18044	1
29	O	60.24828	75.87393	82.12289	-317.80580	-363.38227	484.43082	1
30	H	60.38795	75.91244	83.09195	1863.74748	-1451.84923	1357.29467	1
31	C	61.65325	77.40282	80.62712	503.80731	517.99032	318.51606	1
32	H	61.29855	78.35581	81.08390	640.61020	-2157.10410	-1536.29104	1
33	H	62.71206	77.55748	80.29165	1687.88455	465.60692	2087.56452	1
34	H	61.03870	77.22221	79.71413	-1293.07895	-1899.88581	-1463.57452	1
35	C	63.74166	75.73009	80.34877	-153.07550	-733.68902	248.70981	1
36	O	64.39217	76.29392	81.18812	186.15459	-480.78787	-449.34387	1
37	N	64.01020	75.54346	79.04517	-487.53139	543.18517	42.03850	1
38	C	65.12884	76.17250	78.42322	-699.35871	69.34393	360.10701	1
39	H	65.85133	76.45287	79.22513	2.81126	-221.99807	-2715.58072	1
40	C	65.59376	75.02596	77.42007	-507.46439	-592.59194	122.07761	1
41	H	66.25260	75.40366	76.60671	-1975.08116	525.87560	-1801.71556	1
42	H	66.16093	74.22714	77.94698	1588.27743	-1913.22100	1113.83566	1
43	C	64.21655	74.50414	76.90838	-613.62442	-457.55993	-194.14490	1
44	H	63.79032	75.19366	76.14524	1707.54637	-721.27992	1996.92523	1
45	H	64.26967	73.49871	76.43419	758.23357	2100.81767	1560.55011	1
46	C	63.34908	74.52400	78.23917	-352.41524	704.96076	49.21465	1
47	H	62.28841	74.83603	78.09325	1714.76886	-2070.42778	443.35792	1
48	H	63.37893	73.58525	78.84240	1224.15040	1801.50881	1636.97633	1
49	C	64.64115	77.43643	77.49957	566.85117	537.05831	117.62814	1
50	O	63.50380	77.58443	77.12729	-550.26779	-406.08867	4.21666	1
51	N	65.73100	78.10898	77.12363	566.34832	-425.77725	180.18749	1
52	H	66.60065	77.86695	77.59573	644.44502	2646.80550	-52.73430	1
53	C	65.54158	79.42850	76.56044	612.34801	-281.48662	411.56221	1
54	H	64.53497	79.74635	76.92301	1667.23498	-1490.75142	1556.16753	1
55	C	66.72265	80.31125	77.05639	-714.45746	-175.43074	286.98927	1
56	H	67.68538	79.95757	76.62052	-787.09484	1763.03619	-1922.46060	1
57	O	67.03716	80.05767	78.60521	-429.46514	516.51932	-128.40526	1
58	H	67.08571	80.96305	78.89516	1981.82785	436.16847	-1818.18182	1
59	C	66.45378	81.79508	76.71698	630.79189	-468.94448	76.03230	1
60	H	67.30635	82.44871	77.02849	-1775.71861	2062.30353	131.89849	1
61	H	66.29966	81.94416	75.61500	-1855.14608	88.94118	1993.53760	1
62	H	65.53512	82.17073	77.23272	-1504.82350	-780.94249	-2132.90992	1
63	C	65.62292	79.37011	74.92212	288.57638	618.62814	-397.00270	1
64	O	65.51105	80.43651	74.27904	321.70495	-185.26452	574.37218	1
65	N	65.85838	78.16910	74.47503	-447.05792	-446.53431	367.76425	1
66	H	65.89239	77.53280	75.27334	350.31316	1975.63644	-1843.31522	1
67	C	65.93741	77.71794	73.13555	-511.23061	374.03917	-471.51480	1
68	H	65.81008	76.61711	73.23410	2234.79579	-898.70890	-1273.45190	1
69	C	64.78048	78.42543	72.29361	529.53781	-159.34528	563.72604	1
70	H	64.52835	77.78140	71.40769	654.59388	2347.94251	1217.51488	1
71	H	63.87591	78.43391	72.95784	-1526.55661	2103.42026	817.87394	1
72	O	65.05513	79.74658	71.79391	-554.84278	14.12789	399.58769	1
73	H	65.21544	80.21776	72.69625	1297.06236	2061.84854	1220.68812	1
74	C	67.38439	78.10166	72.48535	-662.15484	-412.13544	123.62687	1
75	O	67.93172	77.34687	71.72222	-540.01537	-317.05804	274.91456	1
76	N	67.76342	79.32442	72.85978	-202.76299	-690.00100	-131.49145	1
77	H	67.12951	79.85665	73.47556	-702.62132	-2617.37191	281.70413	1
78	C	69.05670	79.85433	72.44066	-491.73914	576.34187	222.73509	1
79	H	69.39782	79.11913	71.66798	1977.17978	-1823.58850	-434.68928	1
80	C	68.81423	81.25612	71.89590	-649.50797	-328.66843	306.11224	1
81	H	68.44442	81.88189	72.73904	2075.07803	1452.16490	-1004.45904	1
82	C	70.08247	81.89032	71.35787	-615.18735	-489.99689	-70.96352	1

83	H	69.90348	82.94063	70.99642	-1226.32661	-1724.38906	-1716.47170	1
84	H	70.88983	81.93808	72.14611	2381.64273	-969.84735	900.46860	1
85	H	70.50145	81.30696	70.49205	2122.74991	1702.23946	-141.36228	1
86	C	67.74252	81.26093	70.82188	-501.86074	-479.61276	-376.42482	1
87	H	67.45662	82.30657	70.52148	993.79261	-2246.95401	-1177.81305	1
88	H	68.08914	80.73063	69.89258	42.71279	-626.15391	-2651.37258	1
89	H	66.79963	80.73526	71.16871	-2026.39012	-1590.33709	-887.82922	1
90	C	70.05307	79.90423	73.76302	-672.89153	382.57394	-156.34072	1
91	O	71.14438	80.43127	73.66108	410.04627	221.86223	500.35950	1
92	N	69.51126	79.39308	74.86624	-378.11782	-443.79414	-441.10984	1
93	H	68.63402	78.90995	74.68150	2404.15973	-568.14894	1149.30085	1
94	C	70.44603	78.98352	75.87507	-544.54484	466.16019	331.29119	1
95	H	71.21990	79.78173	75.85155	-1409.80988	-170.17955	2325.32679	1
96	C	69.68980	78.82653	77.25668	-184.48284	116.78282	-758.89137	1
97	H	69.17708	79.77346	77.54440	1893.78641	1861.14652	611.04528	1
98	H	68.88952	78.05513	77.18464	-2170.79665	-974.19311	1327.50117	1
99	C	70.76207	78.43222	78.31932	389.51668	672.81878	-138.49152	1
100	H	71.32035	77.50835	78.00254	510.64577	1933.03327	1851.02484	1
101	H	71.55246	79.21408	78.35687	-2302.30869	-1105.72939	-948.89774	1
102	C	70.18029	78.21606	79.77174	-559.93427	-126.34590	542.30857	1
103	O	70.89135	77.74827	80.62791	-670.36003	-111.83166	76.36448	1
104	N	68.91101	78.62350	79.94316	-216.06729	-537.07037	446.51379	1
105	H	68.21403	79.08372	79.27919	-1251.96487	1074.12894	-2168.52500	1
106	H	68.46135	78.52658	80.86483	-2451.83023	-720.73851	944.84612	1
107	C	71.01221	77.50474	75.45701	546.24052	-563.88337	-85.11809	1
108	O	70.25084	76.58342	75.33354	71.70702	-307.40463	606.69673	1
109	N	72.35144	77.52907	75.35596	479.90863	-504.50129	222.86849	1
110	C	73.12822	76.33490	75.26423	75.51268	-600.91904	506.73700	1
111	H	72.46750	75.56171	74.80708	-2033.61562	1795.30103	254.89480	1
112	C	74.34325	76.84251	74.36749	523.79067	517.99274	284.45581	1
113	H	75.22982	76.17126	74.39886	1599.61665	-1127.00911	1895.98173	1
114	H	74.04869	76.92977	73.29769	-1881.83093	1275.82488	-1501.55016	1
115	C	74.60786	78.24236	75.00107	-600.05639	-404.05026	316.64485	1
116	H	75.19752	78.14701	75.94049	-2597.05260	496.36221	657.73249	1
117	H	75.18297	78.92707	74.33843	-1666.24518	1294.38985	-1723.90591	1
118	C	73.13462	78.75627	75.30021	493.57570	-129.95376	-602.56394	1
119	H	73.01872	79.27403	76.28171	-1469.08415	-637.84797	2204.22581	1
120	H	72.66405	79.38140	74.49000	-1038.97840	1068.88701	-2280.71789	1
121	C	73.60783	75.95747	76.78323	188.88100	241.05089	-727.87821	1
122	O	73.02086	76.38483	77.75348	531.88613	-49.19943	427.07960	1
123	N	74.63096	75.11688	76.74488	708.14833	26.93417	-179.73509	1
124	H	75.00928	74.80940	75.85057	-2232.69501	-1179.09831	1023.94816	1
125	C	75.20541	74.69515	77.97135	-738.32412	259.92548	104.42456	1
126	H	74.79664	75.36112	78.76688	2028.89123	1260.02983	1311.33324	1
127	C	74.78005	73.16688	78.14145	-258.65678	-345.52513	661.28459	1
128	H	75.08072	72.58330	77.24487	-1826.06090	-1801.46097	-918.64554	1
129	C	75.45359	72.59439	79.43281	-541.23400	531.92970	-218.41428	1
130	H	75.17404	71.52802	79.60384	1311.73218	-2219.18200	882.19023	1
131	H	76.56725	72.64062	79.36462	-1048.71298	1223.58118	-2196.97971	1
132	H	75.15251	73.16787	80.34083	419.06414	1903.92898	1903.44670	1
133	C	73.22723	73.11510	78.33769	-423.86431	152.66566	-648.55262	1
134	H	72.85868	72.07047	78.46735	105.68386	-2342.50080	1387.51238	1
135	H	72.90972	73.69780	79.23452	-1695.63603	-1484.73621	-1531.02793	1
136	H	72.69494	73.55304	77.46007	-1853.57121	-487.39031	1936.59343	1
137	C	76.83389	74.72168	77.76569	539.71428	-510.58232	267.58633	1
138	O	77.33549	74.22683	76.78765	-15.93758	-278.34085	-624.49402	1
139	N	77.42820	75.18621	78.88029	-676.81886	12.05292	276.17960	1
140	H	76.75153	75.58231	79.53559	-1694.44250	-373.84189	-2100.66098	1
141	C	78.68506	75.88752	78.69511	412.33078	-664.70360	108.35451	1
142	H	78.49712	76.66963	77.92844	1765.77476	1294.44366	1621.76594	1
143	C	79.03090	76.44995	80.12055	-179.66635	-721.95667	-264.73915	1
144	H	78.32553	77.25751	80.42075	-607.34922	2587.87032	-598.10018	1

145	H	78.89695	75.64043	80.87322	-359.69332	-1479.13954	-2259.74260	1
146	C	80.51200	76.96508	80.14255	-240.01076	616.02425	431.85322	1
147	H	81.18321	76.23926	79.63078	-1359.17131	782.54425	2227.99181	1
148	H	80.62033	77.92538	79.59120	-820.36667	85.81767	-2596.78715	1
149	C	80.92893	77.11321	81.66010	-513.07015	236.18570	-551.87280	1
150	H	80.34120	77.91786	82.15869	1816.11944	-1183.11722	-1650.94321	1
151	H	80.69815	76.17833	82.22100	-1800.04429	-1361.53473	1526.34643	1
152	C	82.44525	77.40994	81.72639	726.08972	-253.19732	-179.64713	1
153	H	83.08895	76.61866	81.29276	1224.27271	-456.51798	-2390.90304	1
154	H	82.74236	78.40063	81.32874	1206.40339	-1150.93514	-2154.90344	1
155	N	82.84588	77.44599	83.24038	329.70796	-633.68968	-155.67358	1
156	H	83.87049	77.63302	83.44121	1348.31305	1938.76845	1359.00643	1
157	H	82.37636	78.17845	83.84823	2096.92035	1446.54551	-966.48890	1
158	H	82.68338	76.55910	83.80067	-1197.07217	-2303.53719	827.28733	1
159	C	79.86049	74.84290	78.26819	-378.01186	-556.17301	-413.96481	1
160	O	80.06850	73.84221	78.91820	-409.44433	-307.55053	-453.30833	1
161	N	80.61455	75.41440	77.33392	-429.02477	524.70884	274.08502	1
162	H	80.25499	76.28952	76.95629	1706.34263	-1425.96036	1574.38926	1
163	C	81.52934	74.67318	76.49751	-45.25864	-626.22952	478.93267	1
164	H	82.52422	75.14739	76.64962	1988.63164	570.90773	1772.87287	1
165	C	81.48357	73.15672	76.91902	551.77128	-20.49526	-564.54996	1
166	H	81.82748	73.04439	77.97766	1434.61535	-1753.10253	1513.99471	1
167	H	80.42454	72.80257	76.91292	-714.67738	1819.09770	1898.36494	1
168	C	82.36741	72.26987	75.97709	446.99263	-555.77305	338.97221	1
169	H	82.00192	72.28793	74.92108	1953.68466	1892.25957	-161.67766	1
170	H	83.42252	72.62362	75.94907	-403.03785	2688.07032	-188.43591	1
171	C	82.25545	70.82069	76.59997	567.86262	335.74681	434.04421	1
172	H	82.60502	70.81030	77.65822	-1080.02275	1568.26081	-1948.78900	1
173	H	81.19146	70.48989	76.63048	-919.54108	2111.34692	1456.13463	1
174	C	83.09782	69.86010	75.72948	195.81897	173.33862	-745.11536	1
175	H	82.77682	69.82250	74.65369	1405.67949	-2301.21089	-390.08113	1
176	H	84.19339	70.01805	75.79354	-940.37328	-1118.32446	2299.72133	1
177	N	82.86771	68.41932	76.29424	319.26422	656.36007	-42.02424	1
178	H	83.40046	67.63087	75.82364	1961.03633	619.91968	1787.09422	1
179	H	83.12526	68.26709	77.31221	854.14343	-2156.80752	1429.08711	1
180	H	81.87408	68.04685	76.26576	1237.02905	-1378.50857	-1998.28500	1
181	C	81.00758	74.84868	74.97237	532.53319	-268.57236	517.55729	1
182	O	79.83076	74.66063	74.66841	266.16714	-290.73804	-558.88002	1
183	N	82.01105	75.12721	74.16510	-226.25352	640.49678	-270.32839	1
184	H	82.95465	75.21922	74.53444	2007.69063	-1035.27229	1523.50231	1
185	C	81.68279	75.50168	72.81794	-540.76542	-573.33303	49.50000	1
186	H	80.65399	75.91526	72.94509	-2374.20950	-1036.76023	843.75774	1
187	C	82.75876	76.55630	72.28349	-77.09082	666.87422	-415.84136	1
188	H	83.73684	76.02253	72.12636	-985.81834	617.19825	2463.91927	1
189	O	83.03830	77.66905	73.14591	293.29899	-391.65602	-477.80926	1
190	H	83.99139	77.52814	73.33494	2528.72714	-681.76262	-751.27122	1
191	C	82.10408	76.89863	70.89312	252.47363	-605.14473	440.05134	1
192	H	82.70789	77.64840	70.32064	-2052.65063	1456.49051	-1043.51830	1
193	H	82.00823	75.98478	70.25692	-2152.98800	-1661.97574	-161.70652	1
194	H	81.08361	77.32952	71.01928	-473.12726	-1584.27339	2165.61725	1
195	C	81.67715	74.13376	71.92759	360.36307	488.46713	505.10056	1
196	O	82.50081	73.89969	71.04864	-200.08817	-528.03552	-385.82850	1
197	N	80.65431	73.44634	72.35342	-597.54095	-226.44775	355.20479	1
198	H	80.06911	73.83212	73.13271	2179.23655	-1300.70981	-991.33835	1
199	C	80.33475	72.16889	71.83534	-687.68921	297.39807	-249.45179	1
200	H	79.47767	71.86373	72.47512	-349.16256	-2467.37713	-1101.72831	1
201	C	79.91529	72.36496	70.30009	672.47345	361.54328	-201.62880	1
202	H	80.67593	72.96903	69.75259	1541.41502	582.18425	2169.97026	1
203	H	79.82870	71.37853	69.78851	-2534.67717	60.25153	997.72295	1
204	C	78.55790	73.07974	70.33986	574.26774	-389.43119	-377.02542	1
205	C	77.41175	72.35699	70.79046	688.82679	-287.33580	-257.96133	1
206	H	77.48871	71.28810	71.06022	331.14182	1470.38163	2269.80013	1

207	C	78.45334	74.46231	70.00019	-383.52382	-675.04808	144.24917	1
208	H	79.34032	75.02643	69.65933	4.09847	1517.59662	2262.86397	1
209	C	76.19751	73.03245	70.90396	-134.76730	428.45285	-649.50303	1
210	H	75.31452	72.47472	71.26178	-903.23433	1600.49020	2011.53387	1
211	C	77.21165	75.09164	70.12168	-335.53281	-615.00040	-364.39058	1
212	H	77.14026	76.16037	69.85475	1596.45398	-1369.33862	1732.02659	1
213	C	76.04551	74.41255	70.58126	585.48547	-340.24194	-406.23938	1
214	O	74.78508	75.04944	70.72553	-419.15649	-173.04408	-511.94141	1
215	H	75.01186	75.94580	70.38221	-1071.84350	1559.71507	-1960.13012	1
216	C	81.63510	71.20186	72.06328	291.41878	-183.13091	710.72246	1
217	O	81.93037	70.81305	73.17682	379.87695	523.47396	-222.23622	1
218	N	82.21564	70.91693	70.90966	564.30591	373.09380	277.24371	1
219	H	81.84394	71.32346	70.05417	-120.59931	-2436.07824	-1214.35098	1
220	C	83.46022	70.21268	70.92534	404.07514	-299.37480	608.84009	1
221	H	83.81033	70.29592	71.98271	-1071.07882	-841.69025	2359.66467	1
222	C	83.09270	68.70888	70.53141	-683.12807	68.71770	-390.13096	1
223	H	82.26422	68.33797	71.17480	2068.88918	1596.58590	770.89603	1
224	H	82.70341	68.66563	69.49026	1379.86429	2342.49779	-179.85638	1
225	C	84.35393	67.81143	70.68475	-176.39967	537.49466	550.97268	1
226	H	85.17179	68.15804	70.00744	-396.28051	1942.22168	1869.33314	1
227	H	84.76875	67.86868	71.71619	-94.44700	586.00678	-2659.20016	1
228	C	83.89158	66.32235	70.32821	-291.69381	-718.18079	-150.72929	1
229	H	83.15464	65.85531	71.02969	-2303.38776	1089.76242	964.62032	1
230	H	83.50859	66.18402	69.28503	884.16729	2568.80533	-207.74283	1
231	N	85.10012	65.61878	70.43003	-594.49522	-252.81478	342.29276	1
232	H	85.93840	66.17044	70.52803	-1735.17426	2084.05705	-263.71605	1
233	C	85.20719	64.35217	70.38795	595.23177	-271.52487	442.22352	1
234	N	84.03561	63.60198	70.23941	585.53813	-424.79750	-105.81303	1
235	H	83.07237	63.91994	70.14154	959.88797	1327.56823	-2177.11905	1
236	H	83.99624	62.58397	70.18304	1578.48647	16.27378	-2220.76233	1
237	N	86.54853	63.96098	70.50412	-452.17763	-390.33541	-421.51853	1
238	H	87.39883	64.51367	70.60110	470.26107	1974.25629	-1817.92087	1
239	H	86.84984	62.98619	70.48343	1856.67307	-1573.97321	-1224.35416	1
240	C	84.43162	70.88546	69.82595	-531.47271	-581.45780	-55.06206	1
241	O	85.30581	70.22860	69.32735	-243.00837	192.73507	609.52485	1
242	N	84.17274	72.19298	69.63760	343.49288	-644.25607	38.09164	1
243	H	83.39272	72.66038	70.16052	-1691.16043	-1535.97525	-1484.73099	1
244	C	84.76813	72.81665	68.43414	542.66492	350.14337	454.42563	1
245	H	85.57381	72.09216	68.15714	1209.57979	-2396.95920	463.86744	1
246	C	83.70543	72.90792	67.34991	-737.14309	145.93010	242.71942	1
247	H	82.82790	73.44469	67.77223	-1050.18303	159.36419	-2509.06125	1
248	C	84.20379	73.68189	66.14438	-706.77696	-252.88343	-245.16230	1
249	H	83.42314	73.75019	65.33673	-1624.64039	-1665.49085	1417.86935	1
250	H	84.49941	74.73451	66.42047	2566.10521	598.51109	693.22305	1
251	H	85.11236	73.19680	65.69013	-1972.69758	107.10018	-1876.34312	1
252	C	83.24133	71.53052	66.91289	412.85148	672.58832	-27.69222	1
253	H	82.43176	71.58739	66.13377	1447.02277	1762.76533	-1490.78944	1
254	H	84.08782	70.93471	66.47048	1320.77379	-145.20455	2378.68491	1
255	H	82.83864	70.93477	67.77820	-1512.10848	1470.52031	1724.75147	1
256	C	85.38995	74.28822	68.81500	-607.11113	499.56689	73.73769	1
257	O	86.13319	74.80821	68.01618	357.97126	460.81534	356.68785	1
258	N	84.96734	74.78602	69.97189	536.55407	-368.62270	332.76306	1
259	H	84.26075	74.28874	70.54295	524.38866	2297.69985	1367.20941	1
260	C	85.88898	75.69966	70.57923	46.50277	-774.29190	-147.97904	1
261	H	86.85192	75.52986	70.04440	1676.51875	1883.29066	1032.55549	1
262	C	85.35291	77.20801	70.35018	-559.41456	-34.19198	-556.30433	1
263	H	84.23591	77.21683	70.40515	-64.66664	395.18769	2695.05373	1
264	H	85.70577	77.88369	71.16555	-2703.44278	-60.40056	333.79418	1
265	C	85.81719	77.71903	69.01466	-519.76435	377.31045	459.42366	1
266	H	85.64894	76.92188	68.25000	-1746.74323	1667.50644	-1261.73691	1
267	C	85.01898	78.95520	68.61792	570.95554	16.46261	-545.27700	1
268	H	85.35573	79.36686	67.63175	2391.58273	28.05277	-1305.07271	1

269	H	83.92467	78.73215	68.52866	175.75588	917.63458	2559.43867	1
270	H	85.12878	79.77471	69.37416	-1063.97851	-2155.34650	1283.00462	1
271	C	87.30128	78.06064	69.04524	193.76014	2.62946	-765.53141	1
272	H	87.64539	78.49121	68.06967	507.39394	-846.55087	2539.60089	1
273	H	87.53495	78.81354	69.84158	1337.57841	1818.19054	1526.01994	1
274	H	87.93140	77.15658	69.24683	1100.88635	-1172.91350	-2199.08909	1
275	C	85.95883	75.42369	72.15595	-549.21115	475.64486	-309.38218	1
276	O	85.36595	74.53626	72.71300	556.06106	-390.37755	-78.24250	1
277	O	86.76105	76.32433	72.90538	-572.27940	-310.19032	-209.75862	1
278	H	87.15810	76.83641	72.14972	-1380.08193	2212.14486	790.85944	1

Listing 61: C00061.xmolout

1		276								
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	1.1117	4447	
		0.2500	300.00	0.00	0.00	0.00	-1293.6252	0.0000	300.0000	
3	H	83.51876	65.34336	81.39617	-2043.14101	-1757.64893	399.89339			1
4	N	83.61168	65.30731	80.38272	426.75047	490.45733	-334.42467			1
5	H	82.63503	65.30755	80.09399	442.25559	-1110.30854	-2448.52907			1
6	C	84.35497	66.38232	79.84253	415.32972	-666.39213	83.73172			1
7	H	85.13301	66.53827	80.62064	879.32219	2491.00447	667.35213			1
8	C	84.98596	65.95044	78.42562	31.35357	477.41777	628.23362			1
9	H	84.18226	65.93996	77.65075	1168.38489	2240.25337	-1019.71136			1
10	H	85.73156	66.70733	78.08227	-360.43770	2534.90498	931.67112			1
11	C	85.62102	64.58846	78.53629	463.18208	512.70242	-382.34388			1
12	H	84.85691	63.88244	78.93364	1725.29117	1863.52247	-987.07854			1
13	C	86.07046	64.10177	77.16421	710.42801	-144.27427	-313.15367			1
14	H	86.51143	63.07287	77.21377	364.20195	-1033.13725	2494.72524			1
15	H	85.21803	64.06409	76.43794	2567.61904	335.80679	847.48802			1
16	H	86.85050	64.77521	76.72431	-2587.99029	680.92867	-512.16411			1
17	C	86.80926	64.59665	79.48815	268.17616	741.64379	-40.42634			1
18	H	87.29953	63.59050	79.54499	1283.54314	-1945.37420	-1411.27812			1
19	H	87.59254	65.33015	79.16591	-1258.57796	1317.15249	-2026.02085			1
20	H	86.50138	64.87320	80.52940	-2502.84526	909.80597	575.92391			1
21	C	83.31565	67.62217	79.75044	619.36578	-458.64843	-172.09273			1
22	O	82.40227	67.74351	80.54775	-81.40433	433.87611	522.34594			1
23	N	83.65860	68.45563	78.77580	175.23996	-622.20190	341.55523			1
24	H	84.44604	68.22366	78.17431	-876.57256	-303.22879	-2561.90213			1
25	C	82.93695	69.66573	78.60845	-571.88214	-534.10783	-106.15033			1
26	H	82.33677	69.79385	79.53869	-2713.20841	-16.25800	-248.80809			1
27	C	84.01947	70.81031	78.30485	166.60354	288.16399	-716.09568			1
28	H	84.60945	70.49961	77.39875	-2097.85574	1636.78449	-586.18044			1
29	O	84.98294	71.04993	79.34308	-317.80580	-363.38227	484.43082			1
30	H	85.81775	70.81626	78.88776	1863.74748	-1451.84923	1357.29467			1
31	C	83.09814	72.02427	77.91814	503.80731	517.99032	318.51606			1
32	H	83.70001	72.90544	77.59528	640.61020	-2157.10410	-1536.29104			1
33	H	82.41183	71.76321	77.07455	1687.88455	465.60692	2087.56452			1
34	H	82.46723	72.35083	78.77710	-1293.07895	-1899.88581	-1463.57452			1
35	C	82.05366	69.52568	77.23589	-153.07550	-733.68902	248.70981			1
36	O	82.61892	69.66692	76.18318	186.15459	-480.78787	-449.34387			1
37	N	80.75186	69.28118	77.47551	-487.53139	543.18517	42.03850			1
38	C	79.85665	69.07844	76.38673	-699.35871	69.34393	360.10701			1
39	H	80.48705	68.87273	75.49066	2.81126	-221.99807	-2715.58072			1
40	C	78.99633	67.85966	76.93231	-507.46439	-592.59194	122.07761			1
41	H	78.02695	67.74179	76.39816	-1975.08116	525.87560	-1801.71556			1
42	H	79.54219	66.89611	76.82573	1588.27743	-1913.22100	1113.83566			1
43	C	78.82639	68.24759	78.43463	-613.62442	-457.55993	-194.14490			1
44	H	78.00918	69.01176	78.55356	1707.54637	-721.27992	1996.92523			1
45	H	78.55131	67.38908	79.08913	758.23357	2100.81767	1560.55011			1
46	C	80.25002	68.85604	78.77838	-352.41524	704.96076	49.21465			1
47	H	80.22729	69.74377	79.45375	1714.76886	-2070.42778	443.35792			1
48	H	81.00563	68.12008	79.17132	1224.15040	1801.50881	1636.97633			1

49	C	78.82656	70.34788	76.16323	566.85117	537.05831	117.62814	1
50	O	78.18441	70.40879	75.14219	-550.26779	-406.08867	4.21666	1
51	N	78.81600	71.16745	77.20700	566.34832	-425.77725	180.18749	1
52	H	79.46582	70.90453	77.94488	644.44502	2646.80550	-52.73430	1
53	C	77.71551	72.03839	77.47262	612.34801	-281.48662	411.56221	1
54	H	78.00929	72.45035	78.46388	1667.23498	-1490.75142	1556.16753	1
55	C	77.68136	73.16241	76.33960	-714.45746	-175.43074	286.98927	1
56	H	77.33797	72.68050	75.38098	-787.09484	1763.03619	-1922.46060	1
57	O	78.94052	73.78026	76.00320	-429.46514	516.51932	-128.40526	1
58	H	79.10153	73.39462	75.11918	1981.82785	436.16847	-1818.18182	1
59	C	76.59648	74.15318	76.90495	630.79189	-468.94448	76.03230	1
60	H	76.23717	74.86212	76.12384	-1775.71861	2062.30353	131.89849	1
61	H	75.69895	73.62851	77.32084	-1855.14608	88.94118	1993.53760	1
62	H	77.01275	74.77101	77.73409	-1504.82350	-780.94249	-2132.90992	1
63	C	76.38962	71.10497	77.58952	288.57638	618.62814	-397.00270	1
64	O	76.38447	70.18588	78.41688	321.70495	-185.26452	574.37218	1
65	N	75.45422	71.44902	76.74037	-447.05792	-446.53431	367.76425	1
66	H	75.70515	72.18197	76.07952	350.31316	1975.63644	-1843.31522	1
67	C	74.06313	71.27341	77.00511	-511.23061	374.03917	-471.51480	1
68	H	73.59504	71.78844	76.13494	2234.79579	-898.70890	-1273.45190	1
69	C	73.77674	69.70705	77.01213	529.53781	-159.34528	563.72604	1
70	H	72.70769	69.52182	76.72490	654.59388	2347.94251	1217.51488	1
71	H	74.40294	69.27095	76.18951	-1526.55661	2103.42026	817.87394	1
72	O	74.03399	69.00039	78.24690	-554.84278	14.12789	399.58769	1
73	H	74.99015	69.34373	78.41867	1297.06236	2061.84854	1220.68812	1
74	C	73.70539	72.01243	78.40968	-662.15484	-412.13544	123.62687	1
75	O	74.50290	72.76458	78.97869	-540.01537	-317.05804	274.91456	1
76	N	72.44562	71.78553	78.72568	-202.76299	-690.00100	-131.49145	1
77	H	72.04374	71.14112	78.04768	-702.62132	-2617.37191	281.70413	1
78	C	71.85370	71.98591	80.03759	-491.73914	576.34187	222.73509	1
79	H	70.88220	71.44192	79.96427	1977.17978	-1823.58850	-434.68928	1
80	C	72.78841	71.40737	81.09229	-649.50797	-328.66843	306.11224	1
81	H	73.80836	71.81680	80.90531	2075.07803	1452.16490	-1004.45904	1
82	C	72.36555	71.80762	82.49329	-615.18735	-489.99689	-70.96352	1
83	H	73.06731	71.40066	83.27275	-1226.32661	-1724.38906	-1716.47170	1
84	H	72.34163	72.92636	82.61399	2381.64273	-969.84735	900.46860	1
85	H	71.33631	71.42589	82.73924	2122.74991	1702.23946	-141.36228	1
86	C	72.87826	69.89755	80.99231	-501.86074	-479.61276	-376.42482	1
87	H	73.58819	69.47073	81.75364	993.79261	-2246.95401	-1177.81305	1
88	H	71.87840	69.40959	81.15933	42.71279	-626.15391	-2651.37258	1
89	H	73.24825	69.57097	79.96363	-2026.39012	-1590.33709	-887.82922	1
90	C	71.61485	73.61334	80.30491	-672.89153	382.57394	-156.34072	1
91	O	70.50245	73.99394	80.56106	410.04627	221.86223	500.35950	1
92	N	72.74195	74.29790	80.27633	-378.11782	-443.79414	-441.10984	1
93	H	73.64720	73.85004	79.97676	2404.15973	-568.14894	1149.30085	1
94	C	72.64647	75.71140	80.39607	-544.54484	466.16019	331.29119	1
95	H	71.59581	75.92716	80.70074	-1409.80988	-170.17955	2325.32679	1
96	C	73.75196	76.13551	81.45506	-184.48284	116.78282	-758.89137	1
97	H	73.64201	75.54044	82.38974	1893.78641	1861.14652	611.04528	1
98	H	74.77228	75.91219	81.06827	-2170.79665	-974.19311	1327.50117	1
99	C	73.57950	77.65878	81.73792	389.51668	672.81878	-138.49152	1
100	H	73.74564	78.24220	80.80397	510.64577	1933.03327	1851.02484	1
101	H	72.52450	77.88137	82.01141	-2302.30869	-1105.72939	-948.89774	1
102	C	74.53348	78.18800	82.87554	-559.93427	-126.34590	542.30857	1
103	O	74.47093	79.34371	83.20635	-670.36003	-111.83166	76.36448	1
104	N	75.35494	77.25103	83.39575	-216.06729	-537.07037	446.51379	1
105	H	75.46577	76.26172	83.14467	-1251.96487	1074.12894	-2168.52500	1
106	H	76.03881	77.43792	84.13734	-2451.83023	-720.73851	944.84612	1
107	C	73.09607	76.33054	78.94095	546.24052	-563.88337	-85.11809	1
108	O	74.24040	76.24134	78.58325	71.70702	-307.40463	606.69673	1
109	N	72.04298	76.85851	78.30108	479.90863	-504.50129	222.86849	1
110	C	72.21637	77.52434	77.04541	75.51268	-600.91904	506.73700	1

111	H	73.18053	77.11321	76.66440	-2033.61562	1795.30103	254.89480	1
112	C	70.91351	77.02470	76.28432	523.79067	517.99274	284.45581	1
113	H	70.67257	77.62321	75.37770	1599.61665	-1127.00911	1895.98173	1
114	H	71.03556	75.97202	75.94589	-1881.83093	1275.82488	-1501.55016	1
115	C	69.83817	77.11627	77.41036	-600.05639	-404.05026	316.64485	1
116	H	69.49705	78.16457	77.56093	-2597.05260	496.36221	657.73249	1
117	H	68.92359	76.51855	77.19861	-1666.24518	1294.38985	-1723.90591	1
118	C	70.65951	76.57486	78.65896	493.57570	-129.95376	-602.56394	1
119	H	70.43707	77.09469	79.62047	-1469.08415	-637.84797	2204.22581	1
120	H	70.60513	75.46942	78.81764	-1038.97840	1068.88701	-2280.71789	1
121	C	72.32884	79.12849	77.34424	188.88100	241.05089	-727.87821	1
122	O	73.24947	79.52245	78.05680	531.88613	-49.19943	427.07960	1
123	N	71.43059	79.83953	76.70436	708.14833	26.93417	-179.73509	1
124	H	70.79532	79.27349	76.14411	-2232.69501	-1179.09831	1023.94816	1
125	C	71.06952	81.20811	77.02550	-738.32412	259.92548	104.42456	1
126	H	70.07216	81.34540	76.51648	2028.89123	1260.02983	1311.33324	1
127	C	71.00399	81.40914	78.53376	-258.65678	-345.52513	661.28459	1
128	H	71.98229	81.09549	78.96784	-1826.06090	-1801.46097	-918.64554	1
129	C	70.77845	82.87027	78.87494	-541.23400	531.92970	-218.41428	1
130	H	70.75487	83.04265	79.98631	1311.73218	-2219.18200	882.19023	1
131	H	71.59153	83.52337	78.45121	-1048.71298	1223.58118	-2196.97971	1
132	H	69.80328	83.24528	78.45672	419.06414	1903.92898	1903.44670	1
133	C	69.92814	80.55208	79.17344	-423.86431	152.66566	-648.55262	1
134	H	69.85506	80.73370	80.28141	105.68386	-2342.50080	1387.51238	1
135	H	68.91494	80.76471	78.73190	-1695.63603	-1484.73621	-1531.02793	1
136	H	70.13609	79.45679	79.02685	-1853.57121	-487.39031	1936.59343	1
137	C	72.21218	82.24458	76.38211	539.71428	-510.58232	267.58633	1
138	O	71.85239	83.14975	75.67877	-15.93758	-278.34085	-624.49402	1
139	N	73.41828	81.93185	76.80570	-676.81886	12.05292	276.17960	1
140	H	73.56285	81.10440	77.43268	-1694.44250	-373.84189	-2100.66098	1
141	C	74.51732	82.73001	76.34874	412.33078	-664.70360	108.35451	1
142	H	74.23846	83.78370	76.57450	1765.77476	1294.44366	1621.76594	1
143	C	75.78176	82.19419	77.12533	-179.66635	-721.95667	-264.73915	1
144	H	75.65069	82.28991	78.22694	-607.34922	2587.87032	-598.10018	1
145	H	75.90929	81.10355	76.93623	-359.69332	-1479.13954	-2259.74260	1
146	C	77.03760	82.98778	76.63052	-240.01076	616.02425	431.85322	1
147	H	77.06409	83.01744	75.51643	-1359.17131	782.54425	2227.99181	1
148	H	77.00517	84.04868	76.96537	-820.36667	85.81767	-2596.78715	1
149	C	78.31492	82.24254	77.18900	-513.07015	236.18570	-551.87280	1
150	H	78.36600	82.31007	78.30017	1816.11944	-1183.11722	-1650.94321	1
151	H	78.27126	81.15406	76.95295	-1800.04429	-1361.53473	1526.34643	1
152	C	79.55499	82.88904	76.52754	726.08972	-253.19732	-179.64713	1
153	H	79.58302	82.80215	75.42277	1224.27271	-456.51798	-2390.90304	1
154	H	79.75020	83.93773	76.82939	1206.40339	-1150.93514	-2154.90344	1
155	N	80.80855	82.08725	77.01054	329.70796	-633.68968	-155.67358	1
156	H	81.74023	82.40202	76.61271	1348.31305	1938.76845	1359.00643	1
157	H	81.01405	82.08269	78.05197	2096.92035	1446.54551	-966.48890	1
158	H	80.82128	81.05218	76.77848	-1197.07217	-2303.53719	827.28733	1
159	C	74.72616	82.52468	74.73704	-378.01186	-556.17301	-413.96481	1
160	O	75.30066	83.38798	74.11080	-409.44433	-307.55053	-453.30833	1
161	N	74.41127	81.27142	74.32945	-429.02477	524.70884	274.08502	1
162	H	73.96054	80.84426	75.14374	1706.34263	-1425.96036	1574.38926	1
163	C	73.75029	81.10587	73.05012	-45.25864	-626.22952	478.93267	1
164	H	72.67232	81.07675	73.31985	1988.63164	570.90773	1772.87287	1
165	C	74.13834	82.26838	72.07361	551.77128	-20.49526	-564.54996	1
166	H	73.73948	83.24109	72.44834	1434.61535	-1753.10253	1513.99471	1
167	H	75.24865	82.38497	72.06649	-714.67738	1819.09770	1898.36494	1
168	C	73.61416	81.98774	70.62090	446.99263	-555.77305	338.97221	1
169	H	74.00465	81.01437	70.24347	1953.68466	1892.25957	-161.67766	1
170	H	72.50431	81.91300	70.59036	-403.03785	2688.07032	-188.43591	1
171	C	74.14137	83.18437	69.73350	567.86262	335.74681	434.04421	1
172	H	73.64648	84.14008	70.02266	-1080.02275	1568.26081	-1948.78900	1

173	H	75.23065	83.34642	69.90465	-919.54108	2111.34692	1456.13463	1
174	C	73.88216	82.85395	68.24509	195.81897	173.33862	-745.11536	1
175	H	74.42854	81.96599	67.86889	1405.67949	-2301.21089	-390.08113	1
176	H	72.81268	82.78964	67.96110	-940.37328	-1118.32446	2299.72133	1
177	N	74.45047	84.04722	67.40412	319.26422	656.36007	-42.02424	1
178	H	74.35846	83.95461	66.35148	1961.03633	619.91968	1787.09422	1
179	H	74.01905	85.00301	67.56820	854.14343	-2156.80752	1429.08711	1
180	H	75.48660	84.25514	67.50452	1237.02905	-1378.50857	-1998.28500	1
181	C	74.29109	79.67068	72.50404	532.53319	-268.57236	517.55729	1
182	O	75.13554	79.60209	71.63555	266.16714	-290.73804	-558.88002	1
183	N	73.66323	78.66232	73.11736	-226.25352	640.49678	-270.32839	1
184	H	73.02892	78.89183	73.88313	2007.69063	-1035.27229	1523.50231	1
185	C	74.25387	77.36364	72.99637	-540.76542	-573.33303	49.50000	1
186	H	74.66222	77.38946	71.95356	-2374.20950	-1036.76023	843.75774	1
187	C	75.41011	77.20600	74.07825	-77.09082	666.87422	-415.84136	1
188	H	74.99245	76.98521	75.10133	-985.81834	617.19825	2463.91927	1
189	O	76.24038	78.36958	74.32576	293.29899	-391.65602	-477.80926	1
190	H	76.00877	78.91602	73.54328	2528.72714	-681.76262	-751.27122	1
191	C	76.14568	75.92019	73.55740	252.47363	-605.14473	440.05134	1
192	H	76.99688	75.63783	74.22120	-2052.65063	1456.49051	-1043.51830	1
193	H	75.45487	75.04293	73.50361	-2152.98800	-1661.97574	-161.70652	1
194	H	76.56582	76.07538	72.52973	-473.12726	-1584.27339	2165.61725	1
195	C	73.05464	76.28054	73.24638	360.36307	488.46713	505.10056	1
196	O	73.21671	75.27843	73.90244	-200.08817	-528.03552	-385.82850	1
197	N	71.98457	76.66228	72.54537	-597.54095	-226.44775	355.20479	1
198	H	72.06222	77.56521	72.07731	2179.23655	-1300.70981	-991.33835	1
199	C	70.72433	76.07259	72.86805	-687.68921	297.39807	-249.45179	1
200	H	70.73105	75.90979	73.96618	-349.16256	-2467.37713	-1101.72831	1
201	C	69.57054	77.03815	72.34262	672.47345	361.54328	-201.62880	1
202	H	69.77831	77.33167	71.28839	1541.41502	582.18425	2169.97026	1
203	H	68.60870	76.47478	72.34163	-2534.67717	60.25153	997.72295	1
204	C	69.42524	78.28927	73.22424	574.26774	-389.43119	-377.02542	1
205	C	68.60595	78.20012	74.38987	688.82679	-287.33580	-257.96133	1
206	H	68.17564	77.23257	74.70508	331.14182	1470.38163	2269.80013	1
207	C	70.02401	79.53150	72.85394	-383.52382	-675.04808	144.24917	1
208	H	70.68972	79.59732	71.97471	4.09847	1517.59662	2262.86397	1
209	C	68.33006	79.37011	75.10299	-134.76730	428.45285	-649.50303	1
210	H	67.67869	79.30697	75.99230	-903.23433	1600.49020	2011.53387	1
211	C	69.71216	80.67561	73.60083	-335.53281	-615.00040	-364.39058	1
212	H	70.15518	81.63967	73.29335	1596.45398	-1369.33862	1732.02659	1
213	C	68.83755	80.64424	74.72327	585.48547	-340.24194	-406.23938	1
214	O	68.47633	81.81504	75.47551	-419.15649	-173.04408	-511.94141	1
215	H	68.98469	82.48619	74.96569	-1071.84350	1559.71507	-1960.13012	1
216	C	70.51920	74.66814	72.07834	291.41878	-183.13091	710.72246	1
217	O	69.63326	73.91157	72.42212	379.87695	523.47396	-222.23622	1
218	N	71.26188	74.58457	70.92534	564.30591	373.09380	277.24371	1
219	H	71.96433	75.31686	71.08108	-120.59931	-2436.07824	-1214.35098	1
220	C	71.71381	73.23427	70.62390	404.07514	-299.37480	608.84009	1
221	H	72.18755	72.86190	71.55795	-1071.07882	-841.69025	2359.66467	1
222	C	70.43831	72.41210	70.21211	-683.12807	68.71770	-390.13096	1
223	H	69.66957	72.44337	71.03218	2068.88918	1596.58590	770.89603	1
224	H	69.95027	72.88401	69.32840	1379.86429	2342.49779	-179.85638	1
225	C	70.84189	70.93705	69.88913	-176.39967	537.49466	550.97268	1
226	H	71.57988	70.89303	69.05689	-396.28051	1942.22168	1869.33314	1
227	H	71.33734	70.44907	70.75749	-94.44700	586.00678	-2659.20016	1
228	C	69.47317	70.20720	69.50866	-291.69381	-718.18079	-150.72929	1
229	H	68.72767	70.11641	70.33940	-2303.38776	1089.76242	964.62032	1
230	H	68.93857	70.63497	68.62228	884.16729	2568.80533	-207.74283	1
231	N	69.88156	68.91249	69.16195	-594.49522	-252.81478	342.29276	1
232	H	70.87427	68.73813	69.14433	-1735.17426	2084.05705	-263.71605	1
233	C	69.08854	67.96467	68.86470	595.23177	-271.52487	442.22352	1
234	N	67.71500	68.23231	68.89031	585.53813	-424.79750	-105.81303	1

235	H	67.22808	69.09735	69.12145	959.88797	1327.56823	-2177.11905	1
236	H	66.98369	67.55438	68.67392	1578.48647	16.27378	-2220.76233	1
237	N	69.79266	66.79252	68.55526	-452.17763	-390.33541	-421.51853	1
238	H	70.79269	66.59824	68.53493	470.26107	1974.25629	-1817.92087	1
239	H	69.33338	65.92052	68.28932	1856.67307	-1573.97321	-1224.35416	1
240	C	72.73264	73.29475	69.37011	-531.47271	-581.45780	-55.06206	1
241	O	73.58209	72.44552	69.23370	-243.00837	192.73507	609.52485	1
242	N	72.46335	74.34074	68.55494	343.49288	-644.25607	38.09164	1
243	H	71.62247	74.84765	68.83704	-1691.16043	-1535.97525	-1484.73099	1
244	C	72.77692	74.12670	67.15574	542.66492	350.14337	454.42563	1
245	H	72.50022	73.07032	66.94402	1209.57979	-2396.95920	463.86744	1
246	C	71.91667	75.17656	66.33902	-737.14309	145.93010	242.71942	1
247	H	71.90341	76.15969	66.85740	-1050.18303	159.36419	-2509.06125	1
248	C	72.50681	75.31581	64.89334	-706.77696	-252.88343	-245.16230	1
249	H	71.90347	76.01283	64.26557	-1624.64039	-1665.49085	1417.86935	1
250	H	73.55183	75.70670	64.91749	2566.10521	598.51109	693.22305	1
251	H	72.53811	74.33275	64.36778	-1972.69758	107.10018	-1876.34312	1
252	C	70.46472	74.60108	66.19339	412.85148	672.58832	-27.69222	1
253	H	69.80037	75.29884	65.63210	1447.02277	1762.76533	-1490.78944	1
254	H	70.46444	73.63061	65.64402	1320.77379	-145.20455	2378.68491	1
255	H	69.99335	74.41876	67.18733	-1512.10848	1470.52031	1724.75147	1
256	C	74.35886	74.36110	66.94811	-607.11113	499.56689	73.73769	1
257	O	74.91882	73.83819	66.01092	357.97126	460.81534	356.68785	1
258	N	74.84546	75.27554	67.80794	536.55407	-368.62270	332.76306	1
259	H	74.18916	75.59774	68.54129	524.38866	2297.69985	1367.20941	1
260	C	76.14361	74.93584	68.36620	46.50277	-774.29190	-147.97904	1
261	H	76.13145	73.82545	68.43265	1676.51875	1883.29066	1032.55549	1
262	C	77.31010	75.46349	67.38919	-559.41456	-34.19198	-556.30433	1
263	H	76.91283	76.28488	66.74576	-64.66664	395.18769	2695.05373	1
264	H	78.15776	75.90252	67.96826	-2703.44278	-60.40056	333.79418	1
265	C	77.78568	74.30407	66.55520	-519.76435	377.31045	459.42366	1
266	H	76.87560	73.80514	66.10712	-1746.74323	1667.50644	-1261.73691	1
267	C	78.67833	74.78074	65.41719	570.95554	16.46261	-545.27700	1
268	H	79.03797	73.92437	64.78969	2391.58273	28.05277	-1305.07271	1
269	H	78.13768	75.48685	64.73528	175.75588	917.63458	2559.43867	1
270	H	79.58580	75.31546	65.79959	-1063.97851	-2155.34650	1283.00462	1
271	C	78.54930	73.29760	67.40513	193.76014	2.62946	-765.53141	1
272	H	78.89061	72.41978	66.79813	507.39394	-846.55087	2539.60089	1
273	H	79.46196	73.75689	67.86551	1337.57841	1818.19054	1526.01994	1
274	H	77.92416	72.89512	68.24306	1100.88635	-1172.91350	-2199.08909	1
275	C	76.11052	75.65607	69.77842	-549.21115	475.64486	-309.38218	1
276	O	75.08325	76.10392	70.24007	556.06106	-390.37755	-78.24250	1
277	O	77.30689	75.69028	70.53490	-572.27940	-310.19032	-209.75862	1
278	H	77.90638	75.21787	69.89336	-1380.08193	2212.14486	790.85944	1

Listing 62: C00062.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.6237	0.0000	300.0000
3	H	56.91105	76.10418	68.20016	-2043.14101	-1757.64893	399.89339		1
4	N	57.44298	76.31099	69.04273	426.75047	490.45733	-334.42467		1
5	H	56.70990	76.56972	69.69955	442.25559	-1110.30854	-2448.52907		1
6	C	58.47584	77.25812	68.89167	415.32972	-666.39213	83.73172		1
7	H	58.94971	76.96582	67.93033	879.32219	2491.00447	667.35213		1
8	C	57.86162	78.74344	68.83012	31.35357	477.41777	628.23362		1
9	H	57.45543	79.01552	69.83401	1168.38489	2240.25337	-1019.71136		1
10	H	58.68321	79.47334	68.63209	-360.43770	2534.90498	931.67112		1
11	C	56.78174	78.85833	67.78390	463.18208	512.70242	-382.34388		1
12	H	55.97233	78.13487	68.02905	1725.29117	1863.52247	-987.07854		1
13	C	56.18879	80.26201	67.79173	710.42801	-144.27427	-313.15367		1
14	H	55.35713	80.36430	67.04759	364.20195	-1033.13725	2494.72524		1

15	H	55.77168	80.53091	68.79643	2567.61904	335.80679	847.48802	1
16	H	56.95863	81.03491	67.53524	-2587.99029	680.92867	-512.16411	1
17	C	57.30741	78.54065	66.39099	268.17616	741.64379	-40.42634	1
18	H	56.51055	78.66089	65.61203	1283.54314	-1945.37420	-1411.27812	1
19	H	58.15423	79.21699	66.10605	-1258.57796	1317.15249	-2026.02085	1
20	H	57.68403	77.48801	66.31771	-2502.84526	909.80597	575.92391	1
21	C	59.49019	77.16854	70.15521	619.36578	-458.64843	-172.09273	1
22	O	60.14366	78.13315	70.49232	-81.40433	433.87611	522.34594	1
23	N	59.51495	75.94595	70.68948	175.23996	-622.20190	341.55523	1
24	H	58.94195	75.23208	70.24069	-876.57256	-303.22879	-2561.90213	1
25	C	60.46814	75.68198	71.71283	-571.88214	-534.10783	-106.15033	1
26	H	60.61822	76.66767	72.20867	-2713.20841	-16.25800	-248.80809	1
27	C	59.82936	74.53415	72.62647	166.60354	288.16399	-716.09568	1
28	H	59.61817	73.64642	71.96892	-2097.85574	1636.78449	-586.18044	1
29	O	58.57569	74.86703	73.25212	-317.80580	-363.38227	484.43082	1
30	H	57.97433	74.22738	72.82272	1863.74748	-1451.84923	1357.29467	1
31	C	61.00270	74.17494	73.60927	503.80731	517.99032	318.51606	1
32	H	60.75589	73.27889	74.22498	640.61020	-2157.10410	-1536.29104	1
33	H	61.95332	73.95226	73.06687	1687.88455	465.60692	2087.56452	1
34	H	61.21095	75.00958	74.31776	-1293.07895	-1899.88581	-1463.57452	1
35	C	61.80906	75.10912	70.97471	-153.07550	-733.68902	248.70981	1
36	O	61.70118	74.24083	70.15053	186.15459	-480.78787	-449.34387	1
37	N	62.91878	75.66051	71.48776	-487.53139	543.18517	42.03850	1
38	C	64.21711	75.28127	71.02356	-699.35871	69.34393	360.10701	1
39	H	64.13517	75.05849	69.93567	2.81126	-221.99807	-2715.58072	1
40	C	65.08691	76.54875	71.42142	-507.46439	-592.59194	122.07761	1
41	H	66.17566	76.32272	71.48717	-1975.08116	525.87560	-1801.71556	1
42	H	64.97463	77.37631	70.68576	1588.27743	-1913.22100	1113.83566	1
43	C	64.44678	76.91652	72.79473	-613.62442	-457.55993	-194.14490	1
44	H	64.75198	76.18597	73.58113	1707.54637	-721.27992	1996.92523	1
45	H	64.71862	77.93072	73.16496	758.23357	2100.81767	1560.55011	1
46	C	62.90536	76.76401	72.43973	-352.41524	704.96076	49.21465	1
47	H	62.24816	76.49532	73.29888	1714.76886	-2070.42778	443.35792	1
48	H	62.46371	77.63135	71.89206	1224.15040	1801.50881	1636.97633	1
49	C	64.77866	74.00993	71.90143	566.85117	537.05831	117.62814	1
50	O	64.64174	73.95431	73.09995	-550.26779	-406.08867	4.21666	1
51	N	65.50164	73.23944	71.09792	566.34832	-425.77725	180.18749	1
52	H	65.53155	73.47018	70.10587	644.44502	2646.80550	-52.73430	1
53	C	65.97855	71.99259	71.57928	612.34801	-281.48662	411.56221	1
54	H	65.79866	72.05468	72.67806	1667.23498	-1490.75142	1556.16753	1
55	C	65.14791	70.83604	70.84883	-714.45746	-175.43074	286.98927	1
56	H	65.37576	70.88873	69.74962	-787.09484	1763.03619	-1922.46060	1
57	O	63.71777	70.92371	70.97690	-429.46514	516.51932	-128.40526	1
58	H	63.45419	71.12132	70.05668	1981.82785	436.16847	-1818.18182	1
59	C	65.78387	69.53006	71.45130	630.79189	-468.94448	76.03230	1
60	H	65.35954	68.61674	70.97332	-1775.71861	2062.30353	131.89849	1
61	H	66.89090	69.49346	71.30548	-1855.14608	88.94118	1993.53760	1
62	H	65.58890	69.45015	72.54579	-1504.82350	-780.94249	-2132.90992	1
63	C	67.55433	71.90604	71.13798	288.57638	618.62814	-397.00270	1
64	O	67.93976	71.14719	70.27783	321.70495	-185.26452	574.37218	1
65	N	68.29341	72.72725	71.89280	-447.05792	-446.53431	367.76425	1
66	H	67.78842	73.40094	72.46922	350.31316	1975.63644	-1843.31522	1
67	C	69.61268	72.96771	71.38694	-511.23061	374.03917	-471.51480	1
68	H	69.94608	71.96389	71.03397	2234.79579	-898.70890	-1273.45190	1
69	C	69.45390	74.03544	70.21126	529.53781	-159.34528	563.72604	1
70	H	70.46225	74.12236	69.72389	654.59388	2347.94251	1217.51488	1
71	H	68.77964	73.62484	69.41489	-1526.55661	2103.42026	817.87394	1
72	O	68.99992	75.33574	70.62488	-554.84278	14.12789	399.58769	1
73	H	69.50778	75.40538	71.51296	1297.06236	2061.84854	1220.68812	1
74	C	70.50525	73.65547	72.56235	-662.15484	-412.13544	123.62687	1
75	O	70.40534	74.85693	72.80437	-540.01537	-317.05804	274.91456	1
76	N	71.28209	72.75788	73.11357	-202.76299	-690.00100	-131.49145	1

77	H	71.21039	71.78422	72.82006	-702.62132	-2617.37191	281.70413	1
78	C	72.19192	73.13494	74.14148	-491.73914	576.34187	222.73509	1
79	H	72.55332	74.15617	73.88650	1977.17978	-1823.58850	-434.68928	1
80	C	71.36845	73.12737	75.50229	-649.50797	-328.66843	306.11224	1
81	H	70.91342	72.12897	75.67887	2075.07803	1452.16490	-1004.45904	1
82	C	72.34644	73.50581	76.66544	-615.18735	-489.99689	-70.96352	1
83	H	71.82621	73.52283	77.65205	-1226.32661	-1724.38906	-1716.47170	1
84	H	73.18532	72.77390	76.74619	2381.64273	-969.84735	900.46860	1
85	H	72.79958	74.51285	76.51067	2122.74991	1702.23946	-141.36228	1
86	C	70.25613	74.22781	75.40185	-501.86074	-479.61276	-376.42482	1
87	H	69.75802	74.40827	76.38384	993.79261	-2246.95401	-1177.81305	1
88	H	70.67476	75.20113	75.04669	42.71279	-626.15391	-2651.37258	1
89	H	69.46296	73.93664	74.67063	-2026.39012	-1590.33709	-887.82922	1
90	C	73.33680	71.95885	74.21512	-672.89153	382.57394	-156.34072	1
91	O	73.01230	70.79175	74.22484	410.04627	221.86223	500.35950	1
92	N	74.52055	72.51478	74.40992	-378.11782	-443.79414	-441.10984	1
93	H	74.53723	73.53300	74.43653	2404.15973	-568.14894	1149.30085	1
94	C	75.75263	71.79667	74.31743	-544.54484	466.16019	331.29119	1
95	H	76.40280	72.30007	75.06484	-1409.80988	-170.17955	2325.32679	1
96	C	75.47510	70.27115	74.61466	-184.48284	116.78282	-758.89137	1
97	H	74.80504	70.17577	75.50213	1893.78641	1861.14652	611.04528	1
98	H	74.91475	69.81033	73.76271	-2170.79665	-974.19311	1327.50117	1
99	C	76.83205	69.53018	74.83934	389.51668	672.81878	-138.49152	1
100	H	77.45527	69.57866	73.91801	510.64577	1933.03327	1851.02484	1
101	H	77.44375	70.05570	75.60697	-2302.30869	-1105.72939	-948.89774	1
102	C	76.61787	68.02809	75.26465	-559.93427	-126.34590	542.30857	1
103	O	77.57348	67.32823	75.48193	-670.36003	-111.83166	76.36448	1
104	N	75.32160	67.65811	75.35632	-216.06729	-537.07037	446.51379	1
105	H	74.46584	68.19320	75.16687	-1251.96487	1074.12894	-2168.52500	1
106	H	75.01317	66.71454	75.61431	-2451.83023	-720.73851	944.84612	1
107	C	76.32649	71.94413	72.79116	546.24052	-563.88337	-85.11809	1
108	O	75.82488	71.31227	71.89739	71.70702	-307.40463	606.69673	1
109	N	77.34682	72.81732	72.73325	479.90863	-504.50129	222.86849	1
110	C	78.00601	73.08515	71.49420	75.51268	-600.91904	506.73700	1
111	H	77.33878	72.72863	70.67328	-2033.61562	1795.30103	254.89480	1
112	C	78.19102	74.66574	71.63110	523.79067	517.99274	284.45581	1
113	H	78.93062	75.08346	70.90866	1599.61665	-1127.00911	1895.98173	1
114	H	77.23239	75.19810	71.44768	-1881.83093	1275.82488	-1501.55016	1
115	C	78.63560	74.80014	73.11742	-600.05639	-404.05026	316.64485	1
116	H	79.71227	74.54444	73.23764	-2597.05260	496.36221	657.73249	1
117	H	78.50986	75.82870	73.52662	-1666.24518	1294.38985	-1723.90591	1
118	C	77.69578	73.72477	73.81770	493.57570	-129.95376	-602.56394	1
119	H	78.19761	73.11419	74.60589	-1469.08415	-637.84797	2204.22581	1
120	H	76.73388	74.12965	74.21129	-1038.97840	1068.88701	-2280.71789	1
121	C	79.50174	72.44507	71.46478	188.88100	241.05089	-727.87821	1
122	O	79.99168	71.81816	72.39002	531.88613	-49.19943	427.07960	1
123	N	80.04845	72.70744	70.27584	708.14833	26.93417	-179.73509	1
124	H	79.45310	73.31941	69.71974	-2232.69501	-1179.09831	1023.94816	1
125	C	81.51066	72.69255	70.11700	-738.32412	259.92548	104.42456	1
126	H	81.76260	71.68752	70.52895	2028.89123	1260.02983	1311.33324	1
127	C	81.87357	72.89328	68.65904	-258.65678	-345.52513	661.28459	1
128	H	81.46932	73.88096	68.34086	-1826.06090	-1801.46097	-918.64554	1
129	C	83.38043	72.92335	68.47405	-541.23400	531.92970	-218.41428	1
130	H	83.66675	73.10598	67.40219	1311.73218	-2219.18200	882.19023	1
131	H	83.84818	73.74207	69.09167	-1048.71298	1223.58118	-2196.97971	1
132	H	83.85721	71.95391	68.78675	419.06414	1903.92898	1903.44670	1
133	C	81.26034	71.83226	67.76371	-423.86431	152.66566	-648.55262	1
134	H	81.50088	72.01182	66.67982	105.68386	-2342.50080	1387.51238	1
135	H	81.63683	70.80491	68.02353	-1695.63603	-1484.73621	-1531.02793	1
136	H	80.14018	71.80840	67.86152	-1853.57121	-487.39031	1936.59343	1
137	C	82.13386	73.91175	71.05092	539.71428	-510.58232	267.58633	1
138	O	82.56142	74.92626	70.56505	-15.93758	-278.34085	-624.49402	1

139	N	82.04467	73.56791	72.33031	-676.81886	12.05292	276.17960	1
140	H	81.60593	72.65428	72.56554	-1694.44250	-373.84189	-2100.66098	1
141	C	83.03417	74.15983	73.19749	412.33078	-664.70360	108.35451	1
142	H	84.00129	74.08068	72.65418	1765.77476	1294.44366	1621.76594	1
143	C	82.61341	75.66150	73.42998	-179.66635	-721.95667	-264.73915	1
144	H	82.52675	76.20402	72.45896	-607.34922	2587.87032	-598.10018	1
145	H	81.60386	75.71365	73.89863	-359.69332	-1479.13954	-2259.74260	1
146	C	83.68948	76.31014	74.36591	-240.01076	616.02425	431.85322	1
147	H	83.85956	75.66575	75.26157	-1359.17131	782.54425	2227.99181	1
148	H	84.67477	76.40168	73.85665	-820.36667	85.81767	-2596.78715	1
149	C	83.11344	77.72145	74.78268	-513.07015	236.18570	-551.87280	1
150	H	82.97339	78.37106	73.88721	1816.11944	-1183.11722	-1650.94321	1
151	H	82.09362	77.58068	75.23919	-1800.04429	-1361.53473	1526.34643	1
152	C	84.03808	78.40364	75.81626	726.08972	-253.19732	-179.64713	1
153	H	84.07909	77.89770	76.80179	1224.27271	-456.51798	-2390.90304	1
154	H	85.06330	78.62300	75.45632	1206.40339	-1150.93514	-2154.90344	1
155	N	83.39951	79.80268	76.11925	329.70796	-633.68968	-155.67358	1
156	H	83.89545	80.38927	76.85003	1348.31305	1938.76845	1359.00643	1
157	H	83.33554	80.48856	75.31181	2096.92035	1446.54551	-966.48890	1
158	H	82.40282	79.81105	76.48841	-1197.07217	-2303.53719	827.28733	1
159	C	82.99779	73.37413	74.63056	-378.01186	-556.17301	-413.96481	1
160	O	84.00658	73.34937	75.30376	-409.44433	-307.55053	-453.30833	1
161	N	81.76459	73.00974	74.93027	-429.02477	524.70884	274.08502	1
162	H	81.06365	73.16733	74.20763	1706.34263	-1425.96036	1574.38926	1
163	C	81.40574	72.14733	76.02492	-45.25864	-626.22952	478.93267	1
164	H	81.25486	71.14368	75.56609	1988.63164	570.90773	1772.87287	1
165	C	82.55045	72.17170	77.10919	551.77128	-20.49526	-564.54996	1
166	H	83.51351	71.81230	76.66506	1434.61535	-1753.10253	1513.99471	1
167	H	82.75044	73.22052	77.42951	-714.67738	1819.09770	1898.36494	1
168	C	82.17116	71.27519	78.33646	446.99263	-555.77305	338.97221	1
169	H	81.24924	71.64468	78.83979	1953.68466	1892.25957	-161.67766	1
170	H	81.95276	70.23274	78.01366	-403.03785	2688.07032	-188.43591	1
171	C	83.41867	71.32005	79.30836	567.86262	335.74681	434.04421	1
172	H	84.36069	71.12317	78.74640	-1080.02275	1568.26081	-1948.78900	1
173	H	83.53827	72.33734	79.74786	-919.54108	2111.34692	1456.13463	1
174	C	83.23307	70.25980	80.41742	195.81897	173.33862	-745.11536	1
175	H	82.39050	70.45690	81.10850	1405.67949	-2301.21089	-390.08113	1
176	H	83.18508	69.21409	80.05378	-940.37328	-1118.32446	2299.72133	1
177	N	84.51989	70.29997	81.31242	319.26422	656.36007	-42.02424	1
178	H	84.54023	69.63995	82.14382	1961.03633	619.91968	1787.09422	1
179	H	85.43027	70.04902	80.83021	854.14343	-2156.80752	1429.08711	1
180	H	84.76790	71.22541	81.76948	1237.02905	-1378.50857	-1998.28500	1
181	C	80.00194	72.75136	76.57100	532.53319	-268.57236	517.55729	1
182	O	79.04869	72.02065	76.82397	266.16714	-290.73804	-558.88002	1
183	N	80.12960	74.04232	76.74527	-226.25352	640.49678	-270.32839	1
184	H	81.02679	74.52128	76.50915	2007.69063	-1035.27229	1523.50231	1
185	C	78.99659	74.91998	76.80108	-540.76542	-573.33303	49.50000	1
186	H	78.21167	74.54433	76.11056	-2374.20950	-1036.76023	843.75774	1
187	C	78.49246	74.83068	78.31271	-77.09082	666.87422	-415.84136	1
188	H	79.39566	74.83444	78.99782	-985.81834	617.19825	2463.91927	1
189	O	77.85093	73.58238	78.65370	293.29899	-391.65602	-477.80926	1
190	H	78.28060	72.96439	77.96570	2528.72714	-681.76262	-751.27122	1
191	C	77.65119	76.13030	78.53277	252.47363	-605.14473	440.05134	1
192	H	77.29368	76.20304	79.58715	-2052.65063	1456.49051	-1043.51830	1
193	H	78.24290	77.05094	78.31944	-2152.98800	-1661.97574	-161.70652	1
194	H	76.75143	76.15244	77.87426	-473.12726	-1584.27339	2165.61725	1
195	C	79.71615	76.29016	76.31743	360.36307	488.46713	505.10056	1
196	O	80.95032	76.32723	76.27838	-200.08817	-528.03552	-385.82850	1
197	N	78.87138	77.25557	76.00215	-597.54095	-226.44775	355.20479	1
198	H	77.86827	77.09888	76.09321	2179.23655	-1300.70981	-991.33835	1
199	C	79.42514	78.46853	75.50029	-687.68921	297.39807	-249.45179	1
200	H	80.34513	78.11258	74.98636	-349.16256	-2467.37713	-1101.72831	1

201	C	78.37778	79.21567	74.55521	672.47345	361.54328	-201.62880	1
202	H	77.35846	79.22958	75.00425	1541.41502	582.18425	2169.97026	1
203	H	78.68784	80.28148	74.44166	-2534.67717	60.25153	997.72295	1
204	C	78.36839	78.51906	73.18356	574.26774	-389.43119	-377.02542	1
205	C	79.59997	78.24431	72.51598	688.82679	-287.33580	-257.96133	1
206	H	80.56686	78.51110	72.97921	331.14182	1470.38163	2269.80013	1
207	C	77.12501	78.18501	72.56899	-383.52382	-675.04808	144.24917	1
208	H	76.16842	78.40048	73.07843	4.09847	1517.59662	2262.86397	1
209	C	79.56259	77.63176	71.26320	-134.76730	428.45285	-649.50303	1
210	H	80.51638	77.40680	70.75371	-903.23433	1600.49020	2011.53387	1
211	C	77.13716	77.59064	71.30379	-335.53281	-615.00040	-364.39058	1
212	H	76.16922	77.34327	70.83396	1596.45398	-1369.33862	1732.02659	1
213	C	78.34402	77.28972	70.60865	585.48547	-340.24194	-406.23938	1
214	O	78.36462	76.64598	69.34086	-419.15649	-173.04408	-511.94141	1
215	H	77.39748	76.63269	69.14859	-1071.84350	1559.71507	-1960.13012	1
216	C	79.81233	79.48065	76.71873	291.41878	-183.13091	710.72246	1
217	O	79.90599	80.67318	76.53348	379.87695	523.47396	-222.23622	1
218	N	80.13596	78.79647	77.81827	564.30591	373.09380	277.24371	1
219	H	80.00342	77.78312	77.76423	-120.59931	-2436.07824	-1214.35098	1
220	C	80.16255	79.51506	79.05435	404.07514	-299.37480	608.84009	1
221	H	80.47384	80.54027	78.74464	-1071.07882	-841.69025	2359.66467	1
222	C	78.68148	79.52335	79.62986	-683.12807	68.71770	-390.13096	1
223	H	77.95334	79.74117	78.81645	2068.88918	1596.58590	770.89603	1
224	H	78.40443	78.51987	80.02375	1379.86429	2342.49779	-179.85638	1
225	C	78.59573	80.59812	80.75525	-176.39967	537.49466	550.97268	1
226	H	79.26422	80.32805	81.60651	-396.28051	1942.22168	1869.33314	1
227	H	78.95480	81.58684	80.39204	-94.44700	586.00678	-2659.20016	1
228	C	77.06823	80.68803	81.22155	-291.69381	-718.18079	-150.72929	1
229	H	76.32890	80.99542	80.43952	-2303.38776	1089.76242	964.62032	1
230	H	76.69172	79.76124	81.72569	884.16729	2568.80533	-207.74283	1
231	N	77.13540	81.69925	82.19043	-594.49522	-252.81478	342.29276	1
232	H	78.03804	81.85578	82.61254	-1735.17426	2084.05705	-263.71605	1
233	C	76.15335	82.39837	82.59476	595.23177	-271.52487	442.22352	1
234	N	74.89468	82.16663	82.03078	585.53813	-424.79750	-105.81303	1
235	H	74.61240	81.48242	81.33040	959.88797	1327.56823	-2177.11905	1
236	H	74.03945	82.65840	82.29250	1578.48647	16.27378	-2220.76233	1
237	N	76.55695	83.30719	83.58317	-452.17763	-390.33541	-421.51853	1
238	H	77.46938	83.47392	84.00471	470.26107	1974.25629	-1817.92087	1
239	H	75.91452	83.95332	84.04324	1856.67307	-1573.97321	-1224.35416	1
240	C	81.16318	78.79260	80.11224	-531.47271	-581.45780	-55.06206	1
241	O	81.21823	79.22480	81.24362	-243.00837	192.73507	609.52485	1
242	N	81.88652	77.81774	79.56971	343.49288	-644.25607	38.09164	1
243	H	81.68519	77.63461	78.58698	-1691.16043	-1535.97525	-1484.73099	1
244	C	82.75010	76.92036	80.33799	542.66492	350.14337	454.42563	1
245	H	83.34834	76.45441	79.52053	1209.57979	-2396.95920	463.86744	1
246	C	83.60110	77.75454	81.27789	-737.14309	145.93010	242.71942	1
247	H	82.91415	78.34223	81.94386	-1050.18303	159.36419	-2509.06125	1
248	C	84.51569	76.91006	82.14416	-706.77696	-252.88343	-245.16230	1
249	H	85.27849	77.54241	82.67666	-1624.64039	-1665.49085	1417.86935	1
250	H	83.94596	76.34326	82.93360	2566.10521	598.51109	693.22305	1
251	H	85.07929	76.15183	81.53453	-1972.69758	107.10018	-1876.34312	1
252	C	84.43207	78.75857	80.49609	412.85148	672.58832	-27.69222	1
253	H	85.00185	79.44952	81.17521	1447.02277	1762.76533	-1490.78944	1
254	H	85.18126	78.24823	79.83143	1320.77379	-145.20455	2378.68491	1
255	H	83.78292	79.39668	79.83554	-1512.10848	1470.52031	1724.75147	1
256	C	81.74187	75.77053	80.98962	-607.11113	499.56689	73.73769	1
257	O	81.15488	75.03680	80.23012	357.97126	460.81534	356.68785	1
258	N	81.76091	75.73804	82.31219	536.55407	-368.62270	332.76306	1
259	H	82.25218	76.47278	82.81976	524.38866	2297.69985	1367.20941	1
260	C	80.90196	74.82180	82.96544	46.50277	-774.29190	-147.97904	1
261	H	80.60109	74.08692	82.18370	1676.51875	1883.29066	1032.55549	1
262	C	81.66427	74.19264	84.24400	-559.41456	-34.19198	-556.30433	1

263	H	82.06177	75.02247	84.87558	-64.66664	395.18769	2695.05373	1
264	H	80.94529	73.63301	84.88954	-2703.44278	-60.40056	333.79418	1
265	C	82.78111	73.29088	83.79155	-519.76435	377.31045	459.42366	1
266	H	83.29695	73.77201	82.93014	-1746.74323	1667.50644	-1261.73691	1
267	C	83.79512	73.09276	84.91171	570.95554	16.46261	-545.27700	1
268	H	84.64274	72.43314	84.59215	2391.58273	28.05277	-1305.07271	1
269	H	84.23878	74.06566	85.24671	175.75588	917.63458	2559.43867	1
270	H	83.32669	72.61571	85.81102	-1063.97851	-2155.34650	1283.00462	1
271	C	82.24295	71.93482	83.35375	193.76014	2.62946	-765.53141	1
272	H	83.06849	71.24309	83.04740	507.39394	-846.55087	2539.60089	1
273	H	81.68151	71.42762	84.18042	1337.57841	1818.19054	1526.01994	1
274	H	81.54323	72.02704	82.48369	1100.88635	-1172.91350	-2199.08909	1
275	C	79.65988	75.66161	83.57499	-549.21115	475.64486	-309.38218	1
276	O	79.76222	76.78323	83.99651	556.06106	-390.37755	-78.24250	1
277	O	78.46214	74.93153	83.75588	-572.27940	-310.19032	-209.75862	1
278	H	78.73042	74.08027	83.31106	-1380.08193	2212.14486	790.85944	1

Listing 63: C00063.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.8935	3574
		0.2500	300.00	0.00	0.00	0.00	-1293.6126	0.0000	300.0000
3	H	72.13158	63.34573	73.50435	-2043.14101	-1757.64893	399.89339		1
4	N	72.14281	64.34379	73.70612	426.75047	490.45733	-334.42467		1
5	H	72.25416	64.34471	74.71876	442.25559	-1110.30854	-2448.52907		1
6	C	73.11976	65.07655	72.99760	415.32972	-666.39213	83.73172		1
7	H	73.24409	64.53631	72.03596	879.32219	2491.00447	667.35213		1
8	C	72.58535	66.58440	72.81604	31.35357	477.41777	628.23362		1
9	H	72.35426	67.02494	73.81493	1168.38489	2240.25337	-1019.71136		1
10	H	73.37868	67.23157	72.36946	-360.43770	2534.90498	931.67112		1
11	C	71.34835	66.56779	71.95218	463.18208	512.70242	-382.34388		1
12	H	70.72253	65.69909	72.25808	1725.29117	1863.52247	-987.07854		1
13	C	70.53730	67.84002	72.16102	710.42801	-144.27427	-313.15367		1
14	H	69.60990	67.84761	71.53193	364.20195	-1033.13725	2494.72524		1
15	H	70.21540	67.95484	73.22842	2567.61904	335.80679	847.48802		1
16	H	71.12779	68.75374	71.89215	-2587.99029	680.92867	-512.16411		1
17	C	71.70954	66.42397	70.48049	268.17616	741.64379	-40.42634		1
18	H	70.79675	66.40582	69.83042	1283.54314	-1945.37420	-1411.27812		1
19	H	72.34890	67.27504	70.12935	-1258.57796	1317.15249	-2026.02085		1
20	H	72.27841	65.47927	70.28197	-2502.84526	909.80597	575.92391		1
21	C	74.48515	65.09018	73.90148	619.36578	-458.64843	-172.09273		1
22	O	75.51991	64.60834	73.49906	-81.40433	433.87611	522.34594		1
23	N	74.26223	65.73131	75.04873	175.23996	-622.20190	341.55523		1
24	H	73.30878	66.02186	75.25958	-876.57256	-303.22879	-2561.90213		1
25	C	75.25520	65.64846	76.06294	-571.88214	-534.10783	-106.15033		1
26	H	76.19985	65.37761	75.53836	-2713.20841	-16.25800	-248.80809		1
27	C	75.26842	67.08448	76.77726	166.60354	288.16399	-716.09568		1
28	H	74.23651	67.29814	77.16863	-2097.85574	1636.78449	-586.18044		1
29	O	75.60980	68.18634	75.91871	-317.80580	-363.38227	484.43082		1
30	H	74.80752	68.74039	75.99645	1863.74748	-1451.84923	1357.29467		1
31	C	76.23198	66.86950	78.00213	503.80731	517.99032	318.51606		1
32	H	76.32907	67.81346	78.59850	640.61020	-2157.10410	-1536.29104		1
33	H	75.86307	66.07013	78.69387	1687.88455	465.60692	2087.56452		1
34	H	77.26160	66.58414	77.68235	-1293.07895	-1899.88581	-1463.57452		1
35	C	74.71164	64.51991	77.11241	-153.07550	-733.68902	248.70981		1
36	O	73.56468	64.55215	77.47052	186.15459	-480.78787	-449.34387		1
37	N	75.69678	63.69412	77.49245	-487.53139	543.18517	42.03850		1
38	C	75.49306	62.77183	78.56850	-699.35871	69.34393	360.10701		1
39	H	74.42808	62.44908	78.52201	2.81126	-221.99807	-2715.58072		1
40	C	76.57757	61.65722	78.24548	-507.46439	-592.59194	122.07761		1
41	H	76.85264	61.05075	79.13737	-1975.08116	525.87560	-1801.71556		1
42	H	76.21137	60.94280	77.47485	1588.27743	-1913.22100	1113.83566		1

43	C	77.75569	62.52248	77.70080	-613.62442	-457.55993	-194.14490	1
44	H	78.29366	63.02638	78.53746	1707.54637	-721.27992	1996.92523	1
45	H	78.51612	61.94043	77.13258	758.23357	2100.81767	1560.55011	1
46	C	76.97635	63.57993	76.80690	-352.41524	704.96076	49.21465	1
47	H	77.44933	64.58832	76.75997	1714.76886	-2070.42778	443.35792	1
48	H	76.73672	63.23615	75.77201	1224.15040	1801.50881	1636.97633	1
49	C	75.86692	63.55365	79.95986	566.85117	537.05831	117.62814	1
50	O	76.98806	64.03265	80.11892	-550.26779	-406.08867	4.21666	1
51	N	74.82378	63.54005	80.75355	566.34832	-425.77725	180.18749	1
52	H	73.99708	63.10552	80.34327	644.44502	2646.80550	-52.73430	1
53	C	74.84560	63.75483	82.15452	612.34801	-281.48662	411.56221	1
54	H	73.86193	63.36029	82.49274	1667.23498	-1490.75142	1556.16753	1
55	C	76.08722	62.94391	82.75718	-714.45746	-175.43074	286.98927	1
56	H	77.03151	63.34868	82.29444	-787.09484	1763.03619	-1922.46060	1
57	O	76.09940	61.52707	82.50817	-429.46514	516.51932	-128.40526	1
58	H	76.91264	61.43909	81.97067	1981.82785	436.16847	-1818.18182	1
59	C	76.00880	63.37767	84.26674	630.79189	-468.94448	76.03230	1
60	H	76.90060	63.03279	84.83983	-1775.71861	2062.30353	131.89849	1
61	H	75.94484	64.48832	84.37596	-1855.14608	88.94118	1993.53760	1
62	H	75.10953	62.94642	84.76496	-1504.82350	-780.94249	-2132.90992	1
63	C	75.01954	65.34237	82.53113	288.57638	618.62814	-397.00270	1
64	O	74.34957	65.81703	83.41840	321.70495	-185.26452	574.37218	1
65	N	76.03413	65.87701	81.87463	-447.05792	-446.53431	367.76425	1
66	H	76.54083	65.30651	81.15226	350.31316	1975.63644	-1843.31522	1
67	C	76.16661	67.29800	81.90445	-511.23061	374.03917	-471.51480	1
68	H	76.02336	67.58729	82.96977	2234.79579	-898.70890	-1273.45190	1
69	C	77.63735	67.55108	81.33887	529.53781	-159.34528	563.72604	1
70	H	77.83657	68.65606	81.36389	654.59388	2347.94251	1217.51488	1
71	H	78.34417	67.07897	82.07198	-1526.55661	2103.42026	817.87394	1
72	O	77.93432	67.07579	79.99467	-554.84278	14.12789	399.58769	1
73	H	77.87876	66.11250	80.14644	1297.06236	2061.84854	1220.68812	1
74	C	74.99039	67.94846	80.98003	-662.15484	-412.13544	123.62687	1
75	O	74.56998	67.47442	79.94849	-540.01537	-317.05804	274.91456	1
76	N	74.66198	69.11142	81.53977	-202.76299	-690.00100	-131.49145	1
77	H	75.09207	69.39462	82.41929	-702.62132	-2617.37191	281.70413	1
78	C	73.44408	69.71394	81.11604	-491.73914	576.34187	222.73509	1
79	H	73.30222	69.39770	80.05619	1977.17978	-1823.58850	-434.68928	1
80	C	72.29584	69.17445	82.08045	-649.50797	-328.66843	306.11224	1
81	H	72.51816	69.45486	83.13257	2075.07803	1452.16490	-1004.45904	1
82	C	70.93163	69.78600	81.61466	-615.18735	-489.99689	-70.96352	1
83	H	70.08663	69.44087	82.25560	-1226.32661	-1724.38906	-1716.47170	1
84	H	70.94826	70.90081	81.65994	2381.64273	-969.84735	900.46860	1
85	H	70.69067	69.49938	80.56408	2122.74991	1702.23946	-141.36228	1
86	C	72.16300	67.61951	81.95322	-501.86074	-479.61276	-376.42482	1
87	H	71.30048	67.22952	82.54376	993.79261	-2246.95401	-1177.81305	1
88	H	72.01238	67.30745	80.89228	42.71279	-626.15391	-2651.37258	1
89	H	73.08395	67.09525	82.32627	-2026.39012	-1590.33709	-887.82922	1
90	C	73.57726	71.32524	81.39003	-672.89153	382.57394	-156.34072	1
91	O	74.12048	71.75509	82.38087	410.04627	221.86223	500.35950	1
92	N	72.81951	71.96625	80.49754	-378.11782	-443.79414	-441.10984	1
93	H	72.41827	71.34780	79.79158	2404.15973	-568.14894	1149.30085	1
94	C	73.14598	73.30135	80.06397	-544.54484	466.16019	331.29119	1
95	H	72.16063	73.75077	79.81901	-1409.80988	-170.17955	2325.32679	1
96	C	73.92904	74.05616	81.20543	-184.48284	116.78282	-758.89137	1
97	H	73.40823	73.91771	82.18285	1893.78641	1861.14652	611.04528	1
98	H	74.94034	73.60153	81.33696	-2170.79665	-974.19311	1327.50117	1
99	C	74.05829	75.57092	80.84088	389.51668	672.81878	-138.49152	1
100	H	74.59380	75.69821	79.86880	510.64577	1933.03327	1851.02484	1
101	H	73.05550	76.01374	80.65394	-2302.30869	-1105.72939	-948.89774	1
102	C	74.79079	76.38804	81.97162	-559.93427	-126.34590	542.30857	1
103	O	74.93617	77.57782	81.85250	-670.36003	-111.83166	76.36448	1
104	N	75.19305	75.63877	83.02168	-216.06729	-537.07037	446.51379	1

105	H	75.11108	74.62802	83.18292	-1251.96487	1074.12894	-2168.52500	1
106	H	75.68826	76.01588	83.83682	-2451.83023	-720.73851	944.84612	1
107	C	74.12525	73.17291	78.77118	546.24052	-563.88337	-85.11809	1
108	O	75.07701	72.43649	78.79232	71.70702	-307.40463	606.69673	1
109	N	73.73147	74.01108	77.79407	479.90863	-504.50129	222.86849	1
110	C	74.58933	74.28371	76.68838	75.51268	-600.91904	506.73700	1
111	H	75.25521	73.39875	76.55816	-2033.61562	1795.30103	254.89480	1
112	C	73.52354	74.54339	75.53524	523.79067	517.99274	284.45581	1
113	H	73.94634	75.10406	74.67214	1599.61665	-1127.00911	1895.98173	1
114	H	73.12474	73.58705	75.13033	-1881.83093	1275.82488	-1501.55016	1
115	C	72.42069	75.33607	76.30188	-600.05639	-404.05026	316.64485	1
116	H	72.70299	76.40756	76.40894	-2597.05260	496.36221	657.73249	1
117	H	71.43110	75.32099	75.79216	-1666.24518	1294.38985	-1723.90591	1
118	C	72.40481	74.60676	77.71308	493.57570	-129.95376	-602.56394	1
119	H	72.28453	75.29213	78.58458	-1469.08415	-637.84797	2204.22581	1
120	H	71.67857	73.76449	77.80064	-1038.97840	1068.88701	-2280.71789	1
121	C	75.40483	75.67551	76.97820	188.88100	241.05089	-727.87821	1
122	O	75.03113	76.50171	77.77427	531.88613	-49.19943	427.07960	1
123	N	76.53638	75.72355	76.21100	708.14833	26.93417	-179.73509	1
124	H	76.44479	74.86647	75.65197	-2232.69501	-1179.09831	1023.94816	1
125	C	76.92784	76.97343	75.51326	-738.32412	259.92548	104.42456	1
126	H	76.16147	77.11811	74.71900	2028.89123	1260.02983	1311.33324	1
127	C	76.96983	78.09384	76.51481	-258.65678	-345.52513	661.28459	1
128	H	77.00223	77.62899	77.52965	-1826.06090	-1801.46097	-918.64554	1
129	C	78.19436	78.97890	76.35359	-541.23400	531.92970	-218.41428	1
130	H	78.20388	79.81889	77.10157	1311.73218	-2219.18200	882.19023	1
131	H	79.14816	78.39563	76.49497	-1048.71298	1223.58118	-2196.97971	1
132	H	78.24153	79.44148	75.32970	419.06414	1903.92898	1903.44670	1
133	C	75.72824	78.96826	76.44012	-423.86431	152.66566	-648.55262	1
134	H	75.68415	79.69585	77.29679	105.68386	-2342.50080	1387.51238	1
135	H	75.69214	79.56739	75.48973	-1695.63603	-1484.73621	-1531.02793	1
136	H	74.78497	78.35407	76.47849	-1853.57121	-487.39031	1936.59343	1
137	C	78.41051	76.58195	74.90397	539.71428	-510.58232	267.58633	1
138	O	79.32284	76.29094	75.64312	-15.93758	-278.34085	-624.49402	1
139	N	78.43479	76.67923	73.58019	-676.81886	12.05292	276.17960	1
140	H	77.58228	76.94901	73.09245	-1694.44250	-373.84189	-2100.66098	1
141	C	79.60661	76.19084	72.92598	412.33078	-664.70360	108.35451	1
142	H	80.07843	75.50671	73.67008	1765.77476	1294.44366	1621.76594	1
143	C	79.17382	75.48867	71.57491	-179.66635	-721.95667	-264.73915	1
144	H	78.36314	74.74651	71.74895	-607.34922	2587.87032	-598.10018	1
145	H	78.75231	76.22866	70.86008	-359.69332	-1479.13954	-2259.74260	1
146	C	80.45317	74.80391	70.98903	-240.01076	616.02425	431.85322	1
147	H	81.27948	75.54812	70.89239	-1359.17131	782.54425	2227.99181	1
148	H	80.83141	74.02265	71.68587	-820.36667	85.81767	-2596.78715	1
149	C	80.12013	74.17606	69.57671	-513.07015	236.18570	-551.87280	1
150	H	79.34107	73.38402	69.66152	1816.11944	-1183.11722	-1650.94321	1
151	H	79.70209	74.94305	68.88475	-1800.04429	-1361.53473	1526.34643	1
152	C	81.44777	73.60025	69.02984	726.08972	-253.19732	-179.64713	1
153	H	82.23387	74.35829	68.84036	1224.27271	-456.51798	-2390.90304	1
154	H	81.86685	72.76432	69.62472	1206.40339	-1150.93514	-2154.90344	1
155	N	81.16165	72.97584	67.62329	329.70796	-633.68968	-155.67358	1
156	H	82.00175	72.55147	67.13364	1348.31305	1938.76845	1359.00643	1
157	H	80.46996	72.17179	67.58255	2096.92035	1446.54551	-966.48890	1
158	H	80.78878	73.62576	66.87142	-1197.07217	-2303.53719	827.28733	1
159	C	80.60758	77.43346	72.54714	-378.01186	-556.17301	-413.96481	1
160	O	81.75759	77.21218	72.23195	-409.44433	-307.55053	-453.30833	1
161	N	79.98168	78.60449	72.54578	-429.02477	524.70884	274.08502	1
162	H	79.00948	78.60252	72.84762	1706.34263	-1425.96036	1574.38926	1
163	C	80.80232	79.76243	72.32194	-45.25864	-626.22952	478.93267	1
164	H	81.77923	79.49426	72.78619	1988.63164	570.90773	1772.87287	1
165	C	80.93988	79.91591	70.75051	551.77128	-20.49526	-564.54996	1
166	H	81.23911	78.94705	70.29109	1434.61535	-1753.10253	1513.99471	1

167	H	79.95679	80.17397	70.29811	-714.67738	1819.09770	1898.36494	1
168	C	81.99178	81.03102	70.44410	446.99263	-555.77305	338.97221	1
169	H	81.68961	81.99602	70.91076	1953.68466	1892.25957	-161.67766	1
170	H	82.98564	80.77630	70.87590	-403.03785	2688.07032	-188.43591	1
171	C	82.06974	81.15731	68.86868	567.86262	335.74681	434.04421	1
172	H	82.39745	80.19502	68.41204	-1080.02275	1568.26081	-1948.78900	1
173	H	81.05946	81.36074	68.43935	-919.54108	2111.34692	1456.13463	1
174	C	83.05259	82.29465	68.50902	195.81897	173.33862	-745.11536	1
175	H	82.73589	83.30255	68.84379	1405.67949	-2301.21089	-390.08113	1
176	H	84.10482	82.11007	68.80405	-940.37328	-1118.32446	2299.72133	1
177	N	83.08437	82.38691	66.94527	319.26422	656.36007	-42.02424	1
178	H	83.70282	83.14565	66.53660	1961.03633	619.91968	1787.09422	1
179	H	83.42697	81.53123	66.41914	854.14343	-2156.80752	1429.08711	1
180	H	82.16158	82.58296	66.45888	1237.02905	-1378.50857	-1998.28500	1
181	C	80.07955	81.08107	72.94184	532.53319	-268.57236	517.55729	1
182	O	80.78364	81.99246	73.38487	266.16714	-290.73804	-558.88002	1
183	N	78.79074	81.04970	72.74031	-226.25352	640.49678	-270.32839	1
184	H	78.44310	80.20596	72.28442	2007.69063	-1035.27229	1523.50231	1
185	C	77.84218	81.82996	73.48760	-540.76542	-573.33303	49.50000	1
186	H	77.58694	81.20102	74.36754	-2374.20950	-1036.76023	843.75774	1
187	C	78.48820	83.21680	73.91267	-77.09082	666.87422	-415.84136	1
188	H	79.13934	83.54343	73.05088	-985.81834	617.19825	2463.91927	1
189	O	79.35119	83.16446	75.05090	293.29899	-391.65602	-477.80926	1
190	H	80.23918	82.95190	74.57200	2528.72714	-681.76262	-751.27122	1
191	C	77.25205	84.17627	74.07001	252.47363	-605.14473	440.05134	1
192	H	77.57307	85.20803	74.34371	-2052.65063	1456.49051	-1043.51830	1
193	H	76.65703	84.25556	73.12683	-2152.98800	-1661.97574	-161.70652	1
194	H	76.56286	83.82244	74.87161	-473.12726	-1584.27339	2165.61725	1
195	C	76.58996	81.90947	72.44780	360.36307	488.46713	505.10056	1
196	O	76.48996	82.76159	71.57940	-200.08817	-528.03552	-385.82850	1
197	N	75.76272	80.91619	72.73157	-597.54095	-226.44775	355.20479	1
198	H	75.99018	80.24899	73.46882	2179.23655	-1300.70981	-991.33835	1
199	C	74.61611	80.73869	71.92774	-687.68921	297.39807	-249.45179	1
200	H	74.47736	81.67935	71.34560	-349.16256	-2467.37713	-1101.72831	1
201	C	74.84848	79.43337	71.02157	672.47345	361.54328	-201.62880	1
202	H	74.89438	78.52931	71.66929	1541.41502	582.18425	2169.97026	1
203	H	73.96702	79.29808	70.35393	-2534.67717	60.25153	997.72295	1
204	C	76.13361	79.53936	70.19026	574.26774	-389.43119	-377.02542	1
205	C	76.29552	80.59652	69.24425	688.82679	-287.33580	-257.96133	1
206	H	75.52018	81.37572	69.13344	331.14182	1470.38163	2269.80013	1
207	C	77.15482	78.55281	70.34792	-383.52382	-675.04808	144.24917	1
208	H	77.04368	77.74131	71.08873	4.09847	1517.59662	2262.86397	1
209	C	77.45292	80.62850	68.46611	-134.76730	428.45285	-649.50303	1
210	H	77.57620	81.44795	67.73669	-903.23433	1600.49020	2011.53387	1
211	C	78.29018	78.62116	69.53733	-335.53281	-615.00040	-364.39058	1
212	H	79.07044	77.85016	69.66141	1596.45398	-1369.33862	1732.02659	1
213	C	78.48069	79.64639	68.56530	585.48547	-340.24194	-406.23938	1
214	O	79.63507	79.71798	67.73943	-419.15649	-173.04408	-511.94141	1
215	H	80.08738	78.88633	68.01873	-1071.84350	1559.71507	-1960.13012	1
216	C	73.40062	80.28209	72.92738	291.41878	-183.13091	710.72246	1
217	O	73.56772	79.44910	73.78863	379.87695	523.47396	-222.23622	1
218	N	72.26369	80.85023	72.52800	564.30591	373.09380	277.24371	1
219	H	72.29119	81.57335	71.80779	-120.59931	-2436.07824	-1214.35098	1
220	C	71.11344	80.64275	73.34280	404.07514	-299.37480	608.84009	1
221	H	71.37949	79.76654	73.98166	-1071.07882	-841.69025	2359.66467	1
222	C	70.90356	81.97311	74.19055	-683.12807	68.71770	-390.13096	1
223	H	71.87592	82.33919	74.59008	2068.88918	1596.58590	770.89603	1
224	H	70.51444	82.79128	73.53553	1379.86429	2342.49779	-179.85638	1
225	C	69.90854	81.65490	75.34379	-176.39967	537.49466	550.97268	1
226	H	68.91773	81.35275	74.93073	-396.28051	1942.22168	1869.33314	1
227	H	70.25805	80.78685	75.94547	-94.44700	586.00678	-2659.20016	1
228	C	69.77974	82.96462	76.26197	-291.69381	-718.18079	-150.72929	1

229	H	70.71390	83.30382	76.77513	-2303.38776	1089.76242	964.62032	1
230	H	69.29598	83.82136	75.72581	884.16729	2568.80533	-207.74283	1
231	N	68.87574	82.45655	77.20169	-594.49522	-252.81478	342.29276	1
232	H	68.10750	81.91836	76.82618	-1735.17426	2084.05705	-263.71605	1
233	C	68.91134	82.63851	78.46393	595.23177	-271.52487	442.22352	1
234	N	69.94196	83.40520	79.01132	585.53813	-424.79750	-105.81303	1
235	H	70.70825	83.89281	78.54997	959.88797	1327.56823	-2177.11905	1
236	H	70.04368	83.62069	80.00382	1578.48647	16.27378	-2220.76233	1
237	N	67.83003	81.99222	79.07699	-452.17763	-390.33541	-421.51853	1
238	H	67.07426	81.43568	78.68107	470.26107	1974.25629	-1817.92087	1
239	H	67.66079	82.01621	80.08295	1856.67307	-1573.97321	-1224.35416	1
240	C	69.78715	80.43518	72.41978	-531.47271	-581.45780	-55.06206	1
241	O	68.68411	80.39820	72.91088	-243.00837	192.73507	609.52485	1
242	N	70.08581	80.25074	71.08967	343.49288	-644.25607	38.09164	1
243	H	71.11298	80.21634	71.11907	-1691.16043	-1535.97525	-1484.73099	1
244	C	69.49242	81.18599	70.10119	542.66492	350.14337	454.42563	1
245	H	69.79705	80.75227	69.12226	1209.57979	-2396.95920	463.86744	1
246	C	68.00038	81.26233	70.28758	-737.14309	145.93010	242.71942	1
247	H	67.80403	81.73444	71.27940	-1050.18303	159.36419	-2509.06125	1
248	C	67.35273	82.11779	69.21121	-706.77696	-252.88343	-245.16230	1
249	H	66.24638	82.22789	69.37563	-1624.64039	-1665.49085	1417.86935	1
250	H	67.79295	83.15254	69.18108	2566.10521	598.51109	693.22305	1
251	H	67.49391	81.67410	68.18815	-1972.69758	107.10018	-1876.34312	1
252	C	67.36056	79.88409	70.30754	412.85148	672.58832	-27.69222	1
253	H	66.24969	79.93828	70.46846	1447.02277	1762.76533	-1490.78944	1
254	H	67.53496	79.32948	69.34562	1320.77379	-145.20455	2378.68491	1
255	H	67.79234	79.25944	71.14022	-1512.10848	1470.52031	1724.75147	1
256	C	70.17872	82.66196	70.37064	-607.11113	499.56689	73.73769	1
257	O	70.13512	83.23291	71.43759	357.97126	460.81534	356.68785	1
258	N	70.76831	83.06272	69.24887	536.55407	-368.62270	332.76306	1
259	H	70.66937	82.47659	68.42071	524.38866	2297.69985	1367.20941	1
260	C	70.99339	84.45969	69.10101	46.50277	-774.29190	-147.97904	1
261	H	70.68260	84.91408	70.07107	1676.51875	1883.29066	1032.55549	1
262	C	72.55443	84.70153	68.76688	-559.41456	-34.19198	-556.30433	1
263	H	72.77447	84.35763	67.72842	-64.66664	395.18769	2695.05373	1
264	H	72.79118	85.79185	68.78106	-2703.44278	-60.40056	333.79418	1
265	C	73.40426	83.94923	69.75654	-519.76435	377.31045	459.42366	1
266	H	73.14145	82.86869	69.69200	-1746.74323	1667.50644	-1261.73691	1
267	C	74.87822	84.11307	69.42192	570.95554	16.46261	-545.27700	1
268	H	75.54224	83.60483	70.21316	2391.58273	28.05277	-1305.07271	1
269	H	75.13210	83.66701	68.42579	175.75588	917.63458	2559.43867	1
270	H	75.17489	85.19290	69.38473	-1063.97851	-2155.34650	1283.00462	1
271	C	73.14553	84.41145	71.18413	193.76014	2.62946	-765.53141	1
272	H	73.83375	83.90908	71.91241	507.39394	-846.55087	2539.60089	1
273	H	73.29637	85.51622	71.29443	1337.57841	1818.19054	1526.01994	1
274	H	72.09050	84.17754	71.50378	1100.88635	-1172.91350	-2199.08909	1
275	C	70.11097	84.92201	67.83503	-549.21115	475.64486	-309.38218	1
276	O	69.44846	84.16226	67.17751	556.06106	-390.37755	-78.24250	1
277	O	70.16243	86.29892	67.50972	-572.27940	-310.19032	-209.75862	1
278	H	70.76145	86.60782	68.24360	-1380.08193	2212.14486	790.85944	1

Listing 64: C00064.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.6118	0.0000	300.0000
3	H	70.86456	70.38264	90.46485	-2043.14101	-1757.64893	399.89339		1
4	N	71.80658	69.99925	90.47458	426.75047	490.45733	-334.42467		1
5	H	71.71069	69.16223	89.90548	442.25559	-1110.30854	-2448.52907		1
6	C	72.83715	70.88415	90.09649	415.32972	-666.39213	83.73172		1
7	H	72.57003	71.84158	90.59306	879.32219	2491.00447	667.35213		1
8	C	74.24872	70.29569	90.60647	31.35357	477.41777	628.23362		1

9	H	74.46175	69.33946	90.07081	1168.38489	2240.25337	-1019.71136	1
10	H	75.07730	70.99155	90.32944	-360.43770	2534.90498	931.67112	1
11	C	74.20722	70.06533	92.09506	463.18208	512.70242	-382.34388	1
12	H	73.30501	69.45528	92.32770	1725.29117	1863.52247	-987.07854	1
13	C	75.44389	69.29722	92.54439	710.42801	-144.27427	-313.15367	1
14	H	75.42718	69.09280	93.64602	364.20195	-1033.13725	2494.72524	1
15	H	75.52980	68.30863	92.02356	2567.61904	335.80679	847.48802	1
16	H	76.38344	69.86829	92.32759	-2587.99029	680.92867	-512.16411	1
17	C	74.11602	71.37792	92.86090	268.17616	741.64379	-40.42634	1
18	H	74.13110	71.21158	93.96911	1283.54314	-1945.37420	-1411.27812	1
19	H	74.97178	72.05872	92.61556	-1258.57796	1317.15249	-2026.02085	1
20	H	73.17161	71.93183	92.62279	-2502.84526	909.80597	575.92391	1
21	C	72.93921	71.03142	88.49148	619.36578	-458.64843	-172.09273	1
22	O	73.89841	71.60576	88.00006	-81.40433	433.87611	522.34594	1
23	N	71.91748	70.48047	87.84853	175.23996	-622.20190	341.55523	1
24	H	71.13713	70.09702	88.37724	-876.57256	-303.22879	-2561.90213	1
25	C	71.87538	70.62607	86.43096	-571.88214	-534.10783	-106.15033	1
26	H	72.94571	70.69310	86.13271	-2713.20841	-16.25800	-248.80809	1
27	C	71.06905	69.37766	85.83846	166.60354	288.16399	-716.09568	1
28	H	70.03775	69.37040	86.28520	-2097.85574	1636.78449	-586.18044	1
29	O	71.63676	68.08280	86.09796	-317.80580	-363.38227	484.43082	1
30	H	70.92395	67.66267	86.62009	1863.74748	-1451.84923	1357.29467	1
31	C	70.98097	69.79086	84.32236	503.80731	517.99032	318.51606	1
32	H	70.41117	69.04037	83.72779	640.61020	-2157.10410	-1536.29104	1
33	H	70.47909	70.77936	84.17740	1687.88455	465.60692	2087.56452	1
34	H	71.99790	69.87582	83.87123	-1293.07895	-1899.88581	-1463.57452	1
35	C	71.01673	71.99345	86.14453	-153.07550	-733.68902	248.70981	1
36	O	69.84411	71.99966	86.40537	186.15459	-480.78787	-449.34387	1
37	N	71.77443	72.95137	85.58836	-487.53139	543.18517	42.03850	1
38	C	71.26571	74.27826	85.43054	-699.35871	69.34393	360.10701	1
39	H	70.56548	74.45232	86.27904	2.81126	-221.99807	-2715.58072	1
40	C	72.59200	75.14778	85.44988	-507.46439	-592.59194	122.07761	1
41	H	72.47090	76.12642	84.93320	-1975.08116	525.87560	-1801.71556	1
42	H	72.90738	75.37711	86.49217	1588.27743	-1913.22100	1113.83566	1
43	C	73.62525	74.20842	84.75019	-613.62442	-457.55993	-194.14490	1
44	H	73.52017	74.25409	83.64295	1707.54637	-721.27992	1996.92523	1
45	H	74.68503	74.46487	84.97584	758.23357	2100.81767	1560.55011	1
46	C	73.19632	72.78923	85.31474	-352.41524	704.96076	49.21465	1
47	H	73.31806	71.94167	84.59864	1714.76886	-2070.42778	443.35792	1
48	H	73.65640	72.50352	86.31431	1224.15040	1801.50881	1636.97633	1
49	C	70.49232	74.41864	83.98911	566.85117	537.05831	117.62814	1
50	O	69.61955	75.24188	83.87131	-550.26779	-406.08867	4.21666	1
51	N	71.04299	73.64020	83.06356	566.34832	-425.77725	180.18749	1
52	H	71.76211	72.97441	83.35590	644.44502	2646.80550	-52.73430	1
53	C	70.35344	73.38809	81.84843	612.34801	-281.48662	411.56221	1
54	H	69.33779	73.83699	81.93959	1667.23498	-1490.75142	1556.16753	1
55	C	71.23003	74.02952	80.66832	-714.45746	-175.43074	286.98927	1
56	H	72.23688	73.52868	80.65504	-787.09484	1763.03619	-1922.46060	1
57	O	71.49262	75.43930	80.76356	-429.46514	516.51932	-128.40526	1
58	H	72.46938	75.44900	80.82268	1981.82785	436.16847	-1818.18182	1
59	C	70.40297	73.58661	79.40730	630.79189	-468.94448	76.03230	1
60	H	70.87680	73.96100	78.47142	-1775.71861	2062.30353	131.89849	1
61	H	70.32519	72.47637	79.32115	-1855.14608	88.94118	1993.53760	1
62	H	69.36585	73.99492	79.43500	-1504.82350	-780.94249	-2132.90992	1
63	C	70.44136	71.75692	81.71863	288.57638	618.62814	-397.00270	1
64	O	71.42235	71.17467	82.13326	321.70495	-185.26452	574.37218	1
65	N	69.38622	71.27097	81.08526	-447.05792	-446.53431	367.76425	1
66	H	68.65698	71.89210	80.73746	350.31316	1975.63644	-1843.31522	1
67	C	69.33793	69.86448	80.84077	-511.23061	374.03917	-471.51480	1
68	H	69.65877	69.39671	81.79656	2234.79579	-898.70890	-1273.45190	1
69	C	67.84026	69.55292	80.39652	529.53781	-159.34528	563.72604	1
70	H	67.77978	68.44342	80.24799	654.59388	2347.94251	1217.51488	1

71	H	67.13277	69.78347	81.23660	-1526.55661	2103.42026	817.87394	1
72	O	67.35719	70.25934	79.21203	-554.84278	14.12789	399.58769	1
73	H	68.13813	70.15177	78.63353	1297.06236	2061.84854	1220.68812	1
74	C	70.36599	69.52392	79.61843	-662.15484	-412.13544	123.62687	1
75	O	70.28974	70.03039	78.51951	-540.01537	-317.05804	274.91456	1
76	N	71.17105	68.50980	80.01761	-202.76299	-690.00100	-131.49145	1
77	H	70.95772	68.30967	80.99866	-702.62132	-2617.37191	281.70413	1
78	C	72.58477	68.74254	79.75966	-491.73914	576.34187	222.73509	1
79	H	72.74597	69.82679	79.94255	1977.17978	-1823.58850	-434.68928	1
80	C	73.36632	67.78524	80.74063	-649.50797	-328.66843	306.11224	1
81	H	72.87599	66.78786	80.78024	2075.07803	1452.16490	-1004.45904	1
82	C	74.83710	67.65340	80.21030	-615.18735	-489.99689	-70.96352	1
83	H	75.45900	67.00559	80.87139	-1226.32661	-1724.38906	-1716.47170	1
84	H	74.84846	67.19892	79.18787	2381.64273	-969.84735	900.46860	1
85	H	75.34149	68.64524	80.13983	2122.74991	1702.23946	-141.36228	1
86	C	73.41860	68.43022	82.16985	-501.86074	-479.61276	-376.42482	1
87	H	74.04616	67.83216	82.87151	993.79261	-2246.95401	-1177.81305	1
88	H	73.83983	69.46247	82.14092	42.71279	-626.15391	-2651.37258	1
89	H	72.40080	68.49971	82.61632	-2026.39012	-1590.33709	-887.82922	1
90	C	72.92788	68.28369	78.24307	-672.89153	382.57394	-156.34072	1
91	O	72.94825	67.11948	77.91553	410.04627	221.86223	500.35950	1
92	N	73.30033	69.35110	77.50832	-378.11782	-443.79414	-441.10984	1
93	H	73.16135	70.26510	77.94214	2404.15973	-568.14894	1149.30085	1
94	C	73.03250	69.18519	76.09329	-544.54484	466.16019	331.29119	1
95	H	73.64813	68.29759	75.82917	-1409.80988	-170.17955	2325.32679	1
96	C	71.49530	68.83108	76.01146	-184.48284	116.78282	-758.89137	1
97	H	71.29745	67.85416	76.51556	1893.78641	1861.14652	611.04528	1
98	H	70.89062	69.57433	76.59427	-2170.79665	-974.19311	1327.50117	1
99	C	71.06354	68.76828	74.51288	389.51668	672.81878	-138.49152	1
100	H	71.38573	69.68842	73.97692	510.64577	1933.03327	1851.02484	1
101	H	71.60378	67.94933	73.98827	-2302.30869	-1105.72939	-948.89774	1
102	C	69.50869	68.57287	74.35103	-559.93427	-126.34590	542.30857	1
103	O	69.04382	68.42014	73.25101	-670.36003	-111.83166	76.36448	1
104	N	68.81899	68.62124	75.51158	-216.06729	-537.07037	446.51379	1
105	H	69.14865	68.74737	76.47624	-1251.96487	1074.12894	-2168.52500	1
106	H	67.80022	68.51851	75.57461	-2451.83023	-720.73851	944.84612	1
107	C	73.52057	70.53115	75.32167	546.24052	-563.88337	-85.11809	1
108	O	74.46588	70.37881	74.59005	71.70702	-307.40463	606.69673	1
109	N	72.82462	71.65638	75.54689	479.90863	-504.50129	222.86849	1
110	C	73.25025	72.87587	74.92959	75.51268	-600.91904	506.73700	1
111	H	73.74690	72.60639	73.96915	-2033.61562	1795.30103	254.89480	1
112	C	71.87339	73.66429	74.81747	523.79067	517.99274	284.45581	1
113	H	72.01109	74.75963	74.67814	1599.61665	-1127.00911	1895.98173	1
114	H	71.25748	73.30413	73.96359	-1881.83093	1275.82488	-1501.55016	1
115	C	71.22596	73.29196	76.18497	-600.05639	-404.05026	316.64485	1
116	H	71.73054	73.84126	77.01538	-2597.05260	496.36221	657.73249	1
117	H	70.13778	73.51995	76.25070	-1666.24518	1294.38985	-1723.90591	1
118	C	71.54869	71.73674	76.24323	493.57570	-129.95376	-602.56394	1
119	H	71.67107	71.31707	77.27062	-1469.08415	-637.84797	2204.22581	1
120	H	70.83719	71.10094	75.66547	-1038.97840	1068.88701	-2280.71789	1
121	C	74.23160	73.69640	75.95558	188.88100	241.05089	-727.87821	1
122	O	74.01036	73.78333	77.14287	531.88613	-49.19943	427.07960	1
123	N	75.19414	74.28684	75.25669	708.14833	26.93417	-179.73509	1
124	H	75.26426	74.09409	74.25823	-2232.69501	-1179.09831	1023.94816	1
125	C	76.16143	75.02020	76.00974	-738.32412	259.92548	104.42456	1
126	H	75.56366	75.46243	76.83960	2028.89123	1260.02983	1311.33324	1
127	C	77.22828	73.98640	76.58309	-258.65678	-345.52513	661.28459	1
128	H	77.72359	73.43711	75.75391	-1826.06090	-1801.46097	-918.64554	1
129	C	78.27123	74.79954	77.42130	-541.23400	531.92970	-218.41428	1
130	H	79.06904	74.14240	77.84056	1311.73218	-2219.18200	882.19023	1
131	H	78.77241	75.58101	76.79858	-1048.71298	1223.58118	-2196.97971	1
132	H	77.78693	75.32527	78.27756	419.06414	1903.92898	1903.44670	1

133	C	76.50898	72.98646	77.55295	-423.86431	152.66566	-648.55262	1
134	H	77.23554	72.31052	78.06305	105.68386	-2342.50080	1387.51238	1
135	H	75.93708	73.52760	78.34577	-1695.63603	-1484.73621	-1531.02793	1
136	H	75.77821	72.34083	77.00613	-1853.57121	-487.39031	1936.59343	1
137	C	76.95137	76.10095	75.07354	539.71428	-510.58232	267.58633	1
138	O	77.48513	77.04718	75.60684	-15.93758	-278.34085	-624.49402	1
139	N	77.03864	75.72479	73.80210	-676.81886	12.05292	276.17960	1
140	H	76.55311	74.88034	73.50215	-1694.44250	-373.84189	-2100.66098	1
141	C	77.45878	76.72616	72.85851	412.33078	-664.70360	108.35451	1
142	H	76.88512	77.63730	73.13428	1765.77476	1294.44366	1621.76594	1
143	C	79.00443	76.92566	73.10148	-179.66635	-721.95667	-264.73915	1
144	H	79.16428	77.39179	74.10225	-607.34922	2587.87032	-598.10018	1
145	H	79.53920	75.95052	73.14348	-359.69332	-1479.13954	-2259.74260	1
146	C	79.57390	77.82823	71.95651	-240.01076	616.02425	431.85322	1
147	H	79.96766	77.21307	71.11484	-1359.17131	782.54425	2227.99181	1
148	H	78.50351	80.01396	71.66786	-820.36667	85.81767	-2596.78715	1
149	C	80.70422	78.73401	72.59157	-513.07015	236.18570	-551.87280	1
150	H	80.29974	79.33752	73.43658	1816.11944	-1183.11722	-1650.94321	1
151	H	81.51349	78.10533	73.02868	-1800.04429	-1361.53473	1526.34643	1
152	C	81.26652	79.65575	71.48439	726.08972	-253.19732	-179.64713	1
153	H	81.77082	79.11493	70.63843	1224.27271	-456.51798	-2390.90304	1
154	H	80.54160	80.39751	71.08077	1206.40339	-1150.93514	-2154.90344	1
155	N	82.39197	80.54094	72.11005	329.70796	-633.68968	-155.67358	1
156	H	82.83120	81.23570	71.43962	1348.31305	1938.76845	1359.00643	1
157	H	82.12680	81.17309	72.92079	2096.92035	1446.54551	-966.48890	1
158	H	83.25169	80.04255	72.48304	-1197.07217	-2303.53719	827.28733	1
159	C	77.14163	76.18115	71.34663	-378.01186	-556.17301	-413.96481	1
160	O	76.42174	76.84008	70.62768	-409.44433	-307.55053	-453.30833	1
161	N	77.75040	75.02719	71.11443	-429.02477	524.70884	274.08502	1
162	H	78.27676	74.64319	71.89888	1706.34263	-1425.96036	1574.38926	1
163	C	77.87596	74.48267	69.80886	-45.25864	-626.22952	478.93267	1
164	H	78.33908	73.48958	70.00695	1988.63164	570.90773	1772.87287	1
165	C	76.42735	74.41161	69.17912	551.77128	-20.49526	-564.54996	1
166	H	75.69159	74.06654	69.94012	1434.61535	-1753.10253	1513.99471	1
167	H	76.08863	75.43064	68.87420	-714.67738	1819.09770	1898.36494	1
168	C	76.46992	73.43245	67.95939	446.99263	-555.77305	338.97221	1
169	H	77.10873	73.84207	67.14498	1953.68466	1892.25957	-161.67766	1
170	H	76.92532	72.45908	68.24957	-403.03785	2688.07032	-188.43591	1
171	C	74.98014	73.22347	67.47040	567.86262	335.74681	434.04421	1
172	H	74.33479	72.87487	68.30931	-1080.02275	1568.26081	-1948.78900	1
173	H	74.53626	74.18700	67.12910	-919.54108	2111.34692	1456.13463	1
174	C	74.98777	72.18312	66.32667	195.81897	173.33862	-745.11536	1
175	H	75.51926	72.50748	65.41001	1405.67949	-2301.21089	-390.08113	1
176	H	75.32920	71.17145	66.62411	-940.37328	-1118.32446	2299.72133	1
177	N	73.50179	71.97901	65.87457	319.26422	656.36007	-42.02424	1
178	H	73.35227	71.29206	65.08026	1961.03633	619.91968	1787.09422	1
179	H	72.82283	71.60769	66.60108	854.14343	-2156.80752	1429.08711	1
180	H	72.98700	72.83342	65.51182	1237.02905	-1378.50857	-1998.28500	1
181	C	78.84812	75.46136	68.91098	532.53319	-268.57236	517.55729	1
182	O	78.42026	76.10016	67.95050	266.16714	-290.73804	-558.88002	1
183	N	80.06126	75.40095	69.40783	-226.25352	640.49678	-270.32839	1
184	H	80.10556	74.80873	70.23620	2007.69063	-1035.27229	1523.50231	1
185	C	81.24469	75.80510	68.74013	-540.76542	-573.33303	49.50000	1
186	H	82.05677	75.36362	69.35921	-2374.20950	-1036.76023	843.75774	1
187	C	81.21265	75.21324	67.25115	-77.09082	666.87422	-415.84136	1
188	H	80.26895	75.55534	66.74165	-985.81834	617.19825	2463.91927	1
189	O	81.20852	73.77727	67.16472	293.29899	-391.65602	-477.80926	1
190	H	80.34367	73.61768	66.73586	2528.72714	-681.76262	-751.27122	1
191	C	82.44203	75.94130	66.59574	252.47363	-605.14473	440.05134	1
192	H	82.54344	75.68057	65.51672	-2052.65063	1456.49051	-1043.51830	1
193	H	82.34983	77.05201	66.65808	-2152.98800	-1661.97574	-161.70652	1
194	H	83.39781	75.65907	67.09554	-473.12726	-1584.27339	2165.61725	1

195	C	81.34416	77.43652	68.69921	360.36307	488.46713	505.10056	1
196	O	82.33643	77.96842	69.15313	-200.08817	-528.03552	-385.82850	1
197	N	80.31400	77.98483	68.08081	-597.54095	-226.44775	355.20479	1
198	H	79.50811	77.39593	67.74165	2179.23655	-1300.70981	-991.33835	1
199	C	80.34050	79.39014	67.90800	-687.68921	297.39807	-249.45179	1
200	H	81.40417	79.70190	68.02817	-349.16256	-2467.37713	-1101.72831	1
201	C	79.68332	79.71578	66.48075	672.47345	361.54328	-201.62880	1
202	H	78.72992	79.15365	66.35108	1541.41502	582.18425	2169.97026	1
203	H	79.43617	80.80028	66.41479	-2534.67717	60.25153	997.72295	1
204	C	80.71384	79.32330	65.41541	574.26774	-389.43119	-377.02542	1
205	C	81.74971	80.25341	65.09948	688.82679	-287.33580	-257.96133	1
206	H	81.78840	81.24265	65.59057	331.14182	1470.38163	2269.80013	1
207	C	80.67730	78.03979	64.79069	-383.52382	-675.04808	144.24917	1
208	H	79.88613	77.31192	65.04578	4.09847	1517.59662	2262.86397	1
209	C	82.71534	79.88441	64.16480	-134.76730	428.45285	-649.50303	1
210	H	83.51629	80.60398	63.92044	-903.23433	1600.49020	2011.53387	1
211	C	81.66795	77.71805	63.85959	-335.53281	-615.00040	-364.39058	1
212	H	81.63199	76.72394	63.38079	1596.45398	-1369.33862	1732.02659	1
213	C	82.71702	78.61818	63.51080	585.48547	-340.24194	-406.23938	1
214	O	83.72978	78.30213	62.56829	-419.15649	-173.04408	-511.94141	1
215	H	83.43950	77.39623	62.30894	-1071.84350	1559.71507	-1960.13012	1
216	C	79.35244	80.09377	69.00926	291.41878	-183.13091	710.72246	1
217	O	79.56941	81.22431	69.38360	379.87695	523.47396	-222.23622	1
218	N	78.37435	79.26611	69.35772	564.30591	373.09380	277.24371	1
219	H	78.37909	78.33789	68.93341	-120.59931	-2436.07824	-1214.35098	1
220	C	77.16003	79.77629	69.90498	404.07514	-299.37480	608.84009	1
221	H	76.56024	78.83686	70.02201	-1071.07882	-841.69025	2359.66467	1
222	C	77.54459	80.44839	71.29101	-683.12807	68.71770	-390.13096	1
223	H	78.76365	78.45571	71.51077	2068.88918	1596.58590	770.89603	1
224	H	77.74824	81.54289	71.17131	1379.86429	2342.49779	-179.85638	1
225	C	76.40163	80.19253	72.31903	-176.39967	537.49466	550.97268	1
226	H	75.58947	80.94771	72.23367	-396.28051	1942.22168	1869.33314	1
227	H	75.91662	79.20722	72.13994	-94.44700	586.00678	-2659.20016	1
228	C	77.08737	80.23753	73.76186	-291.69381	-718.18079	-150.72929	1
229	H	77.84555	79.43692	73.95985	-2303.38776	1089.76242	964.62032	1
230	H	77.53351	81.21846	74.06560	884.16729	2568.80533	-207.74283	1
231	N	75.97630	79.98189	74.57973	-594.49522	-252.81478	342.29276	1
232	H	75.11666	79.73367	74.11446	-1735.17426	2084.05705	-263.71605	1
233	C	75.98728	80.02570	75.85065	595.23177	-271.52487	442.22352	1
234	N	77.18873	80.36823	76.48135	585.53813	-424.79750	-105.81303	1
235	H	78.10663	80.52638	76.06803	959.88797	1327.56823	-2177.11905	1
236	H	77.33433	80.38739	77.49095	1578.48647	16.27378	-2220.76233	1
237	N	74.72183	79.71754	76.36750	-452.17763	-390.33541	-421.51853	1
238	H	73.85560	79.45243	75.90108	470.26107	1974.25629	-1817.92087	1
239	H	74.52080	79.67859	77.36734	1856.67307	-1573.97321	-1224.35416	1
240	C	76.51377	80.80924	68.82491	-531.47271	-581.45780	-55.06206	1
241	O	76.84467	80.82771	67.65255	-243.00837	192.73507	609.52485	1
242	N	75.48392	81.46956	69.37117	343.49288	-644.25607	38.09164	1
243	H	75.44927	81.24043	70.36284	-1691.16043	-1535.97525	-1484.73099	1
244	C	75.02242	82.77321	68.87553	542.66492	350.14337	454.42563	1
245	H	74.29348	83.09371	69.65745	1209.57979	-2396.95920	463.86744	1
246	C	76.19669	83.72696	68.77306	-737.14309	145.93010	242.71942	1
247	H	76.89520	83.31398	68.00973	-1050.18303	159.36419	-2509.06125	1
248	C	75.76567	85.11542	68.33644	-706.77696	-252.88343	-245.16230	1
249	H	76.64672	85.79441	68.17167	-1624.64039	-1665.49085	1417.86935	1
250	H	75.17337	85.08217	67.36943	2566.10521	598.51109	693.22305	1
251	H	75.11039	85.60537	69.10792	-1972.69758	107.10018	-1876.34312	1
252	C	76.96117	83.84490	70.08019	412.85148	672.58832	-27.69222	1
253	H	77.83786	84.54292	69.98830	1447.02277	1762.76533	-1490.78944	1
254	H	76.30839	84.23708	70.90774	1320.77379	-145.20455	2378.68491	1
255	H	77.36297	82.84305	70.41452	-1512.10848	1470.52031	1724.75147	1
256	C	74.29857	82.55026	67.41043	-607.11113	499.56689	73.73769	1

257	O	74.10518	83.50150	66.67486	357.97126	460.81534	356.68785	1
258	N	73.92231	81.29805	67.22877	536.55407	-368.62270	332.76306	1
259	H	74.17778	80.64215	67.96397	524.38866	2297.69985	1367.20941	1
260	C	73.33011	80.91390	66.00170	46.50277	-774.29190	-147.97904	1
261	H	73.00478	81.86919	65.52954	1676.51875	1883.29066	1032.55549	1
262	C	74.40270	80.10272	65.10374	-559.41456	-34.19198	-556.30433	1
263	H	74.64420	79.13918	65.61264	-64.66664	395.18769	2695.05373	1
264	H	73.94684	79.82391	64.12412	-2703.44278	-60.40056	333.79418	1
265	C	75.66037	80.90102	64.89974	-519.76435	377.31045	459.42366	1
266	H	76.10350	81.12088	65.92255	-1746.74323	1667.50644	-1261.73691	1
267	C	76.67938	80.09272	64.10645	570.95554	16.46261	-545.27700	1
268	H	77.64161	80.65262	63.97766	2391.58273	28.05277	-1305.07271	1
269	H	76.92588	79.12591	64.61661	175.75588	917.63458	2559.43867	1
270	H	76.30119	79.84181	63.08210	-1063.97851	-2155.34650	1283.00462	1
271	C	75.38253	82.21663	64.19021	193.76014	2.62946	-765.53141	1
272	H	76.33080	82.74671	63.91417	507.39394	-846.55087	2539.60089	1
273	H	74.79890	82.06563	63.24520	1337.57841	1818.19054	1526.01994	1
274	H	74.78928	82.91751	64.85317	1100.88635	-1172.91350	-2199.08909	1
275	C	72.15230	79.86710	66.34205	-549.21115	475.64486	-309.38218	1
276	O	72.06381	79.27848	67.38750	556.06106	-390.37755	-78.24250	1
277	O	71.27354	79.57012	65.27177	-572.27940	-310.19032	-209.75862	1
278	H	71.62382	80.21887	64.60119	-1380.08193	2212.14486	790.85944	1

Listing 65: C00065.xmolout

1		276								
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100	
		0.2500	300.00	0.00	0.00	0.00	-1293.6047	0.0000	300.0000	
3	H	77.68201	85.57534	79.91449	-2043.14101	-1757.64893	399.89339			1
4	N	78.18837	86.21783	80.52109	426.75047	490.45733	-334.42467			1
5	H	78.65034	85.58419	81.17055	442.25559	-1110.30854	-2448.52907			1
6	C	79.06743	87.11451	79.87739	415.32972	-666.39213	83.73172			1
7	H	78.61109	87.32671	78.88829	879.32219	2491.00447	667.35213			1
8	C	79.20590	88.40956	80.82071	31.35357	477.41777	628.23362			1
9	H	79.60463	88.09689	81.81617	1168.38489	2240.25337	-1019.71136			1
10	H	79.94675	89.13219	80.40016	-360.43770	2534.90498	931.67112			1
11	C	77.84304	89.04307	80.96662	463.18208	512.70242	-382.34388			1
12	H	77.11046	88.23434	81.18950	1725.29117	1863.52247	-987.07854			1
13	C	77.82974	90.03299	82.12342	710.42801	-144.27427	-313.15367			1
14	H	76.81887	90.49870	82.25719	364.20195	-1033.13725	2494.72524			1
15	H	78.09925	89.54016	83.09351	2567.61904	335.80679	847.48802			1
16	H	78.56002	90.86741	81.96048	-2587.99029	680.92867	-512.16411			1
17	C	77.41851	89.74546	79.68490	268.17616	741.64379	-40.42634			1
18	H	76.41156	90.22632	79.79122	1283.54314	-1945.37420	-1411.27812			1
19	H	78.14231	90.55163	79.39768	-1258.57796	1317.15249	-2026.02085			1
20	H	77.35556	89.03354	78.82192	-2502.84526	909.80597	575.92391			1
21	C	80.52176	86.35302	79.79438	619.36578	-458.64843	-172.09273			1
22	O	81.17408	86.08732	80.77790	-81.40433	433.87611	522.34594			1
23	N	80.78194	86.10612	78.51304	175.23996	-622.20190	341.55523			1
24	H	80.13981	86.47716	77.81298	-876.57256	-303.22879	-2561.90213			1
25	C	81.93392	85.38037	78.10396	-571.88214	-534.10783	-106.15033			1
26	H	81.84768	85.36415	76.99422	-2713.20841	-16.25800	-248.80809			1
27	C	83.18004	86.27414	78.58477	166.60354	288.16399	-716.09568			1
28	H	83.18639	86.24471	79.71055	-2097.85574	1636.78449	-586.18044			1
29	O	83.10444	87.66268	78.21002	-317.80580	-363.38227	484.43082			1
30	H	82.98190	88.07862	79.08650	1863.74748	-1451.84923	1357.29467			1
31	C	84.45583	85.54436	78.03034	503.80731	517.99032	318.51606			1
32	H	85.38802	86.07046	78.34410	640.61020	-2157.10410	-1536.29104			1
33	H	84.53902	84.47884	78.38961	1687.88455	465.60692	2087.56452			1
34	H	84.45551	85.51796	76.91545	-1293.07895	-1899.88581	-1463.57452			1
35	C	81.93123	83.89141	78.74506	-153.07550	-733.68902	248.70981			1
36	O	82.99269	83.31042	78.77366	186.15459	-480.78787	-449.34387			1

37	N	80.72706	83.39898	79.06749	-487.53139	543.18517	42.03850	1
38	C	80.58736	82.40227	80.08542	-699.35871	69.34393	360.10701	1
39	H	81.31831	82.64841	80.88877	2.81126	-221.99807	-2715.58072	1
40	C	79.05843	82.53815	80.47932	-507.46439	-592.59194	122.07761	1
41	H	78.65445	81.61825	80.95943	-1975.08116	525.87560	-1801.71556	1
42	H	78.89632	83.37136	81.19861	1588.27743	-1913.22100	1113.83566	1
43	C	78.40382	82.84768	79.09557	-613.62442	-457.55993	-194.14490	1
44	H	78.30260	81.92002	78.48830	1707.54637	-721.27992	1996.92523	1
45	H	77.38490	83.28914	79.17182	758.23357	2100.81767	1560.55011	1
46	C	79.47241	83.84323	78.47192	-352.41524	704.96076	49.21465	1
47	H	79.57293	83.82086	77.36118	1714.76886	-2070.42778	443.35792	1
48	H	79.37019	84.90316	78.81132	1224.15040	1801.50881	1636.97633	1
49	C	80.85861	80.91119	79.45245	566.85117	537.05831	117.62814	1
50	O	81.12174	79.98418	80.18258	-550.26779	-406.08867	4.21666	1
51	N	80.63670	80.90629	78.14058	566.34832	-425.77725	180.18749	1
52	H	80.43316	81.81514	77.73043	644.44502	2646.80550	-52.73430	1
53	C	80.85348	79.71950	77.40392	612.34801	-281.48662	411.56221	1
54	H	81.26837	78.99645	78.14497	1667.23498	-1490.75142	1556.16753	1
55	C	79.45959	79.25782	76.75807	-714.45746	-175.43074	286.98927	1
56	H	79.12417	80.03369	76.01617	-787.09484	1763.03619	-1922.46060	1
57	O	78.36519	79.08624	77.67155	-429.46514	516.51932	-128.40526	1
58	H	77.71200	79.72016	77.31200	1981.82785	436.16847	-1818.18182	1
59	C	79.91921	77.96638	75.98782	630.79189	-468.94448	76.03230	1
60	H	79.08674	77.53232	75.38387	-1775.71861	2062.30353	131.89849	1
61	H	80.77013	78.17325	75.29334	-1855.14608	88.94118	1993.53760	1
62	H	80.25753	77.17470	76.69589	-1504.82350	-780.94249	-2132.90992	1
63	C	81.84806	80.08588	76.14065	288.57638	618.62814	-397.00270	1
64	O	82.69763	79.26844	75.85209	321.70495	-185.26452	574.37218	1
65	N	81.42302	81.15082	75.47621	-447.05792	-446.53431	367.76425	1
66	H	80.61966	81.59376	75.92217	350.31316	1975.63644	-1843.31522	1
67	C	82.20399	81.95156	74.59608	-511.23061	374.03917	-471.51480	1
68	H	81.42995	82.64023	74.18814	2234.79579	-898.70890	-1273.45190	1
69	C	83.24603	82.82266	75.45802	529.53781	-159.34528	563.72604	1
70	H	83.72323	83.53164	74.72690	654.59388	2347.94251	1217.51488	1
71	H	82.65171	83.44430	76.17974	-1526.55661	2103.42026	817.87394	1
72	O	84.29597	82.11039	76.15264	-554.84278	14.12789	399.58769	1
73	H	83.94490	82.15838	77.06980	1297.06236	2061.84854	1220.68812	1
74	C	82.93153	81.12029	73.42244	-662.15484	-412.13544	123.62687	1
75	O	83.74718	81.65421	72.71223	-540.01537	-317.05804	274.91456	1
76	N	82.38044	79.89005	73.25838	-202.76299	-690.00100	-131.49145	1
77	H	81.77357	79.65189	74.05658	-702.62132	-2617.37191	281.70413	1
78	C	83.19339	78.79681	72.69232	-491.73914	576.34187	222.73509	1
79	H	83.56478	79.23491	71.73660	1977.17978	-1823.58850	-434.68928	1
80	C	84.31996	78.46126	73.64310	-649.50797	-328.66843	306.11224	1
81	H	83.86518	78.02828	74.57038	2075.07803	1452.16490	-1004.45904	1
82	C	85.26380	77.42964	73.05187	-615.18735	-489.99689	-70.96352	1
83	H	86.06678	77.13237	73.78065	-1226.32661	-1724.38906	-1716.47170	1
84	H	84.70575	76.48982	72.75827	2381.64273	-969.84735	900.46860	1
85	H	85.77741	77.81648	72.12970	2122.74991	1702.23946	-141.36228	1
86	C	85.10731	79.68589	74.07448	-501.86074	-479.61276	-376.42482	1
87	H	85.98567	79.41987	74.72366	993.79261	-2246.95401	-1177.81305	1
88	H	85.49784	80.26259	73.18861	42.71279	-626.15391	-2651.37258	1
89	H	84.45234	80.39662	74.66551	-2026.39012	-1590.33709	-887.82922	1
90	C	82.18701	77.50276	72.48940	-672.89153	382.57394	-156.34072	1
91	O	82.63072	76.36722	72.50185	410.04627	221.86223	500.35950	1
92	N	80.93923	77.87592	72.28965	-378.11782	-443.79414	-441.10984	1
93	H	80.81086	78.88355	72.23629	2404.15973	-568.14894	1149.30085	1
94	C	79.89109	76.92567	72.14359	-544.54484	466.16019	331.29119	1
95	H	80.23917	76.02806	72.69908	-1409.80988	-170.17955	2325.32679	1
96	C	78.59443	77.63200	72.71292	-184.48284	116.78282	-758.89137	1
97	H	78.75706	77.93747	73.77176	1893.78641	1861.14652	611.04528	1
98	H	78.38935	78.57355	72.15431	-2170.79665	-974.19311	1327.50117	1

99	C	77.38628	76.64983	72.59058	389.51668	672.81878	-138.49152	1
100	H	77.21309	76.38318	71.52169	510.64577	1933.03327	1851.02484	1
101	H	77.62412	75.67483	73.07167	-2302.30869	-1105.72939	-948.89774	1
102	C	76.06567	77.23755	73.20747	-559.93427	-126.34590	542.30857	1
103	O	75.02451	76.64074	73.06825	-670.36003	-111.83166	76.36448	1
104	N	76.23539	78.39484	73.87710	-216.06729	-537.07037	446.51379	1
105	H	77.09552	78.92468	74.06045	-1251.96487	1074.12894	-2168.52500	1
106	H	75.48840	78.87773	74.38889	-2451.83023	-720.73851	944.84612	1
107	C	79.70937	76.67429	70.53222	546.24052	-563.88337	-85.11809	1
108	O	79.24032	77.54367	69.84732	71.70702	-307.40463	606.69673	1
109	N	80.11440	75.44231	70.18913	479.90863	-504.50129	222.86849	1
110	C	80.30526	75.09049	68.81432	75.51268	-600.91904	506.73700	1
111	H	80.65754	76.01150	68.29539	-2033.61562	1795.30103	254.89480	1
112	C	81.36935	73.91411	68.90630	523.79067	517.99274	284.45581	1
113	H	81.33060	73.22957	68.02940	1599.61665	-1127.00911	1895.98173	1
114	H	82.40831	74.30970	68.95335	-1881.83093	1275.82488	-1501.55016	1
115	C	80.97358	73.22080	70.24711	-600.05639	-404.05026	316.64485	1
116	H	80.08188	72.56804	70.11179	-2597.05260	496.36221	657.73249	1
117	H	81.77679	72.57839	70.67369	-1666.24518	1294.38985	-1723.90591	1
118	C	80.63308	74.48057	71.15201	493.57570	-129.95376	-602.56394	1
119	H	79.84964	74.30298	71.92674	-1469.08415	-637.84797	2204.22581	1
120	H	81.52658	74.99436	71.62731	-1038.97840	1068.88701	-2280.71789	1
121	C	78.91641	74.53250	68.15614	188.88100	241.05089	-727.87821	1
122	O	78.84314	74.44566	66.95632	531.88613	-49.19943	427.07960	1
123	N	78.05703	74.11369	69.07337	708.14833	26.93417	-179.73509	1
124	H	78.19889	74.24214	70.09333	-2232.69501	-1179.09831	1023.94816	1
125	C	76.72740	73.77302	68.67476	-738.32412	259.92548	104.42456	1
126	H	76.46596	74.36585	67.77007	2028.89123	1260.02983	1311.33324	1
127	C	76.70314	72.20388	68.40460	-258.65678	-345.52513	661.28459	1
128	H	77.17164	71.66303	69.25480	-1826.06090	-1801.46097	-918.64554	1
129	C	75.22677	71.73315	68.18538	-541.23400	531.92970	-218.41428	1
130	H	75.17838	70.65083	67.91840	1311.73218	-2219.18200	882.19023	1
131	H	74.60057	71.87570	69.12027	-1048.71298	1223.58118	-2196.97971	1
132	H	74.73370	72.29931	67.36003	419.06414	1903.92898	1903.44670	1
133	C	77.46378	71.89120	67.07092	-423.86431	152.66566	-648.55262	1
134	H	77.43085	70.80513	66.81888	105.68386	-2342.50080	1387.51238	1
135	H	77.02506	72.44853	66.20994	-1695.63603	-1484.73621	-1531.02793	1
136	H	78.53868	72.18793	67.13749	-1853.57121	-487.39031	1936.59343	1
137	C	75.94799	74.14918	70.05609	539.71428	-510.58232	267.58633	1
138	O	76.61462	74.22377	71.07969	-15.93758	-278.34085	-624.49402	1
139	N	74.65696	74.35377	69.86357	-676.81886	12.05292	276.17960	1
140	H	74.29606	74.22334	68.91828	-1694.44250	-373.84189	-2100.66098	1
141	C	73.77145	74.45827	70.97286	412.33078	-664.70360	108.35451	1
142	H	74.48732	74.61971	71.81653	1765.77476	1294.44366	1621.76594	1
143	C	72.81425	75.68749	70.68161	-179.66635	-721.95667	-264.73915	1
144	H	73.36100	76.47021	70.10992	-607.34922	2587.87032	-598.10018	1
145	H	71.97647	75.36916	70.02179	-359.69332	-1479.13954	-2259.74260	1
146	C	72.26660	76.28911	72.01809	-240.01076	616.02425	431.85322	1
147	H	71.88285	75.49782	72.70246	-1359.17131	782.54425	2227.99181	1
148	H	73.08546	76.80551	72.59245	-820.36667	85.81767	-2596.78715	1
149	C	71.10702	77.28670	71.61655	-513.07015	236.18570	-551.87280	1
150	H	71.52309	78.23955	71.21553	1816.11944	-1183.11722	-1650.94321	1
151	H	70.48645	76.85940	70.79562	-1800.04429	-1361.53473	1526.34643	1
152	C	70.22650	77.53644	72.86267	726.08972	-253.19732	-179.64713	1
153	H	69.69464	76.63824	73.23636	1224.27271	-456.51798	-2390.90304	1
154	H	70.73795	78.05123	73.70053	1206.40339	-1150.93514	-2154.90344	1
155	N	69.08133	78.51077	72.42333	329.70796	-633.68968	-155.67358	1
156	H	68.36235	78.74549	73.16677	1348.31305	1938.76845	1359.00643	1
157	H	69.36677	79.47828	72.09261	2096.92035	1446.54551	-966.48890	1
158	H	68.45621	78.18321	71.63042	-1197.07217	-2303.53719	827.28733	1
159	C	72.95154	73.04563	71.05753	-378.01186	-556.17301	-413.96481	1
160	O	73.47470	72.00067	70.71829	-409.44433	-307.55053	-453.30833	1

161	N	71.75592	73.21220	71.59063	-429.02477	524.70884	274.08502	1
162	H	71.41943	74.14747	71.79740	1706.34263	-1425.96036	1574.38926	1
163	C	70.84714	72.09589	71.59859	-45.25864	-626.22952	478.93267	1
164	H	70.83818	71.75006	70.54159	1988.63164	570.90773	1772.87287	1
165	C	71.47621	71.01484	72.55624	551.77128	-20.49526	-564.54996	1
166	H	72.45469	70.65802	72.15504	1434.61535	-1753.10253	1513.99471	1
167	H	71.71233	71.45156	73.55168	-714.67738	1819.09770	1898.36494	1
168	C	70.45208	69.82830	72.68603	446.99263	-555.77305	338.97221	1
169	H	69.43583	70.19658	72.95686	1953.68466	1892.25957	-161.67766	1
170	H	70.33988	69.29425	71.71492	-403.03785	2688.07032	-188.43591	1
171	C	71.02077	68.88476	73.79366	567.86262	335.74681	434.04421	1
172	H	72.08936	68.64681	73.59953	-1080.02275	1568.26081	-1948.78900	1
173	H	71.00153	69.37324	74.79191	-919.54108	2111.34692	1456.13463	1
174	C	70.13965	67.54866	73.78452	195.81897	173.33862	-745.11536	1
175	H	69.06870	67.69660	74.07538	1405.67949	-2301.21089	-390.08113	1
176	H	70.20201	67.00173	72.81091	-940.37328	-1118.32446	2299.72133	1
177	N	70.71149	66.68206	74.76888	319.26422	656.36007	-42.02424	1
178	H	69.36968	64.43813	75.97378	1961.03633	619.91968	1787.09422	2
179	H	71.71655	66.71511	74.89840	854.14343	-2156.80752	1429.08711	1
180	H	70.36109	66.79144	75.71517	1237.02905	-1378.50857	-1998.28500	1
181	C	69.38636	72.60996	72.12492	532.53319	-268.57236	517.55729	1
182	O	68.48443	72.73030	71.29127	266.16714	-290.73804	-558.88002	1
183	N	69.35743	72.78956	73.41653	-226.25352	640.49678	-270.32839	1
184	H	70.26802	72.70196	73.86156	2007.69063	-1035.27229	1523.50231	1
185	C	68.18979	73.12644	74.17599	-540.76542	-573.33303	49.50000	1
186	H	68.23381	74.23298	74.27097	-2374.20950	-1036.76023	843.75774	1
187	C	66.87061	72.67747	73.39650	-77.09082	666.87422	-415.84136	1
188	H	67.11955	71.73858	72.82498	-985.81834	617.19825	2463.91927	1
189	O	66.42371	73.62563	72.42839	293.29899	-391.65602	-477.80926	1
190	H	67.03220	73.35093	71.63564	2528.72714	-681.76262	-751.27122	1
191	C	65.86192	72.32027	74.54866	252.47363	-605.14473	440.05134	1
192	H	64.87100	72.00550	74.14493	-2052.65063	1456.49051	-1043.51830	1
193	H	66.24202	71.48803	75.19049	-2152.98800	-1661.97574	-161.70652	1
194	H	65.68988	73.19555	75.22130	-473.12726	-1584.27339	2165.61725	1
195	C	68.31149	72.43287	75.63771	360.36307	488.46713	505.10056	1
196	O	67.54912	72.82976	76.49891	-200.08817	-528.03552	-385.82850	1
197	N	69.20135	71.45215	75.69875	-597.54095	-226.44775	355.20479	1
198	H	69.74292	71.26786	74.85577	2179.23655	-1300.70981	-991.33835	1
199	C	69.44164	70.71299	76.88021	-687.68921	297.39807	-249.45179	1
200	H	70.46221	70.29049	76.74738	-349.16256	-2467.37713	-1101.72831	1
201	C	69.24727	71.57263	78.21815	672.47345	361.54328	-201.62880	1
202	H	68.21497	72.01859	78.24553	1541.41502	582.18425	2169.97026	1
203	H	69.32797	70.88891	79.09838	-2534.67717	60.25153	997.72295	1
204	C	70.31189	72.67731	78.27614	574.26774	-389.43119	-377.02542	1
205	C	71.66003	72.36055	78.61857	688.82679	-287.33580	-257.96133	1
206	H	71.95884	71.32016	78.84065	331.14182	1470.38163	2269.80013	1
207	C	69.92986	74.01910	77.97538	-383.52382	-675.04808	144.24917	1
208	H	68.88507	74.25233	77.69070	4.09847	1517.59662	2262.86397	1
209	C	72.58841	73.39934	78.67078	-134.76730	428.45285	-649.50303	1
210	H	73.63244	73.16133	78.93891	-903.23433	1600.49020	2011.53387	1
211	C	70.89662	75.02461	78.04638	-335.53281	-615.00040	-364.39058	1
212	H	70.59147	76.06169	77.82196	1596.45398	-1369.33862	1732.02659	1
213	C	72.25184	74.75670	78.39767	585.48547	-340.24194	-406.23938	1
214	O	73.24390	75.76817	78.47557	-419.15649	-173.04408	-511.94141	1
215	H	72.69809	76.55612	78.24511	-1071.84350	1559.71507	-1960.13012	1
216	C	68.31105	69.56338	77.11521	291.41878	-183.13091	710.72246	1
217	O	68.13735	69.13546	78.24061	379.87695	523.47396	-222.23622	1
218	N	67.72316	69.16979	75.98817	564.30591	373.09380	277.24371	1
219	H	68.01930	69.60872	75.11675	-120.59931	-2436.07824	-1214.35098	1
220	C	66.77763	68.12165	76.07354	404.07514	-299.37480	608.84009	1
221	H	66.37966	68.20869	77.10964	-1071.07882	-841.69025	2359.66467	1
222	C	65.74459	68.29209	74.90426	-683.12807	68.71770	-390.13096	1

223	H	65.26876	69.29891	74.93456	2068.88918	1596.58590	770.89603	1
224	H	66.26060	68.23065	73.91882	1379.86429	2342.49779	-179.85638	1
225	C	64.67414	67.15867	75.03780	-176.39967	537.49466	550.97268	1
226	H	65.16563	66.15722	75.05131	-396.28051	1942.22168	1869.33314	1
227	H	64.11473	67.23931	75.99617	-94.44700	586.00678	-2659.20016	1
228	C	63.70342	67.31095	73.77958	-291.69381	-718.18079	-150.72929	1
229	H	63.22980	68.31645	73.64578	-2303.38776	1089.76242	964.62032	1
230	H	64.16233	67.01185	72.80245	884.16729	2568.80533	-207.74283	1
231	N	62.68246	66.39459	74.06660	-594.49522	-252.81478	342.29276	1
232	H	62.86670	65.72164	74.79423	-1735.17426	2084.05705	-263.71605	1
233	C	61.56292	66.34766	73.46520	595.23177	-271.52487	442.22352	1
234	N	61.32878	67.27734	72.44492	585.53813	-424.79750	-105.81303	1
235	H	61.94183	68.00078	72.07260	959.88797	1327.56823	-2177.11905	1
236	H	60.47640	67.32571	71.88664	1578.48647	16.27378	-2220.76233	1
237	N	60.75455	65.32072	73.97430	-452.17763	-390.33541	-421.51853	1
238	H	60.92052	64.64425	74.71740	470.26107	1974.25629	-1817.92087	1
239	H	59.81637	65.12568	73.62322	1856.67307	-1573.97321	-1224.35416	1
240	C	67.60134	66.66576	75.84146	-531.47271	-581.45780	-55.06206	1
241	O	67.43176	65.99267	74.80161	-243.00837	192.73507	609.52485	1
242	N	68.37081	66.38429	76.82074	343.49288	-644.25607	38.09164	1
243	H	68.35903	67.08075	77.54994	-1691.16043	-1535.97525	-1484.73099	1
244	C	70.17755	63.75833	75.60728	542.66492	350.14337	454.42563	2
245	H	69.87712	62.73400	75.93316	1209.57979	-2396.95920	463.86744	2
246	C	70.28462	63.81329	74.10441	-737.14309	145.93010	242.71942	2
247	H	70.75756	64.78284	73.82621	-1050.18303	159.36419	-2509.06125	2
248	C	71.15257	62.68517	73.56704	-706.77696	-252.88343	-245.16230	2
249	H	71.26948	62.74305	72.45356	-1624.64039	-1665.49085	1417.86935	2
250	H	72.18353	62.72206	74.01903	2566.10521	598.51109	693.22305	2
251	H	70.71946	61.67907	73.80508	-1972.69758	107.10018	-1876.34312	2
252	C	68.90060	63.76768	73.48105	412.85148	672.58832	-27.69222	2
253	H	68.93746	63.89804	72.36855	1447.02277	1762.76533	-1490.78944	2
254	H	68.38476	62.79378	73.68492	1320.77379	-145.20455	2378.68491	2
255	H	68.23399	64.61306	73.91356	-1512.10848	1470.52031	1724.75147	2
256	C	71.59563	64.17000	76.29125	-607.11113	499.56689	73.73769	2
257	O	72.65739	63.90179	75.77358	357.97126	460.81534	356.68785	2
258	N	71.37744	64.81990	77.43393	536.55407	-368.62270	332.76306	2
259	H	70.41192	64.95285	77.73849	524.38866	2297.69985	1367.20941	2
260	C	72.43636	64.82573	78.38041	46.50277	-774.29190	-147.97904	2
261	H	73.29437	64.33959	77.86042	1676.51875	1883.29066	1032.55549	2
262	C	72.73832	66.34921	78.82514	-559.41456	-34.19198	-556.30433	2
263	H	71.85779	66.76343	79.37195	-64.66664	395.18769	2695.05373	2
264	H	73.58861	66.37860	79.54744	-2703.44278	-60.40056	333.79418	2
265	C	73.03574	67.18000	77.60569	-519.76435	377.31045	459.42366	2
266	H	72.13683	67.16467	76.94976	-1746.74323	1667.50644	-1261.73691	2
267	C	73.31776	68.62368	78.00209	570.95554	16.46261	-545.27700	2
268	H	73.52377	69.26706	77.10822	2391.58273	28.05277	-1305.07271	2
269	H	72.45005	69.07772	78.54636	175.75588	917.63458	2559.43867	2
270	H	74.20875	68.69914	78.67729	-1063.97851	-2155.34650	1283.00462	2
271	C	74.20795	66.61036	76.81945	193.76014	2.62946	-765.53141	2
272	H	74.50511	67.28078	75.97234	507.39394	-846.55087	2539.60089	2
273	H	75.11268	66.47311	77.46663	1337.57841	1818.19054	1526.01994	2
274	H	73.95373	65.60701	76.37573	1100.88635	-1172.91350	-2199.08909	2
275	C	71.91894	64.03707	79.68923	-549.21115	475.64486	-309.38218	2
276	O	70.76289	63.77686	79.89604	556.06106	-390.37755	-78.24250	2
277	O	72.90984	63.73737	80.65494	-572.27940	-310.19032	-209.75862	2
278	H	73.70904	64.07738	80.16564	-1380.08193	2212.14486	790.85944	2

Listing 66: C00066.xmolout

1	276								
2	150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100	
	0.2500	300.00	0.00	0.00	0.00	-1293.6022	0.0000	300.0000	

3	H	79.78072	61.88150	67.99571	-2043.14101	-1757.64893	399.89339	1
4	N	79.48041	62.84407	67.84501	426.75047	490.45733	-334.42467	1
5	H	79.07510	63.05209	68.75748	442.25559	-1110.30854	-2448.52907	1
6	C	80.54964	63.70911	67.49957	415.32972	-666.39213	83.73172	1
7	H	81.42382	63.36009	68.09132	879.32219	2491.00447	667.35213	1
8	C	80.81239	63.61287	65.91464	31.35357	477.41777	628.23362	1
9	H	79.92400	64.02815	65.38013	1168.38489	2240.25337	-1019.71136	1
10	H	81.67028	64.27175	65.63703	-360.43770	2534.90498	931.67112	1
11	C	81.06401	62.19297	65.47205	463.18208	512.70242	-382.34388	1
12	H	80.21818	61.56013	65.82255	1725.29117	1863.52247	-987.07854	1
13	C	81.12022	62.12159	63.95112	710.42801	-144.27427	-313.15367	1
14	H	81.28436	61.07325	63.59079	364.20195	-1033.13725	2494.72524	1
15	H	80.17035	62.48936	63.48358	2567.61904	335.80679	847.48802	1
16	H	81.95460	62.74719	63.54069	-2587.99029	680.92867	-512.16411	1
17	C	82.35899	61.64620	66.05570	268.17616	741.64379	-40.42634	1
18	H	82.56368	60.60273	65.70120	1283.54314	-1945.37420	-1411.27812	1
19	H	83.23977	62.27435	65.76256	-1258.57796	1317.15249	-2026.02085	1
20	H	82.33075	61.61630	67.17541	-2502.84526	909.80597	575.92391	1
21	C	80.13574	65.24317	67.83333	619.36578	-458.64843	-172.09273	1
22	O	80.98812	66.08670	67.99831	-81.40433	433.87611	522.34594	1
23	N	78.80946	65.42940	67.73192	175.23996	-622.20190	341.55523	1
24	H	78.25386	64.58026	67.62970	-876.57256	-303.22879	-2561.90213	1
25	C	78.28745	66.59864	68.37442	-571.88214	-534.10783	-106.15033	1
26	H	79.04382	67.39505	68.18287	-2713.20841	-16.25800	-248.80809	1
27	C	76.85194	66.86054	67.72744	166.60354	288.16399	-716.09568	1
28	H	76.18980	65.98738	67.97910	-2097.85574	1636.78449	-586.18044	1
29	O	76.82704	66.97458	66.28985	-317.80580	-363.38227	484.43082	1
30	H	76.29225	66.19424	66.04757	1863.74748	-1451.84923	1357.29467	1
31	C	76.34939	68.13428	68.49945	503.80731	517.99032	318.51606	1
32	H	75.30802	68.40002	68.20219	640.61020	-2157.10410	-1536.29104	1
33	H	76.34712	67.99202	69.62531	1687.88455	465.60692	2087.56452	1
34	H	76.98630	69.02143	68.27566	-1293.07895	-1899.88581	-1463.57452	1
35	C	78.12296	66.22180	69.95269	-153.07550	-733.68902	248.70981	1
36	O	77.70207	65.14092	70.26625	186.15459	-480.78787	-449.34387	1
37	N	78.43823	67.27270	70.72002	-487.53139	543.18517	42.03850	1
38	C	78.14729	67.29117	72.12528	-699.35871	69.34393	360.10701	1
39	H	78.45663	66.29805	72.52436	2.81126	-221.99807	-2715.58072	1
40	C	79.00547	68.51913	72.64737	-507.46439	-592.59194	122.07761	1
41	H	78.56031	69.00238	73.54650	-1975.08116	525.87560	-1801.71556	1
42	H	80.03117	68.20042	72.93873	1588.27743	-1913.22100	1113.83566	1
43	C	79.04262	69.45998	71.40336	-613.62442	-457.55993	-194.14490	1
44	H	78.08564	70.01716	71.29326	1707.54637	-721.27992	1996.92523	1
45	H	79.85579	70.21954	71.43969	758.23357	2100.81767	1560.55011	1
46	C	79.22942	68.39471	70.23753	-352.41524	704.96076	49.21465	1
47	H	78.85107	68.71007	69.23599	1714.76886	-2070.42778	443.35792	1
48	H	80.26905	68.00137	70.12800	1224.15040	1801.50881	1636.97633	1
49	C	76.55384	67.55559	72.35516	566.85117	537.05831	117.62814	1
50	O	75.82470	68.03082	71.50891	-550.26779	-406.08867	4.21666	1
51	N	76.27148	67.24824	73.61543	566.34832	-425.77725	180.18749	1
52	H	77.02560	66.89181	74.20022	644.44502	2646.80550	-52.73430	1
53	C	74.90320	67.03208	73.95379	612.34801	-281.48662	411.56221	1
54	H	74.38935	66.78108	72.99833	1667.23498	-1490.75142	1556.16753	1
55	C	74.88319	65.89300	75.07247	-714.45746	-175.43074	286.98927	1
56	H	75.47980	66.25105	75.95631	-787.09484	1763.03619	-1922.46060	1
57	O	75.46387	64.63290	74.68888	-429.46514	516.51932	-128.40526	1
58	H	76.18901	64.54840	75.33931	1981.82785	436.16847	-1818.18182	1
59	C	73.35891	65.85807	75.46060	630.79189	-468.94448	76.03230	1
60	H	73.16746	65.15141	76.30086	-1775.71861	2062.30353	131.89849	1
61	H	72.99154	66.86086	75.78040	-1855.14608	88.94118	1993.53760	1
62	H	72.72695	65.53140	74.60249	-1504.82350	-780.94249	-2132.90992	1
63	C	74.32988	68.40521	74.64455	288.57638	618.62814	-397.00270	1
64	O	74.86931	68.95071	75.57780	321.70495	-185.26452	574.37218	1

65	N	73.14640	68.66914	74.10292	-447.05792	-446.53431	367.76425	1
66	H	72.78744	68.13374	73.31357	350.31316	1975.63644	-1843.31522	1
67	C	72.44176	69.80145	74.59687	-511.23061	374.03917	-471.51480	1
68	H	72.82024	69.96420	75.63391	2234.79579	-898.70890	-1273.45190	1
69	C	72.90290	71.00065	73.62455	529.53781	-159.34528	563.72604	1
70	H	72.44913	71.95135	74.01466	654.59388	2347.94251	1217.51488	1
71	H	74.01421	71.08989	73.76250	-1526.55661	2103.42026	817.87394	1
72	O	72.58010	70.87620	72.22087	-554.84278	14.12789	399.58769	1
73	H	73.19525	70.15287	71.98158	1297.06236	2061.84854	1220.68812	1
74	C	70.86231	69.45074	74.48458	-662.15484	-412.13544	123.62687	1
75	O	70.36755	68.82173	73.58161	-540.01537	-317.05804	274.91456	1
76	N	70.20942	70.06117	75.50718	-202.76299	-690.00100	-131.49145	1
77	H	70.86274	70.44962	76.19000	-702.62132	-2617.37191	281.70413	1
78	C	68.94322	69.45472	75.95604	-491.73914	576.34187	222.73509	1
79	H	68.57644	69.01964	74.99535	1977.17978	-1823.58850	-434.68928	1
80	C	69.21088	68.40548	77.01248	-649.50797	-328.66843	306.11224	1
81	H	69.79332	68.88236	77.83232	2075.07803	1452.16490	-1004.45904	1
82	C	67.92290	67.86342	77.60477	-615.18735	-489.99689	-70.96352	1
83	H	68.11779	67.08513	78.39294	-1226.32661	-1724.38906	-1716.47170	1
84	H	67.31533	68.69171	78.08635	2381.64273	-969.84735	900.46860	1
85	H	67.27355	67.38757	76.81922	2122.74991	1702.23946	-141.36228	1
86	C	70.03753	67.25309	76.46754	-501.86074	-479.61276	-376.42482	1
87	H	70.26359	66.48657	77.25849	993.79261	-2246.95401	-1177.81305	1
88	H	69.50225	66.72340	75.63208	42.71279	-626.15391	-2651.37258	1
89	H	71.01913	67.60969	76.05212	-2026.39012	-1590.33709	-887.82922	1
90	C	68.02954	70.72736	76.49708	-672.89153	382.57394	-156.34072	1
91	O	67.37825	70.66305	77.51668	410.04627	221.86223	500.35950	1
92	N	68.08488	71.70634	75.61083	-378.11782	-443.79414	-441.10984	1
93	H	68.67587	71.48864	74.80957	2404.15973	-568.14894	1149.30085	1
94	C	67.43278	72.95702	75.78207	-544.54484	466.16019	331.29119	1
95	H	67.66831	73.50625	74.84140	-1409.80988	-170.17955	2325.32679	1
96	C	65.88095	72.65850	76.00201	-184.48284	116.78282	-758.89137	1
97	H	65.54913	71.82567	75.34220	1893.78641	1861.14652	611.04528	1
98	H	65.71687	72.30660	77.04857	-2170.79665	-974.19311	1327.50117	1
99	C	65.07102	73.95774	75.70946	389.51668	672.81878	-138.49152	1
100	H	65.38461	74.77106	76.40445	510.64577	1933.03327	1851.02484	1
101	H	65.32788	74.34936	74.70060	-2302.30869	-1105.72939	-948.89774	1
102	C	63.51050	73.76698	75.81096	-559.93427	-126.34590	542.30857	1
103	O	62.78859	74.70898	75.60798	-670.36003	-111.83166	76.36448	1
104	N	63.12060	72.51063	76.11612	-216.06729	-537.07037	446.51379	1
105	H	63.68798	71.68389	76.33625	-1251.96487	1074.12894	-2168.52500	1
106	H	62.14202	72.23173	76.24729	-2451.83023	-720.73851	944.84612	1
107	C	67.90217	73.72076	77.13364	546.24052	-563.88337	-85.11809	1
108	O	67.00467	74.18068	77.82858	71.70702	-307.40463	606.69673	1
109	N	69.21583	73.86393	77.27003	479.90863	-504.50129	222.86849	1
110	C	69.82984	74.23531	78.51807	75.51268	-600.91904	506.73700	1
111	H	69.25457	73.67931	79.29394	-2033.61562	1795.30103	254.89480	1
112	C	71.33469	73.77419	78.33361	523.79067	517.99274	284.45581	1
113	H	72.04059	74.38631	78.94049	1599.61665	-1127.00911	1895.98173	1
114	H	71.47502	72.71728	78.65354	-1881.83093	1275.82488	-1501.55016	1
115	C	71.56180	73.92684	76.79618	-600.05639	-404.05026	316.64485	1
116	H	71.77857	74.99952	76.49930	-2597.05260	496.36221	657.73249	1
117	H	72.40872	73.31399	76.40995	-1666.24518	1294.38985	-1723.90591	1
118	C	70.15440	73.46597	76.22648	493.57570	-129.95376	-602.56394	1
119	H	69.84341	73.94780	75.26982	-1469.08415	-637.84797	2204.22581	1
120	H	70.03826	72.36135	76.13567	-1038.97840	1068.88701	-2280.71789	1
121	C	69.79203	75.83861	78.78009	188.88100	241.05089	-727.87821	1
122	O	70.71783	76.38927	79.31230	531.88613	-49.19943	427.07960	1
123	N	68.63663	76.36392	78.34733	708.14833	26.93417	-179.73509	1
124	H	67.90605	75.69423	78.01974	-2232.69501	-1179.09831	1023.94816	1
125	C	68.26291	77.75944	78.58954	-738.32412	259.92548	104.42456	1
126	H	67.23684	77.82767	78.15591	2028.89123	1260.02983	1311.33324	1

127	C	68.24868	77.97095	80.09214	-258.65678	-345.52513	661.28459	1
128	H	69.26041	77.70614	80.47961	-1826.06090	-1801.46097	-918.64554	1
129	C	67.94654	79.40778	80.47326	-541.23400	531.92970	-218.41428	1
130	H	67.86950	79.53652	81.58819	1311.73218	-2219.18200	882.19023	1
131	H	68.74692	80.11220	80.10903	-1048.71298	1223.58118	-2196.97971	1
132	H	66.97358	79.75679	80.02903	419.06414	1903.92898	1903.44670	1
133	C	67.24123	77.04765	80.75658	-423.86431	152.66566	-648.55262	1
134	H	67.24913	77.15154	81.87578	105.68386	-2342.50080	1387.51238	1
135	H	66.19358	77.26328	80.40911	-1695.63603	-1484.73621	-1531.02793	1
136	H	67.45134	75.96916	80.51531	-1853.57121	-487.39031	1936.59343	1
137	C	69.30558	78.76399	77.78342	539.71428	-510.58232	267.58633	1
138	O	69.17704	79.95977	77.88150	-15.93758	-278.34085	-624.49402	1
139	N	70.14331	78.09582	76.99898	-676.81886	12.05292	276.17960	1
140	H	70.13488	77.08175	77.12220	-1694.44250	-373.84189	-2100.66098	1
141	C	71.29839	78.77607	76.49872	412.33078	-664.70360	108.35451	1
142	H	70.96017	79.78183	76.16013	1765.77476	1294.44366	1621.76594	1
143	C	72.32747	78.85397	77.70192	-179.66635	-721.95667	-264.73915	1
144	H	71.90448	79.42972	78.55535	-607.34922	2587.87032	-598.10018	1
145	H	72.53824	77.83662	78.10301	-359.69332	-1479.13954	-2259.74260	1
146	C	73.61923	79.53179	77.13474	-240.01076	616.02425	431.85322	1
147	H	73.97541	78.99632	76.22517	-1359.17131	782.54425	2227.99181	1
148	H	73.40758	80.57486	76.80892	-820.36667	85.81767	-2596.78715	1
149	C	74.73417	79.50567	78.25109	-513.07015	236.18570	-551.87280	1
150	H	74.39606	80.03599	79.17088	1816.11944	-1183.11722	-1650.94321	1
151	H	74.95859	78.46175	78.56983	-1800.04429	-1361.53473	1526.34643	1
152	C	75.99222	80.18514	77.64614	726.08972	-253.19732	-179.64713	1
153	H	76.39923	79.69319	76.73787	1224.27271	-456.51798	-2390.90304	1
154	H	75.88574	81.27464	77.46536	1206.40339	-1150.93514	-2154.90344	1
155	N	77.09987	80.05299	78.71480	329.70796	-633.68968	-155.67358	1
156	H	78.00498	80.56236	78.49214	1348.31305	1938.76845	1359.00643	1
157	H	76.85981	80.41255	79.74528	2096.92035	1446.54551	-966.48890	1
158	H	77.48396	79.07331	78.87061	-1197.07217	-2303.53719	827.28733	1
159	C	71.97794	77.81717	75.36611	-378.01186	-556.17301	-413.96481	1
160	O	72.07162	76.61282	75.49692	-409.44433	-307.55053	-453.30833	1
161	N	72.47629	78.59104	74.41512	-429.02477	524.70884	274.08502	1
162	H	72.33905	79.60134	74.44118	1706.34263	-1425.96036	1574.38926	1
163	C	73.32298	77.99833	73.44437	-45.25864	-626.22952	478.93267	1
164	H	73.58663	76.98395	73.82628	1988.63164	570.90773	1772.87287	1
165	C	72.47009	77.96973	72.10820	551.77128	-20.49526	-564.54996	1
166	H	71.48014	77.49869	72.29968	1434.61535	-1753.10253	1513.99471	1
167	H	72.24625	79.00402	71.76361	-714.67738	1819.09770	1898.36494	1
168	C	73.25964	77.17453	71.01862	446.99263	-555.77305	338.97221	1
169	H	74.19656	77.70685	70.72632	1953.68466	1892.25957	-161.67766	1
170	H	73.57540	76.17754	71.40002	-403.03785	2688.07032	-188.43591	1
171	C	72.26899	77.02098	69.79397	567.86262	335.74681	434.04421	1
172	H	71.33150	76.50887	70.11122	-1080.02275	1568.26081	-1948.78900	1
173	H	71.95325	78.02009	69.41516	-919.54108	2111.34692	1456.13463	1
174	C	72.97342	76.21254	68.68095	195.81897	173.33862	-745.11536	1
175	H	73.82642	76.73249	68.20094	1405.67949	-2301.21089	-390.08113	1
176	H	73.26989	75.18507	68.97234	-940.37328	-1118.32446	2299.72133	1
177	N	71.92700	76.00657	67.53312	319.26422	656.36007	-42.02424	1
178	H	72.27383	75.47159	66.68572	1961.03633	619.91968	1787.09422	1
179	H	71.04863	75.46225	67.77624	854.14343	-2156.80752	1429.08711	1
180	H	71.52669	76.87905	67.08030	1237.02905	-1378.50857	-1998.28500	1
181	C	74.57947	79.04963	73.21376	532.53319	-268.57236	517.55729	1
182	O	74.37986	80.23625	73.11790	266.16714	-290.73804	-558.88002	1
183	N	75.69182	78.33853	73.11935	-226.25352	640.49678	-270.32839	1
184	H	75.56975	77.32959	73.20669	2007.69063	-1035.27229	1523.50231	1
185	C	76.92784	78.82641	72.62873	-540.76542	-573.33303	49.50000	1
186	H	77.47862	77.90322	72.34319	-2374.20950	-1036.76023	843.75774	1
187	C	76.62672	79.78798	71.38848	-77.09082	666.87422	-415.84136	1
188	H	76.02811	80.66906	71.75978	-985.81834	617.19825	2463.91927	1

189	O	75.86366	79.20198	70.31271	293.29899	-391.65602	-477.80926	1
190	H	75.05260	79.74887	70.35040	2528.72714	-681.76262	-751.27122	1
191	C	78.07483	80.27151	71.01364	252.47363	-605.14473	440.05134	1
192	H	78.05036	81.03972	70.20593	-2052.65063	1456.49051	-1043.51830	1
193	H	78.60170	80.72392	71.88735	-2152.98800	-1661.97574	-161.70652	1
194	H	78.70427	79.42796	70.64654	-473.12726	-1584.27339	2165.61725	1
195	C	77.69032	79.65570	73.82519	360.36307	488.46713	505.10056	1
196	O	77.27606	80.71072	74.24696	-200.08817	-528.03552	-385.82850	1
197	N	78.84024	79.04141	74.09931	-597.54095	-226.44775	355.20479	1
198	H	78.98490	78.12934	73.66795	2179.23655	-1300.70981	-991.33835	1
199	C	79.41762	79.31870	75.39124	-687.68921	297.39807	-249.45179	1
200	H	78.62029	79.12834	76.14182	-349.16256	-2467.37713	-1101.72831	1
201	C	80.71347	78.41331	75.56137	672.47345	361.54328	-201.62880	1
202	H	81.42070	78.61656	74.72403	1541.41502	582.18425	2169.97026	1
203	H	81.23005	78.70431	76.50616	-2534.67717	60.25153	997.72295	1
204	C	80.35652	76.91911	75.60337	574.26774	-389.43119	-377.02542	1
205	C	79.86741	76.35031	76.81713	688.82679	-287.33580	-257.96133	1
206	H	79.70888	76.98021	77.71494	331.14182	1470.38163	2269.80013	1
207	C	80.55719	76.11424	74.44190	-383.52382	-675.04808	144.24917	1
208	H	80.93211	76.56126	73.50316	4.09847	1517.59662	2262.86397	1
209	C	79.61510	74.97800	76.84412	-134.76730	428.45285	-649.50303	1
210	H	79.24957	74.52664	77.78316	-903.23433	1600.49020	2011.53387	1
211	C	80.28951	74.74557	74.52270	-335.53281	-615.00040	-364.39058	1
212	H	80.45971	74.12544	73.62517	1596.45398	-1369.33862	1732.02659	1
213	C	79.81738	74.12816	75.71766	585.48547	-340.24194	-406.23938	1
214	O	79.54788	72.73714	75.80643	-419.15649	-173.04408	-511.94141	1
215	H	79.81807	72.45721	74.89997	-1071.84350	1559.71507	-1960.13012	1
216	C	79.97273	80.84028	75.40371	291.41878	-183.13091	710.72246	1
217	O	80.74406	81.26850	74.57685	379.87695	523.47396	-222.23622	1
218	N	79.58818	81.42482	76.56024	564.30591	373.09380	277.24371	1
219	H	78.87747	80.92800	77.10261	-120.59931	-2436.07824	-1214.35098	1
220	C	79.54733	82.86245	76.47426	404.07514	-299.37480	608.84009	1
221	H	80.45052	83.11253	75.87193	-1071.07882	-841.69025	2359.66467	1
222	C	78.19628	83.21332	75.73257	-683.12807	68.71770	-390.13096	1
223	H	78.03077	82.52107	74.86246	2068.88918	1596.58590	770.89603	1
224	H	77.31576	83.06242	76.39665	1379.86429	2342.49779	-179.85638	1
225	C	78.30604	84.70534	75.28943	-176.39967	537.49466	550.97268	1
226	H	78.51559	85.35866	76.16596	-396.28051	1942.22168	1869.33314	1
227	H	79.16233	84.85230	74.59401	-94.44700	586.00678	-2659.20016	1
228	C	76.92621	85.10583	74.59220	-291.69381	-718.18079	-150.72929	1
229	H	76.69343	84.58953	73.62612	-2303.38776	1089.76242	964.62032	1
230	H	76.02026	85.04131	75.24762	884.16729	2568.80533	-207.74283	1
231	N	77.17094	86.46214	74.32356	-594.49522	-252.81478	342.29276	1
232	H	78.02515	86.85005	74.69387	-1735.17426	2084.05705	-263.71605	1
233	C	76.39740	87.22608	73.66403	595.23177	-271.52487	442.22352	1
234	N	75.21312	86.67776	73.16167	585.53813	-424.79750	-105.81303	1
235	H	74.85564	85.72666	73.24346	959.88797	1327.56823	-2177.11905	1
236	H	74.51449	87.18881	72.62108	1578.48647	16.27378	-2220.76233	1
237	N	76.92816	88.52098	73.58220	-452.17763	-390.33541	-421.51853	1
238	H	77.79300	88.91309	73.95185	470.26107	1974.25629	-1817.92087	1
239	H	76.46222	89.28747	73.09530	1856.67307	-1573.97321	-1224.35416	1
240	C	79.57194	83.46068	77.99595	-531.47271	-581.45780	-55.06206	1
241	O	80.54618	84.05073	78.40155	-243.00837	192.73507	609.52485	1
242	N	78.41720	83.24060	78.62241	343.49288	-644.25607	38.09164	1
243	H	77.71291	82.67092	78.15536	-1691.16043	-1535.97525	-1484.73099	1
244	C	78.40137	83.40571	80.04152	542.66492	350.14337	454.42563	1
245	H	79.31458	84.00656	80.26813	1209.57979	-2396.95920	463.86744	1
246	C	77.02097	84.10292	80.41607	-737.14309	145.93010	242.71942	1
247	H	76.16925	83.44054	80.14949	-1050.18303	159.36419	-2509.06125	1
248	C	77.02393	84.41689	81.95003	-706.77696	-252.88343	-245.16230	1
249	H	76.09043	84.94123	82.26311	-1624.64039	-1665.49085	1417.86935	1
250	H	77.09954	83.48171	82.55434	2566.10521	598.51109	693.22305	1

251	H	77.88291	85.06926	82.23406	-1972.69758	107.10018	-1876.34312	1
252	C	76.92910	85.45642	79.63184	412.85148	672.58832	-27.69222	1
253	H	75.98006	85.99972	79.85057	1447.02277	1762.76533	-1490.78944	1
254	H	77.77262	86.13722	79.89412	1320.77379	-145.20455	2378.68491	1
255	H	76.97354	85.28857	78.52955	-1512.10848	1470.52031	1724.75147	1
256	C	78.43523	81.88498	80.63045	-607.11113	499.56689	73.73769	1
257	O	77.38640	81.31967	80.98318	357.97126	460.81534	356.68785	1
258	N	79.65695	81.43054	80.57702	536.55407	-368.62270	332.76306	1
259	H	80.36255	82.07385	80.21071	524.38866	2297.69985	1367.20941	1
260	C	80.03699	80.18857	81.14889	46.50277	-774.29190	-147.97904	1
261	H	81.14791	80.23606	81.13080	1676.51875	1883.29066	1032.55549	1
262	C	79.43613	80.07162	82.64398	-559.41456	-34.19198	-556.30433	1
263	H	78.32387	80.19816	82.60988	-64.66664	395.18769	2695.05373	1
264	H	79.62082	79.05433	83.06492	-2703.44278	-60.40056	333.79418	1
265	C	80.06998	81.13626	83.49530	-519.76435	377.31045	459.42366	1
266	H	79.97901	82.10848	82.95930	-1746.74323	1667.50644	-1261.73691	1
267	C	79.35898	81.26058	84.83738	570.95554	16.46261	-545.27700	1
268	H	79.81736	82.06076	85.47419	2391.58273	28.05277	-1305.07271	1
269	H	78.27545	81.51617	84.71103	175.75588	917.63458	2559.43867	1
270	H	79.40958	80.30535	85.42061	-1063.97851	-2155.34650	1283.00462	1
271	C	81.54611	80.84465	83.73560	193.76014	2.62946	-765.53141	1
272	H	82.01768	81.61611	84.39691	507.39394	-846.55087	2539.60089	1
273	H	81.69378	79.84986	84.22924	1337.57841	1818.19054	1526.01994	1
274	H	82.12960	80.82985	82.78000	1100.88635	-1172.91350	-2199.08909	1
275	C	79.48525	79.01035	80.20565	-549.21115	475.64486	-309.38218	1
276	O	78.96240	78.01454	80.63131	556.06106	-390.37755	-78.24250	1
277	O	79.75394	79.14023	78.81466	-572.27940	-310.19032	-209.75862	1
278	H	80.08981	80.07988	78.81857	-1380.08193	2212.14486	790.85944	1

Listing 67: C00067.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.6016	0.0000	300.0000
3	H	56.82512	72.04113	75.69816	-2043.14101	-1757.64893	399.89339		1
4	N	57.31295	72.25636	76.56732	426.75047	490.45733	-334.42467		1
5	H	57.45118	71.32655	76.98118	442.25559	-1110.30854	-2448.52907		1
6	C	58.54639	72.92617	76.38301	415.32972	-666.39213	83.73172		1
7	H	58.62160	73.04659	75.28013	879.32219	2491.00447	667.35213		1
8	C	58.53295	74.35071	77.13764	31.35357	477.41777	628.23362		1
9	H	58.53729	74.17884	78.24043	1168.38489	2240.25337	-1019.71136		1
10	H	59.46556	74.92153	76.91306	-360.43770	2534.90498	931.67112		1
11	C	57.32020	75.14809	76.73812	463.18208	512.70242	-382.34388		1
12	H	56.41732	74.52234	76.92028	1725.29117	1863.52247	-987.07854		1
13	C	57.22550	76.40944	77.58873	710.42801	-144.27427	-313.15367		1
14	H	56.31364	77.01061	77.33951	364.20195	-1033.13725	2494.72524		1
15	H	57.17780	76.16878	78.68198	2567.61904	335.80679	847.48802		1
16	H	58.11335	77.07562	77.43551	-2587.99029	680.92867	-512.16411		1
17	C	57.35760	75.53272	75.26531	268.17616	741.64379	-40.42634		1
18	H	56.47254	76.15792	74.97974	1283.54314	-1945.37420	-1411.27812		1
19	H	58.27558	76.12497	75.01633	-1258.57796	1317.15249	-2026.02085		1
20	H	57.35319	74.63102	74.60061	-2502.84526	909.80597	575.92391		1
21	C	59.63309	71.89669	76.99581	619.36578	-458.64843	-172.09273		1
22	O	59.35383	70.71489	77.17075	-81.40433	433.87611	522.34594		1
23	N	60.77256	72.52537	77.22141	175.23996	-622.20190	341.55523		1
24	H	60.79504	73.52647	77.03823	-876.57256	-303.22879	-2561.90213		1
25	C	61.99138	71.81908	77.40706	-571.88214	-534.10783	-106.15033		1
26	H	61.80858	70.78859	77.03159	-2713.20841	-16.25800	-248.80809		1
27	C	63.05658	72.66949	76.56704	166.60354	288.16399	-716.09568		1
28	H	62.98637	73.74380	76.89194	-2097.85574	1636.78449	-586.18044		1
29	O	62.84454	72.67575	75.14251	-317.80580	-363.38227	484.43082		1
30	H	62.66899	73.62353	74.97947	1863.74748	-1451.84923	1357.29467		1

31	C	64.42999	72.08515	77.05901	503.80731	517.99032	318.51606	1
32	H	65.29169	72.61912	76.59404	640.61020	-2157.10410	-1536.29104	1
33	H	64.53453	72.18568	78.17018	1687.88455	465.60692	2087.56452	1
34	H	64.52960	71.00305	76.79605	-1293.07895	-1899.88581	-1463.57452	1
35	C	62.34141	71.87408	79.00367	-153.07550	-733.68902	248.70981	1
36	O	62.78685	72.89572	79.45899	186.15459	-480.78787	-449.34387	1
37	N	62.09418	70.70682	79.63199	-487.53139	543.18517	42.03850	1
38	C	62.11025	70.64147	81.05445	-699.35871	69.34393	360.10701	1
39	H	62.10518	71.68797	81.43696	2.81126	-221.99807	-2715.58072	1
40	C	60.80200	69.77747	81.32096	-507.46439	-592.59194	122.07761	1
41	H	60.77507	69.33865	82.34328	-1975.08116	525.87560	-1801.71556	1
42	H	59.88105	70.39187	81.21073	1588.27743	-1913.22100	1113.83566	1
43	C	60.90294	68.70490	80.19234	-613.62442	-457.55993	-194.14490	1
44	H	61.62008	67.89645	80.46746	1707.54637	-721.27992	1996.92523	1
45	H	59.93415	68.20400	79.96591	758.23357	2100.81767	1560.55011	1
46	C	61.45262	69.57115	78.98207	-352.41524	704.96076	49.21465	1
47	H	62.22420	69.06187	78.35688	1714.76886	-2070.42778	443.35792	1
48	H	60.64301	70.00985	78.30667	1224.15040	1801.50881	1636.97633	1
49	C	63.38358	69.73585	81.58283	566.85117	537.05831	117.62814	1
50	O	63.64175	68.66813	81.08282	-550.26779	-406.08867	4.21666	1
51	N	63.96750	70.36478	82.59107	566.34832	-425.77725	180.18749	1
52	H	63.56169	71.25382	82.87980	644.44502	2646.80550	-52.73430	1
53	C	64.96926	69.74582	83.38791	612.34801	-281.48662	411.56221	1
54	H	65.25126	70.55323	84.09998	1667.23498	-1490.75142	1556.16753	1
55	C	64.30463	68.50203	84.14483	-714.45746	-175.43074	286.98927	1
56	H	64.08762	67.70471	83.38350	-787.09484	1763.03619	-1922.46060	1
57	O	63.06335	68.77873	84.81955	-429.46514	516.51932	-128.40526	1
58	H	62.45479	68.18193	84.34068	1981.82785	436.16847	-1818.18182	1
59	C	65.46892	68.02874	85.09003	630.79189	-468.94448	76.03230	1
60	H	65.18304	67.11748	85.66529	-1775.71861	2062.30353	131.89849	1
61	H	66.40509	67.78145	84.51080	-1855.14608	88.94118	1993.53760	1
62	H	65.73495	68.81557	85.83426	-1504.82350	-780.94249	-2132.90992	1
63	C	66.20028	69.29611	82.41476	288.57638	618.62814	-397.00270	1
64	O	66.91470	68.35043	82.67986	321.70495	-185.26452	574.37218	1
65	N	66.35052	70.19098	81.44536	-447.05792	-446.53431	367.76425	1
66	H	65.63176	70.90956	81.37301	350.31316	1975.63644	-1843.31522	1
67	C	67.18978	69.85678	80.34109	-511.23061	374.03917	-471.51480	1
68	H	67.88107	69.09359	80.76915	2234.79579	-898.70890	-1273.45190	1
69	C	66.22755	69.23978	79.23831	529.53781	-159.34528	563.72604	1
70	H	66.87015	68.90097	78.38564	654.59388	2347.94251	1217.51488	1
71	H	65.74166	68.32601	79.67045	-1526.55661	2103.42026	817.87394	1
72	O	65.16674	70.12861	78.71175	-554.84278	14.12789	399.58769	1
73	H	64.46627	69.91277	79.35791	1297.06236	2061.84854	1220.68812	1
74	C	67.94518	71.27321	79.99272	-662.15484	-412.13544	123.62687	1
75	O	68.87564	71.58660	80.70280	-540.01537	-317.05804	274.91456	1
76	N	67.38309	71.91619	78.98480	-202.76299	-690.00100	-131.49145	1
77	H	66.55746	71.48691	78.54764	-702.62132	-2617.37191	281.70413	1
78	C	67.79808	73.20807	78.57761	-491.73914	576.34187	222.73509	1
79	H	66.96853	73.55464	77.92276	1977.17978	-1823.58850	-434.68928	1
80	C	68.02807	74.11201	79.86374	-649.50797	-328.66843	306.11224	1
81	H	68.69125	73.58059	80.59751	2075.07803	1452.16490	-1004.45904	1
82	C	68.66203	75.48828	79.46682	-615.18735	-489.99689	-70.96352	1
83	H	68.69654	76.19008	80.33288	-1226.32661	-1724.38906	-1716.47170	1
84	H	69.71168	75.35458	79.11312	2381.64273	-969.84735	900.46860	1
85	H	68.08974	75.99082	78.65210	2122.74991	1702.23946	-141.36228	1
86	C	66.62137	74.40315	80.49129	-501.86074	-479.61276	-376.42482	1
87	H	66.70385	75.01002	81.42337	993.79261	-2246.95401	-1177.81305	1
88	H	65.96488	74.96420	79.78569	42.71279	-626.15391	-2651.37258	1
89	H	66.09225	73.45662	80.75389	-2026.39012	-1590.33709	-887.82922	1
90	C	69.21692	73.07153	77.75501	-672.89153	382.57394	-156.34072	1
91	O	70.29606	73.05319	78.30577	410.04627	221.86223	500.35950	1
92	N	68.96266	73.04935	76.45034	-378.11782	-443.79414	-441.10984	1

93	H	67.99889	73.09645	76.12249	2404.15973	-568.14894	1149.30085	1
94	C	70.06869	72.93781	75.56483	-544.54484	466.16019	331.29119	1
95	H	70.93905	72.73833	76.23681	-1409.80988	-170.17955	2325.32679	1
96	C	69.71073	71.79071	74.52342	-184.48284	116.78282	-758.89137	1
97	H	69.32886	70.88988	75.05493	1893.78641	1861.14652	611.04528	1
98	H	68.88921	72.12649	73.84866	-2170.79665	-974.19311	1327.50117	1
99	C	70.99034	71.45373	73.69760	389.51668	672.81878	-138.49152	1
100	H	71.29927	72.35179	73.11278	510.64577	1933.03327	1851.02484	1
101	H	71.84890	71.25687	74.37683	-2302.30869	-1105.72939	-948.89774	1
102	C	70.79963	70.22460	72.72972	-559.93427	-126.34590	542.30857	1
103	O	71.73349	69.84013	72.07515	-670.36003	-111.83166	76.36448	1
104	N	69.55557	69.69939	72.73610	-216.06729	-537.07037	446.51379	1
105	H	68.71525	70.00790	73.23913	-1251.96487	1074.12894	-2168.52500	1
106	H	69.26164	68.91705	72.14121	-2451.83023	-720.73851	944.84612	1
107	C	70.21947	74.28721	74.64658	546.24052	-563.88337	-85.11809	1
108	O	69.98088	74.18477	73.47146	71.70702	-307.40463	606.69673	1
109	N	70.59958	75.36677	75.34834	479.90863	-504.50129	222.86849	1
110	C	70.97556	76.59480	74.72774	75.51268	-600.91904	506.73700	1
111	H	70.58732	76.60453	73.68269	-2033.61562	1795.30103	254.89480	1
112	C	70.31709	77.63015	75.74966	523.79067	517.99274	284.45581	1
113	H	70.69474	78.66816	75.62086	1599.61665	-1127.00911	1895.98173	1
114	H	69.21156	77.67232	75.63575	-1881.83093	1275.82488	-1501.55016	1
115	C	70.72862	76.98573	77.10671	-600.05639	-404.05026	316.64485	1
116	H	71.79758	77.19821	77.33915	-2597.05260	496.36221	657.73249	1
117	H	70.13342	77.35170	77.97320	-1666.24518	1294.38985	-1723.90591	1
118	C	70.51667	75.44050	76.80207	493.57570	-129.95376	-602.56394	1
119	H	71.30944	74.77051	77.21603	-1469.08415	-637.84797	2204.22581	1
120	H	69.51212	75.03056	77.06851	-1038.97840	1068.88701	-2280.71789	1
121	C	72.59222	76.79560	74.86464	188.88100	241.05089	-727.87821	1
122	O	73.26102	76.21967	75.71887	531.88613	-49.19943	427.07960	1
123	N	72.97291	77.71976	74.01448	708.14833	26.93417	-179.73509	1
124	H	72.22365	78.06046	73.41581	-2232.69501	-1179.09831	1023.94816	1
125	C	74.32092	78.24788	73.93102	-738.32412	259.92548	104.42456	1
126	H	74.24504	79.09450	73.20727	2028.89123	1260.02983	1311.33324	1
127	C	74.76639	78.67347	75.32762	-258.65678	-345.52513	661.28459	1
128	H	74.63223	77.79955	76.01211	-1826.06090	-1801.46097	-918.64554	1
129	C	76.22503	79.07366	75.35895	-541.23400	531.92970	-218.41428	1
130	H	76.55168	79.36598	76.39546	1311.73218	-2219.18200	882.19023	1
131	H	76.91482	78.21396	75.01578	-1048.71298	1223.58118	-2196.97971	1
132	H	76.42841	79.95270	74.68707	419.06414	1903.92898	1903.44670	1
133	C	73.90210	79.79625	75.87128	-423.86431	152.66566	-648.55262	1
134	H	74.18981	80.07119	76.92344	105.68386	-2342.50080	1387.51238	1
135	H	73.99029	80.72763	75.24725	-1695.63603	-1484.73621	-1531.02793	1
136	H	72.81573	79.50575	75.88600	-1853.57121	-487.39031	1936.59343	1
137	C	75.26683	77.00906	73.33491	539.71428	-510.58232	267.58633	1
138	O	75.65311	77.06749	72.19777	-15.93758	-278.34085	-624.49402	1
139	N	75.45486	76.06252	74.23642	-676.81886	12.05292	276.17960	1
140	H	74.92885	76.07324	75.13892	-1694.44250	-373.84189	-2100.66098	1
141	C	76.42318	75.05875	73.95394	412.33078	-664.70360	108.35451	1
142	H	76.29592	74.33524	74.79106	1765.77476	1294.44366	1621.76594	1
143	C	76.02361	74.48511	72.52693	-179.66635	-721.95667	-264.73915	1
144	H	74.94666	74.68192	72.32430	-607.34922	2587.87032	-598.10018	1
145	H	76.57693	75.03035	71.72733	-359.69332	-1479.13954	-2259.74260	1
146	C	76.32209	72.95049	72.46770	-240.01076	616.02425	431.85322	1
147	H	77.38230	72.73238	72.73043	-1359.17131	782.54425	2227.99181	1
148	H	75.70356	72.38975	73.20385	-820.36667	85.81767	-2596.78715	1
149	C	76.00626	72.48817	70.98804	-513.07015	236.18570	-551.87280	1
150	H	74.90838	72.49254	70.79597	1816.11944	-1183.11722	-1650.94321	1
151	H	76.44510	73.19833	70.25020	-1800.04429	-1361.53473	1526.34643	1
152	C	76.60129	71.07437	70.79260	726.08972	-253.19732	-179.64713	1
153	H	77.70489	71.02276	70.88375	1224.27271	-456.51798	-2390.90304	1
154	H	76.13158	70.28316	71.41061	1206.40339	-1150.93514	-2154.90344	1

155	N	76.30745	70.65312	69.31448	329.70796	-633.68968	-155.67358	1
156	H	76.69939	69.71431	69.01457	1348.31305	1938.76845	1359.00643	1
157	H	75.28471	70.54370	69.05584	2096.92035	1446.54551	-966.48890	1
158	H	76.66608	71.28841	68.54301	-1197.07217	-2303.53719	827.28733	1
159	C	77.89928	75.76582	73.93454	-378.01186	-556.17301	-413.96481	1
160	O	78.10632	76.86133	74.42607	-409.44433	-307.55053	-453.30833	1
161	N	78.74984	74.96001	73.33083	-429.02477	524.70884	274.08502	1
162	H	78.38841	74.07521	72.98121	1706.34263	-1425.96036	1574.38926	1
163	C	80.14837	75.23024	73.32250	-45.25864	-626.22952	478.93267	1
164	H	80.54370	74.54611	72.53788	1988.63164	570.90773	1772.87287	1
165	C	80.29491	76.76727	72.97153	551.77128	-20.49526	-564.54996	1
166	H	79.44797	77.06355	72.31184	1434.61535	-1753.10253	1513.99471	1
167	H	80.17882	77.39371	73.88897	-714.67738	1819.09770	1898.36494	1
168	C	81.66455	77.06807	72.26532	446.99263	-555.77305	338.97221	1
169	H	82.47025	77.27212	73.00885	1953.68466	1892.25957	-161.67766	1
170	H	82.00811	76.19835	71.65932	-403.03785	2688.07032	-188.43591	1
171	C	81.43115	78.31289	71.34783	567.86262	335.74681	434.04421	1
172	H	80.68412	78.09782	70.55248	-1080.02275	1568.26081	-1948.78900	1
173	H	81.01490	79.16564	71.92778	-919.54108	2111.34692	1456.13463	1
174	C	82.84325	78.70480	70.71147	195.81897	173.33862	-745.11536	1
175	H	83.60579	78.97811	71.49348	1405.67949	-2301.21089	-390.08113	1
176	H	83.27836	77.91348	70.00834	-940.37328	-1118.32446	2299.72133	1
177	N	82.62189	79.86612	69.90225	319.26422	656.36007	-42.02424	1
178	H	85.09872	80.66994	69.97350	1961.03633	619.91968	1787.09422	2
179	H	83.22757	79.94131	69.08987	854.14343	-2156.80752	1429.08711	1
180	H	82.79869	80.75072	70.36968	1237.02905	-1378.50857	-1998.28500	1
181	C	80.72361	74.86082	74.80774	532.53319	-268.57236	517.55729	1
182	O	80.07884	74.27730	75.64811	266.16714	-290.73804	-558.88002	1
183	N	82.02117	75.18528	74.84733	-226.25352	640.49678	-270.32839	1
184	H	82.39451	75.65427	74.02421	2007.69063	-1035.27229	1523.50231	1
185	C	82.56310	75.46967	76.13844	-540.76542	-573.33303	49.50000	1
186	H	81.81978	75.04511	76.85259	-2374.20950	-1036.76023	843.75774	1
187	C	83.99242	74.76431	76.20198	-77.09082	666.87422	-415.84136	1
188	H	84.63585	75.15030	75.36338	-985.81834	617.19825	2463.91927	1
189	O	84.01037	73.33142	76.04424	293.29899	-391.65602	-477.80926	1
190	H	84.49602	73.23701	75.20195	2528.72714	-681.76262	-751.27122	1
191	C	84.51717	75.30683	77.58144	252.47363	-605.14473	440.05134	1
192	H	85.58385	75.03223	77.75131	-2052.65063	1456.49051	-1043.51830	1
193	H	84.44113	76.41734	77.64231	-2152.98800	-1661.97574	-161.70652	1
194	H	83.92840	74.88978	78.43107	-473.12726	-1584.27339	2165.61725	1
195	C	82.67649	77.10703	76.21318	360.36307	488.46713	505.10056	1
196	O	81.82904	77.73539	76.79823	-200.08817	-528.03552	-385.82850	1
197	N	83.74091	77.55681	75.55337	-597.54095	-226.44775	355.20479	1
198	H	84.36517	76.91560	75.06537	2179.23655	-1300.70981	-991.33835	1
199	C	83.94335	78.94103	75.45441	-687.68921	297.39807	-249.45179	1
200	H	83.08214	79.44714	75.94506	-349.16256	-2467.37713	-1101.72831	1
201	C	85.37211	79.27619	76.08828	672.47345	361.54328	-201.62880	1
202	H	86.14235	78.54983	75.74119	1541.41502	582.18425	2169.97026	1
203	H	85.70203	80.28945	75.76221	-2534.67717	60.25153	997.72295	1
204	C	85.21418	79.22846	77.61517	574.26774	-389.43119	-377.02542	1
205	C	84.46908	80.26287	78.25712	688.82679	-287.33580	-257.96133	1
206	H	84.06125	81.10865	77.67440	331.14182	1470.38163	2269.80013	1
207	C	85.75578	78.14951	78.37705	-383.52382	-675.04808	144.24917	1
208	H	86.35240	77.35859	77.88758	4.09847	1517.59662	2262.86397	1
209	C	84.24926	80.17362	79.63101	-134.76730	428.45285	-649.50303	1
210	H	83.66367	80.96857	80.12494	-903.23433	1600.49020	2011.53387	1
211	C	85.50009	78.09969	79.74993	-335.53281	-615.00040	-364.39058	1
212	H	85.90549	77.24968	80.32606	1596.45398	-1369.33862	1732.02659	1
213	C	84.73847	79.09699	80.42621	585.48547	-340.24194	-406.23938	1
214	O	84.46975	79.05585	81.81921	-419.15649	-173.04408	-511.94141	1
215	H	84.91903	78.20939	82.05092	-1071.84350	1559.71507	-1960.13012	1
216	C	84.16035	79.24959	73.82545	291.41878	-183.13091	710.72246	1

217	O	84.82116	78.44401	73.09547	379.87695	523.47396	-222.23622	1
218	N	83.67426	80.36592	73.46439	564.30591	373.09380	277.24371	1
219	H	83.21383	80.84455	74.21942	-120.59931	-2436.07824	-1214.35098	1
220	C	85.91716	80.23777	70.58827	404.07514	-299.37480	608.84009	2
221	H	85.47338	80.03499	71.59108	-1071.07882	-841.69025	2359.66467	2
222	C	87.07571	81.28282	70.69979	-683.12807	68.71770	-390.13096	2
223	H	86.78033	82.12591	71.36607	2068.88918	1596.58590	770.89603	2
224	H	87.97996	80.82227	71.16007	1379.86429	2342.49779	-179.85638	2
225	C	87.38284	81.80895	69.25599	-176.39967	537.49466	550.97268	2
226	H	87.69579	80.97323	68.58702	-396.28051	1942.22168	1869.33314	2
227	H	86.47347	82.24616	68.78739	-94.44700	586.00678	-2659.20016	2
228	C	88.53595	82.90019	69.40946	-291.69381	-718.18079	-150.72929	2
229	H	88.29034	83.76838	70.07339	-2303.38776	1089.76242	964.62032	2
230	H	89.53672	82.50590	69.72130	884.16729	2568.80533	-207.74283	2
231	N	88.65444	83.39434	68.10238	-594.49522	-252.81478	342.29276	2
232	H	88.03682	83.00299	67.40827	-1735.17426	2084.05705	-263.71605	2
233	C	89.47775	84.29458	67.74519	595.23177	-271.52487	442.22352	2
234	N	90.32678	84.82472	68.72328	585.53813	-424.79750	-105.81303	2
235	H	90.39739	84.59240	69.71311	959.88797	1327.56823	-2177.11905	2
236	H	91.02919	85.54637	68.55900	1578.48647	16.27378	-2220.76233	2
237	N	89.35169	84.58080	66.37840	-452.17763	-390.33541	-421.51853	2
238	H	88.73012	84.19557	65.66893	470.26107	1974.25629	-1817.92087	2
239	H	89.92219	85.27875	65.89965	1856.67307	-1573.97321	-1224.35416	2
240	C	86.44742	78.88946	69.93573	-531.47271	-581.45780	-55.06206	2
241	O	87.08342	78.83124	68.91782	-243.00837	192.73507	609.52485	2
242	N	86.04707	77.88222	70.74986	343.49288	-644.25607	38.09164	2
243	H	85.49501	78.10091	71.64120	-1691.16043	-1535.97525	-1484.73099	2
244	C	86.25617	76.47693	70.35573	542.66492	350.14337	454.42563	2
245	H	87.34241	76.39792	70.11862	1209.57979	-2396.95920	463.86744	2
246	C	85.79947	75.60730	71.50541	-737.14309	145.93010	242.71942	2
247	H	84.72842	75.84097	71.70368	-1050.18303	159.36419	-2509.06125	2
248	C	85.90520	74.13155	71.16228	-706.77696	-252.88343	-245.16230	2
249	H	85.50567	73.48282	71.98915	-1624.64039	-1665.49085	1417.86935	2
250	H	85.32915	73.87497	70.22703	2566.10521	598.51109	693.22305	2
251	H	86.97190	73.82399	70.98549	-1972.69758	107.10018	-1876.34312	2
252	C	86.56596	75.89430	72.78455	412.85148	672.58832	-27.69222	2
253	H	86.25447	75.21116	73.62118	1447.02277	1762.76533	-1490.78944	2
254	H	87.67354	75.76401	72.64172	1320.77379	-145.20455	2378.68491	2
255	H	86.39461	76.95344	73.13589	-1512.10848	1470.52031	1724.75147	2
256	C	85.30176	76.20101	69.03822	-607.11113	499.56689	73.73769	2
257	O	84.18160	76.66058	68.92543	357.97126	460.81534	356.68785	2
258	N	85.93462	75.35994	68.24272	536.55407	-368.62270	332.76306	2
259	H	86.84215	75.00316	68.53520	524.38866	2297.69985	1367.20941	2
260	C	85.31967	75.01554	67.01285	46.50277	-774.29190	-147.97904	2
261	H	84.59733	75.84434	66.83069	1676.51875	1883.29066	1032.55549	2
262	C	86.46515	74.83656	65.89137	-559.41456	-34.19198	-556.30433	2
263	H	87.03478	73.89949	66.09976	-64.66664	395.18769	2695.05373	2
264	H	86.00703	74.69346	64.88373	-2703.44278	-60.40056	333.79418	2
265	C	87.39606	76.02055	65.90292	-519.76435	377.31045	459.42366	2
266	H	87.74808	76.18356	66.94691	-1746.74323	1667.50644	-1261.73691	2
267	C	88.61091	75.74805	65.02481	570.95554	16.46261	-545.27700	2
268	H	89.33193	76.60574	65.03873	2391.58273	28.05277	-1305.07271	2
269	H	89.17092	74.83835	65.36342	175.75588	917.63458	2559.43867	2
270	H	88.31827	75.57813	63.95680	-1063.97851	-2155.34650	1283.00462	2
271	C	86.69506	77.29045	65.44089	193.76014	2.62946	-765.53141	2
272	H	87.39694	78.16425	65.42352	507.39394	-846.55087	2539.60089	2
273	H	86.27374	77.17986	64.40840	1337.57841	1818.19054	1526.01994	2
274	H	85.84828	77.56257	66.12335	1100.88635	-1172.91350	-2199.08909	2
275	C	84.58421	73.59202	67.22977	-549.21115	475.64486	-309.38218	2
276	O	84.83013	72.83694	68.13340	556.06106	-390.37755	-78.24250	2
277	O	83.67522	73.22445	66.20965	-572.27940	-310.19032	-209.75862	2
278	H	83.71738	74.05642	65.66027	-1380.08193	2212.14486	790.85944	2

Listing 68: C00068.xmolout

1	276							
2	150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
	0.2500	300.00	0.00	0.00	0.00	-1293.6004	0.0000	300.0000
3	H	60.36614	78.27556	70.64603	-2043.14101	-1757.64893	399.89339	1
4	N	60.50544	79.18841	71.07076	426.75047	490.45733	-334.42467	1
5	H	60.49184	78.96866	72.06287	442.25559	-1110.30854	-2448.52907	1
6	C	61.61101	79.93883	70.60383	415.32972	-666.39213	83.73172	1
7	H	61.65826	79.68466	69.52035	879.32219	2491.00447	667.35213	1
8	C	61.33517	81.51980	70.84406	31.35357	477.41777	628.23362	1
9	H	61.22878	81.71685	71.93664	1168.38489	2240.25337	-1019.71136	1
10	H	62.21575	82.11718	70.50896	-360.43770	2534.90498	931.67112	1
11	C	60.09234	81.92926	70.11074	463.18208	512.70242	-382.34388	1
12	H	59.28061	81.21346	70.37523	1725.29117	1863.52247	-987.07854	1
13	C	59.66322	83.33092	70.53097	710.42801	-144.27427	-313.15367	1
14	H	58.72358	83.64917	70.01082	364.20195	-1033.13725	2494.72524	1
15	H	59.47070	83.39285	71.63269	2567.61904	335.80679	847.48802	1
16	H	60.44936	84.09125	70.28871	-2587.99029	680.92867	-512.16411	1
17	C	60.29671	81.90108	68.60089	268.17616	741.64379	-40.42634	1
18	H	59.37999	82.24071	68.05387	1283.54314	-1945.37420	-1411.27812	1
19	H	61.13776	82.57099	68.28658	-1258.57796	1317.15249	-2026.02085	1
20	H	60.53789	80.87132	68.23293	-2502.84526	909.80597	575.92391	1
21	C	62.92879	79.52656	71.38078	619.36578	-458.64843	-172.09273	1
22	O	63.96294	80.28460	71.44491	-81.40433	433.87611	522.34594	1
23	N	62.89634	78.32644	71.88457	175.23996	-622.20190	341.55523	1
24	H	62.04554	77.77143	71.82930	-876.57256	-303.22879	-2561.90213	1
25	C	63.95344	78.07927	72.82363	-571.88214	-534.10783	-106.15033	1
26	H	63.48755	78.30574	73.80165	-2713.20841	-16.25800	-248.80809	1
27	C	64.29733	76.55171	72.68262	166.60354	288.16399	-716.09568	1
28	H	64.58199	76.34142	71.61507	-2097.85574	1636.78449	-586.18044	1
29	O	63.21970	75.62764	72.98430	-317.80580	-363.38227	484.43082	1
30	H	63.11990	75.16104	72.13534	1863.74748	-1451.84923	1357.29467	1
31	C	65.57728	76.46565	73.59671	503.80731	517.99032	318.51606	1
32	H	66.05045	75.45797	73.54124	640.61020	-2157.10410	-1536.29104	1
33	H	66.34474	77.21755	73.28888	1687.88455	465.60692	2087.56452	1
34	H	65.33098	76.65765	74.66664	-1293.07895	-1899.88581	-1463.57452	1
35	C	65.22465	79.11571	72.39881	-153.07550	-733.68902	248.70981	1
36	O	66.05359	78.69803	71.56901	186.15459	-480.78787	-449.34387	1
37	N	65.59203	79.84244	73.51506	-487.53139	543.18517	42.03850	1
38	C	66.56748	80.85732	73.41381	-699.35871	69.34393	360.10701	1
39	H	66.60823	81.10163	72.32605	2.81126	-221.99807	-2715.58072	1
40	C	66.00027	81.99100	74.38392	-507.46439	-592.59194	122.07761	1
41	H	66.78889	82.69685	74.72836	-1975.08116	525.87560	-1801.71556	1
42	H	65.21204	82.59934	73.88650	1588.27743	-1913.22100	1113.83566	1
43	C	65.40939	81.12217	75.53087	-613.62442	-457.55993	-194.14490	1
44	H	66.21408	80.74557	76.20153	1707.54637	-721.27992	1996.92523	1
45	H	64.68109	81.66386	76.17441	758.23357	2100.81767	1560.55011	1
46	C	64.74661	79.93770	74.68489	-352.41524	704.96076	49.21465	1
47	H	64.73995	78.94398	75.19532	1714.76886	-2070.42778	443.35792	1
48	H	63.72162	80.16326	74.29996	1224.15040	1801.50881	1636.97633	1
49	C	68.03567	80.34815	73.99521	566.85117	537.05831	117.62814	1
50	O	68.57207	80.93858	74.89904	-550.26779	-406.08867	4.21666	1
51	N	68.47506	79.32033	73.28851	566.34832	-425.77725	180.18749	1
52	H	67.89766	78.97398	72.51698	644.44502	2646.80550	-52.73430	1
53	C	69.75523	78.78507	73.57698	612.34801	-281.48662	411.56221	1
54	H	70.14018	79.33026	74.47079	1667.23498	-1490.75142	1556.16753	1
55	C	69.51570	77.21442	73.81817	-714.45746	-175.43074	286.98927	1
56	H	68.94295	76.80946	72.93987	-787.09484	1763.03619	-1922.46060	1
57	O	68.73900	76.89184	74.98564	-429.46514	516.51932	-128.40526	1

58	H	67.94952	76.48524	74.57795	1981.82785	436.16847	-1818.18182	1
59	C	70.97057	76.62209	73.80277	630.79189	-468.94448	76.03230	1
60	H	70.96655	75.51933	73.96409	-1775.71861	2062.30353	131.89849	1
61	H	71.49327	76.81302	72.83632	-1855.14608	88.94118	1993.53760	1
62	H	71.59648	77.07101	74.60543	-1504.82350	-780.94249	-2132.90992	1
63	C	70.65698	78.97222	72.22782	288.57638	618.62814	-397.00270	1
64	O	70.17327	78.97911	71.11874	321.70495	-185.26452	574.37218	1
65	N	71.95116	79.03309	72.55063	-447.05792	-446.53431	367.76425	1
66	H	72.22584	78.96200	73.52892	350.31316	1975.63644	-1843.31522	1
67	C	72.85417	78.80533	71.45373	-511.23061	374.03917	-471.51480	1
68	H	72.25980	78.08667	70.84281	2234.79579	-898.70890	-1273.45190	1
69	C	72.97987	80.20344	70.68273	529.53781	-159.34528	563.72604	1
70	H	73.41275	79.97965	69.67043	654.59388	2347.94251	1217.51488	1
71	H	71.93074	80.56244	70.51363	-1526.55661	2103.42026	817.87394	1
72	O	73.80803	81.21749	71.31758	-554.84278	14.12789	399.58769	1
73	H	73.12789	81.65320	71.86427	1297.06236	2061.84854	1220.68812	1
74	C	74.23037	78.17728	72.01672	-662.15484	-412.13544	123.62687	1
75	O	74.21723	77.24561	72.78212	-540.01537	-317.05804	274.91456	1
76	N	75.29264	78.71351	71.37731	-202.76299	-690.00100	-131.49145	1
77	H	75.07883	79.57214	70.85824	-702.62132	-2617.37191	281.70413	1
78	C	76.66328	78.46726	71.83979	-491.73914	576.34187	222.73509	1
79	H	76.71687	77.35948	71.93431	1977.17978	-1823.58850	-434.68928	1
80	C	77.58288	79.02957	70.77853	-649.50797	-328.66843	306.11224	1
81	H	77.33688	80.10874	70.65408	2075.07803	1452.16490	-1004.45904	1
82	C	79.05143	78.92623	71.14922	-615.18735	-489.99689	-70.96352	1
83	H	79.71391	79.33419	70.33706	-1226.32661	-1724.38906	-1716.47170	1
84	H	79.28533	79.50205	72.08866	2381.64273	-969.84735	900.46860	1
85	H	79.35765	77.85878	71.32434	2122.74991	1702.23946	-141.36228	1
86	C	77.35991	78.35324	69.43541	-501.86074	-479.61276	-376.42482	1
87	H	77.98109	78.82124	68.62384	993.79261	-2246.95401	-1177.81305	1
88	H	77.62918	77.26258	69.47430	42.71279	-626.15391	-2651.37258	1
89	H	76.28430	78.41679	69.11515	-2026.39012	-1590.33709	-887.82922	1
90	C	76.89960	79.18487	73.32238	-672.89153	382.57394	-156.34072	1
91	O	77.97124	79.07051	73.86729	410.04627	221.86223	500.35950	1
92	N	75.82297	79.81905	73.73990	-378.11782	-443.79414	-441.10984	1
93	H	75.02854	79.79369	73.09915	2404.15973	-568.14894	1149.30085	1
94	C	75.81428	80.55580	74.96890	-544.54484	466.16019	331.29119	1
95	H	76.69564	81.23106	74.89331	-1409.80988	-170.17955	2325.32679	1
96	C	74.41863	81.30288	74.97771	-184.48284	116.78282	-758.89137	1
97	H	74.38165	82.10399	74.20491	1893.78641	1861.14652	611.04528	1
98	H	73.60714	80.59599	74.69613	-2170.79665	-974.19311	1327.50117	1
99	C	74.17795	81.88207	76.40642	389.51668	672.81878	-138.49152	1
100	H	74.57216	81.17536	77.17409	510.64577	1933.03327	1851.02484	1
101	H	74.78382	82.80174	76.56294	-2302.30869	-1105.72939	-948.89774	1
102	C	72.65857	82.17342	76.70332	-559.93427	-126.34590	542.30857	1
103	O	72.35541	82.69873	77.74334	-670.36003	-111.83166	76.36448	1
104	N	71.80616	81.75527	75.74225	-216.06729	-537.07037	446.51379	1
105	H	71.99208	81.30993	74.83590	-1251.96487	1074.12894	-2168.52500	1
106	H	70.78430	81.83507	75.81120	-2451.83023	-720.73851	944.84612	1
107	C	76.00230	79.57336	76.25434	546.24052	-563.88337	-85.11809	1
108	O	76.57340	80.06964	77.19160	71.70702	-307.40463	606.69673	1
109	N	75.31841	78.41977	76.21651	479.90863	-504.50129	222.86849	1
110	C	75.67088	77.38620	77.14694	75.51268	-600.91904	506.73700	1
111	H	76.09056	77.94792	78.01409	-2033.61562	1795.30103	254.89480	1
112	C	74.30650	76.63625	77.43003	523.79067	517.99274	284.45581	1
113	H	74.44441	75.53812	77.56495	1599.61665	-1127.00911	1895.98173	1
114	H	73.83653	77.00576	78.36907	-1881.83093	1275.82488	-1501.55016	1
115	C	73.41737	76.97317	76.18864	-600.05639	-404.05026	316.64485	1
116	H	73.57050	76.23146	75.36977	-2597.05260	496.36221	657.73249	1
117	H	72.32924	76.95910	76.42592	-1666.24518	1294.38985	-1723.90591	1
118	C	73.93712	78.40032	75.74144	493.57570	-129.95376	-602.56394	1
119	H	73.97212	78.55896	74.63728	-1469.08415	-637.84797	2204.22581	1

120	H	73.42546	79.26206	76.23191	-1038.97840	1068.88701	-2280.71789	1
121	C	76.77020	76.33209	76.55033	188.88100	241.05089	-727.87821	1
122	O	77.52669	75.77870	77.31114	531.88613	-49.19943	427.07960	1
123	N	76.71938	76.16952	75.19363	708.14833	26.93417	-179.73509	1
124	H	75.87624	76.68283	74.92290	-2232.69501	-1179.09831	1023.94816	1
125	C	77.09213	74.83766	74.64782	-738.32412	259.92548	104.42456	1
126	H	76.60349	74.10964	75.33583	2028.89123	1260.02983	1311.33324	1
127	C	76.60474	74.74840	73.22268	-258.65678	-345.52513	661.28459	1
128	H	76.83339	75.71919	72.73003	-1826.06090	-1801.46097	-918.64554	1
129	C	77.30595	73.64772	72.44490	-541.23400	531.92970	-218.41428	1
130	H	76.98396	73.62624	71.36773	1311.73218	-2219.18200	882.19023	1
131	H	78.42437	73.77996	72.45905	-1048.71298	1223.58118	-2196.97971	1
132	H	77.09103	72.63356	72.88065	419.06414	1903.92898	1903.44670	1
133	C	75.10402	74.52813	73.14633	-423.86431	152.66566	-648.55262	1
134	H	74.73257	74.55594	72.08488	105.68386	-2342.50080	1387.51238	1
135	H	74.80976	73.53260	73.58301	-1695.63603	-1484.73621	-1531.02793	1
136	H	74.53781	75.31913	73.72249	-1853.57121	-487.39031	1936.59343	1
137	C	78.72886	74.70548	74.66923	539.71428	-510.58232	267.58633	1
138	O	79.24066	73.58994	74.58617	-15.93758	-278.34085	-624.49402	1
139	N	79.31615	75.87583	74.68132	-676.81886	12.05292	276.17960	1
140	H	78.68011	76.66266	74.79297	-1694.44250	-373.84189	-2100.66098	1
141	C	80.72119	76.01679	74.45181	412.33078	-664.70360	108.35451	1
142	H	80.91788	75.28131	73.63859	1765.77476	1294.44366	1621.76594	1
143	C	80.94046	77.53148	74.06804	-179.66635	-721.95667	-264.73915	1
144	H	80.30022	77.81681	73.20410	-607.34922	2587.87032	-598.10018	1
145	H	80.61722	78.19380	74.90388	-359.69332	-1479.13954	-2259.74260	1
146	C	82.45775	77.74379	73.74508	-240.01076	616.02425	431.85322	1
147	H	83.07943	77.49624	74.63706	-1359.17131	782.54425	2227.99181	1
148	H	82.80024	77.06670	72.93077	-820.36667	85.81767	-2596.78715	1
149	C	82.63741	79.26128	73.33938	-513.07015	236.18570	-551.87280	1
150	H	82.15515	79.47266	72.35708	1816.11944	-1183.11722	-1650.94321	1
151	H	82.13192	79.92867	74.07484	-1800.04429	-1361.53473	1526.34643	1
152	C	84.15525	79.55500	73.29650	726.08972	-253.19732	-179.64713	1
153	H	84.67037	79.45192	74.27260	1224.27271	-456.51798	-2390.90304	1
154	H	84.71325	79.00261	72.51442	1206.40339	-1150.93514	-2154.90344	1
155	N	84.32657	81.06562	72.92306	329.70796	-633.68968	-155.67358	1
156	H	85.32583	81.42010	72.89215	1348.31305	1938.76845	1359.00643	1
157	H	83.96581	81.37396	71.97362	2096.92035	1446.54551	-966.48890	1
158	H	83.87443	81.77447	73.57110	-1197.07217	-2303.53719	827.28733	1
159	C	81.53007	75.61132	75.81098	-378.01186	-556.17301	-413.96481	1
160	O	82.17888	76.41237	76.43591	-409.44433	-307.55053	-453.30833	1
161	N	81.43556	74.28815	75.98723	-429.02477	524.70884	274.08502	1
162	H	80.75926	73.74088	75.39265	1706.34263	-1425.96036	1574.38926	1
163	C	81.76079	73.83695	77.30663	-45.25864	-626.22952	478.93267	1
164	H	82.36234	74.66207	77.76018	1988.63164	570.90773	1772.87287	1
165	C	80.38372	73.59071	78.05787	551.77128	-20.49526	-564.54996	1
166	H	79.67287	74.43362	77.89348	1434.61535	-1753.10253	1513.99471	1
167	H	79.87661	72.69072	77.64332	-714.67738	1819.09770	1898.36494	1
168	C	80.71165	73.40218	79.57410	446.99263	-555.77305	338.97221	1
169	H	81.66142	72.81673	79.69126	1953.68466	1892.25957	-161.67766	1
170	H	80.89287	74.38302	80.06917	-403.03785	2688.07032	-188.43591	1
171	C	79.51430	72.62811	80.25910	567.86262	335.74681	434.04421	1
172	H	78.58602	73.24443	80.25096	-1080.02275	1568.26081	-1948.78900	1
173	H	79.26648	71.69929	79.69532	-919.54108	2111.34692	1456.13463	1
174	C	79.94880	72.28735	81.70391	195.81897	173.33862	-745.11536	1
175	H	80.78025	71.55810	81.78077	1405.67949	-2301.21089	-390.08113	1
176	H	80.16045	73.16766	82.34279	-940.37328	-1118.32446	2299.72133	1
177	N	78.74191	71.57319	82.40009	319.26422	656.36007	-42.02424	1
178	H	78.91472	71.25252	83.39640	1961.03633	619.91968	1787.09422	1
179	H	77.85026	72.13765	82.51454	854.14343	-2156.80752	1429.08711	1
180	H	78.38188	70.68065	81.95224	1237.02905	-1378.50857	-1998.28500	1
181	C	82.52553	72.39820	77.25188	532.53319	-268.57236	517.55729	1

182	O	82.81701	71.84842	78.31183	266.16714	-290.73804	-558.88002	1
183	N	82.69129	71.94992	76.02379	-226.25352	640.49678	-270.32839	1
184	H	82.38079	72.60622	75.31014	2007.69063	-1035.27229	1523.50231	1
185	C	83.51325	70.84602	75.67498	-540.76542	-573.33303	49.50000	1
186	H	83.62532	70.94239	74.57236	-2374.20950	-1036.76023	843.75774	1
187	C	84.91602	71.01952	76.42507	-77.09082	666.87422	-415.84136	1
188	H	84.72724	71.04640	77.53541	-985.81834	617.19825	2463.91927	1
189	O	85.62471	72.23166	76.10049	293.29899	-391.65602	-477.80926	1
190	H	85.60549	72.69362	76.96155	2528.72714	-681.76262	-751.27122	1
191	C	85.67752	69.69095	76.07209	252.47363	-605.14473	440.05134	1
192	H	86.68437	69.66077	76.55035	-2052.65063	1456.49051	-1043.51830	1
193	H	85.12089	68.78553	76.41509	-2152.98800	-1661.97574	-161.70652	1
194	H	85.83112	69.58920	74.97242	-473.12726	-1584.27339	2165.61725	1
195	C	82.78607	69.43787	76.06456	360.36307	488.46713	505.10056	1
196	O	83.08501	68.44853	75.43529	-200.08817	-528.03552	-385.82850	1
197	N	81.94738	69.52590	77.09443	-597.54095	-226.44775	355.20479	1
198	H	81.85560	70.41643	77.61033	2179.23655	-1300.70981	-991.33835	1
199	C	81.33607	68.30159	77.48880	-687.68921	297.39807	-249.45179	1
200	H	82.13332	67.54211	77.32165	-349.16256	-2467.37713	-1101.72831	1
201	C	80.78207	68.42862	78.97894	672.47345	361.54328	-201.62880	1
202	H	80.08561	69.29557	79.05091	1541.41502	582.18425	2169.97026	1
203	H	80.19287	67.51557	79.22684	-2534.67717	60.25153	997.72295	1
204	C	81.94009	68.59501	79.97393	574.26774	-389.43119	-377.02542	1
205	C	82.64814	67.45106	80.44987	688.82679	-287.33580	-257.96133	1
206	H	82.38990	66.43766	80.09239	331.14182	1470.38163	2269.80013	1
207	C	82.28975	69.90189	80.42681	-383.52382	-675.04808	144.24917	1
208	H	81.75721	70.78842	80.03674	4.09847	1517.59662	2262.86397	1
209	C	83.66787	67.64174	81.38199	-134.76730	428.45285	-649.50303	1
210	H	84.21216	66.75759	81.75695	-903.23433	1600.49020	2011.53387	1
211	C	83.31786	70.04184	81.36195	-335.53281	-615.00040	-364.39058	1
212	H	83.57641	71.05875	81.70550	1596.45398	-1369.33862	1732.02659	1
213	C	84.03940	68.92570	81.87677	585.48547	-340.24194	-406.23938	1
214	O	85.08338	69.05403	82.82968	-419.15649	-173.04408	-511.94141	1
215	H	85.07223	70.03184	82.95800	-1071.84350	1559.71507	-1960.13012	1
216	C	80.01580	67.97113	76.57026	291.41878	-183.13091	710.72246	1
217	O	79.81891	66.81822	76.25273	379.87695	523.47396	-222.23622	1
218	N	79.24694	69.03516	76.38817	564.30591	373.09380	277.24371	1
219	H	79.64644	69.91188	76.72225	-120.59931	-2436.07824	-1214.35098	1
220	C	78.10144	69.01030	75.55183	404.07514	-299.37480	608.84009	1
221	H	77.96532	70.07161	75.24593	-1071.07882	-841.69025	2359.66467	1
222	C	78.40457	67.99141	74.37852	-683.12807	68.71770	-390.13096	1
223	H	79.43974	68.13785	73.99324	2068.88918	1596.58590	770.89603	1
224	H	78.37123	66.94012	74.77235	1379.86429	2342.49779	-179.85638	1
225	C	77.34961	68.18059	73.24198	-176.39967	537.49466	550.97268	1
226	H	76.31391	68.04832	73.62670	-396.28051	1942.22168	1869.33314	1
227	H	77.38837	69.20663	72.81392	-94.44700	586.00678	-2659.20016	1
228	C	77.71369	67.07262	72.14963	-291.69381	-718.18079	-150.72929	1
229	H	78.72733	67.16849	71.68349	-2303.38776	1089.76242	964.62032	1
230	H	77.60161	66.01341	72.49633	884.16729	2568.80533	-207.74283	1
231	N	76.76389	67.28352	71.14166	-594.49522	-252.81478	342.29276	1
232	H	76.04666	67.96664	71.32877	-1735.17426	2084.05705	-263.71605	1
233	C	76.74818	66.66896	70.02929	595.23177	-271.52487	442.22352	1
234	N	77.75047	65.72027	69.79574	585.53813	-424.79750	-105.81303	1
235	H	78.51495	65.42308	70.40080	959.88797	1327.56823	-2177.11905	1
236	H	77.83806	65.16163	68.94635	1578.48647	16.27378	-2220.76233	1
237	N	75.67599	67.09166	69.23083	-452.17763	-390.33541	-421.51853	1
238	H	74.94378	67.77989	69.39895	470.26107	1974.25629	-1817.92087	1
239	H	75.49327	66.71343	68.30042	1856.67307	-1573.97321	-1224.35416	1
240	C	76.80644	68.39926	76.36206	-531.47271	-581.45780	-55.06206	1
241	O	76.64586	67.21117	76.53447	-243.00837	192.73507	609.52485	1
242	N	75.99672	69.38677	76.71549	343.49288	-644.25607	38.09164	1
243	H	76.26789	70.35741	76.56041	-1691.16043	-1535.97525	-1484.73099	1

244	C	74.86207	69.03357	77.51428	542.66492	350.14337	454.42563	1
245	H	74.59284	68.02399	77.12689	1209.57979	-2396.95920	463.86744	1
246	C	75.32909	68.92464	79.02949	-737.14309	145.93010	242.71942	1
247	H	75.80636	69.86964	79.36700	-1050.18303	159.36419	-2509.06125	1
248	C	74.08741	68.57496	79.91753	-706.77696	-252.88343	-245.16230	1
249	H	74.36914	68.43553	80.98797	-1624.64039	-1665.49085	1417.86935	1
250	H	73.31775	69.39100	79.87440	2566.10521	598.51109	693.22305	1
251	H	73.59220	67.63462	79.57823	-1972.69758	107.10018	-1876.34312	1
252	C	76.33120	67.72160	79.13091	412.85148	672.58832	-27.69222	1
253	H	76.57934	67.47435	80.18997	1447.02277	1762.76533	-1490.78944	1
254	H	75.90983	66.79975	78.65967	1320.77379	-145.20455	2378.68491	1
255	H	77.29119	67.94126	78.60260	-1512.10848	1470.52031	1724.75147	1
256	C	73.71956	70.17126	77.25293	-607.11113	499.56689	73.73769	1
257	O	72.97265	70.54101	78.13564	357.97126	460.81534	356.68785	1
258	N	73.67703	70.42173	75.94853	536.55407	-368.62270	332.76306	1
259	H	74.39834	69.94144	75.40942	524.38866	2297.69985	1367.20941	1
260	C	73.06999	71.59172	75.41743	46.50277	-774.29190	-147.97904	1
261	H	73.10179	71.42356	74.31910	1676.51875	1883.29066	1032.55549	1
262	C	71.57158	71.75824	75.99607	-559.41456	-34.19198	-556.30433	1
263	H	71.59180	71.62750	77.11506	-64.66664	395.18769	2695.05373	1
264	H	71.16868	72.78174	75.80434	-2703.44278	-60.40056	333.79418	1
265	C	70.70317	70.71319	75.35344	-519.76435	377.31045	459.42366	1
266	H	71.21818	69.72995	75.44628	-1746.74323	1667.50644	-1261.73691	1
267	C	69.35920	70.62611	76.06680	570.95554	16.46261	-545.27700	1
268	H	68.70371	69.83555	75.61882	2391.58273	28.05277	-1305.07271	1
269	H	69.48328	70.38044	77.15311	175.75588	917.63458	2559.43867	1
270	H	68.79856	71.59442	76.00777	-1063.97851	-2155.34650	1283.00462	1
271	C	70.47525	71.01637	73.87799	193.76014	2.62946	-765.53141	1
272	H	69.80723	70.25534	73.39916	507.33994	-846.55087	2539.60089	1
273	H	69.99418	72.01782	73.73388	1337.57841	1818.19054	1526.01994	1
274	H	71.43383	71.02387	73.29931	1100.88635	-1172.91350	-2199.08909	1
275	C	73.95331	72.87015	75.80735	-549.21115	475.64486	-309.38218	1
276	O	75.01455	72.83227	76.37093	556.06106	-390.37755	-78.24250	1
277	O	73.44466	74.11142	75.32129	-572.27940	-310.19032	-209.75862	1
278	H	72.62021	73.76730	74.88476	-1380.08193	2212.14486	790.85944	1

Listing 69: C00069.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	1.0580	4232
		0.2500	300.00	0.00	0.00	0.00	-1293.5989	0.0000	300.0000
3	H	73.71273	64.84398	68.89238	-2043.14101	-1757.64893	399.89339		1
4	N	74.70404	64.68363	68.71632	426.75047	490.45733	-334.42467		1
5	H	74.69908	64.18461	67.81947	442.25559	-1110.30854	-2448.52907		1
6	C	75.46415	65.87047	68.62716	415.32972	-666.39213	83.73172		1
7	H	74.91973	66.66471	69.18367	879.32219	2491.00447	667.35213		1
8	C	76.93896	65.58563	69.22041	31.35357	477.41777	628.23362		1
9	H	77.36024	64.66912	68.74308	1168.38489	2240.25337	-1019.71136		1
10	H	77.63519	66.41994	68.96175	-360.43770	2534.90498	931.67112		1
11	C	76.83969	65.41320	70.71226	463.18208	512.70242	-382.34388		1
12	H	75.96959	64.75286	70.92929	1725.29117	1863.52247	-987.07854		1
13	C	78.09699	64.74882	71.25954	710.42801	-144.27427	-313.15367		1
14	H	78.03729	64.59883	72.36836	364.20195	-1033.13725	2494.72524		1
15	H	78.26820	63.74251	70.79724	2567.61904	335.80679	847.48802		1
16	H	79.01032	65.36571	71.05752	-2587.99029	680.92867	-512.16411		1
17	C	76.62911	66.75435	71.40270	268.17616	741.64379	-40.42634		1
18	H	76.55154	66.64009	72.51462	1283.54314	-1945.37420	-1411.27812		1
19	H	77.47710	67.45849	71.20014	-1258.57796	1317.15249	-2026.02085		1
20	H	75.69161	67.25932	71.05495	-2502.84526	909.80597	575.92391		1
21	C	75.57772	66.13423	67.02650	619.36578	-458.64843	-172.09273		1
22	O	75.33472	65.28014	66.19862	-81.40433	433.87611	522.34594		1
23	N	76.08116	67.35354	66.85261	175.23996	-622.20190	341.55523		1

24	H	76.20829	67.94147	67.67683	-876.57256	-303.22879	-2561.90213	1
25	C	75.99066	67.96611	65.56349	-571.88214	-534.10783	-106.15033	1
26	H	75.97819	67.05868	64.91378	-2713.20841	-16.25800	-248.80809	1
27	C	74.60288	68.78487	65.51840	166.60354	288.16399	-716.09568	1
28	H	74.82342	69.85257	65.22865	-2097.85574	1636.78449	-586.18044	1
29	O	73.85823	68.89187	66.73712	-317.80580	-363.38227	484.43082	1
30	H	73.90086	69.85714	66.90345	1863.74748	-1451.84923	1357.29467	1
31	C	73.90215	68.04606	64.31952	503.80731	517.99032	318.51606	1
32	H	73.61946	67.00519	64.60263	640.61020	-2157.10410	-1536.29104	1
33	H	72.96907	68.56693	64.00365	1687.88455	465.60692	2087.56452	1
34	H	74.56121	67.97243	63.42325	-1293.07895	-1899.88581	-1463.57452	1
35	C	77.32073	68.87380	65.43304	-153.07550	-733.68902	248.70981	1
36	O	78.31573	68.52232	66.01975	186.15459	-480.78787	-449.34387	1
37	N	77.21669	69.89953	64.56988	-487.53139	543.18517	42.03850	1
38	C	78.29485	70.84801	64.56360	-699.35871	69.34393	360.10701	1
39	H	79.20526	70.24898	64.80474	2.81126	-221.99807	-2715.58072	1
40	C	78.24767	71.45567	63.09817	-507.46439	-592.59194	122.07761	1
41	H	78.62190	72.50319	63.05432	-1975.08116	525.87560	-1801.71556	1
42	H	78.87956	70.86741	62.39592	1588.27743	-1913.22100	1113.83566	1
43	C	76.73475	71.32821	62.73951	-613.62442	-457.55993	-194.14490	1
44	H	76.13869	72.13080	63.22857	1707.54637	-721.27992	1996.92523	1
45	H	76.52510	71.39326	61.64813	758.23357	2100.81767	1560.55011	1
46	C	76.40548	69.90225	63.36102	-352.41524	704.96076	49.21465	1
47	H	75.33351	69.75500	63.62098	1714.76886	-2070.42778	443.35792	1
48	H	76.75580	69.03391	62.75487	1224.15040	1801.50881	1636.97633	1
49	C	78.05327	72.02618	65.67838	566.85117	537.05831	117.62814	1
50	O	79.02520	72.69542	66.03293	-550.26779	-406.08867	4.21666	1
51	N	76.78408	72.16939	65.98752	566.34832	-425.77725	180.18749	1
52	H	76.23254	71.46498	65.50136	644.44502	2646.80550	-52.73430	1
53	C	76.29100	72.85550	67.13094	612.34801	-281.48662	411.56221	1
54	H	75.22534	72.54031	67.18299	1667.23498	-1490.75142	1556.16753	1
55	C	77.12939	72.29716	68.37839	-714.45746	-175.43074	286.98927	1
56	H	78.22883	72.36051	68.14383	-787.09484	1763.03619	-1922.46060	1
57	O	76.87988	70.91141	68.68509	-429.46514	516.51932	-128.40526	1
58	H	77.73559	70.50709	68.43884	1981.82785	436.16847	-1818.18182	1
59	C	76.77457	73.32898	69.50664	630.79189	-468.94448	76.03230	1
60	H	77.24697	73.04293	70.47554	-1775.71861	2062.30353	131.89849	1
61	H	77.13188	74.37695	69.25937	-1855.14608	88.94118	1993.53760	1
62	H	75.67342	73.38014	69.67905	-1504.82350	-780.94249	-2132.90992	1
63	C	76.40745	74.46712	66.92410	288.57638	618.62814	-397.00270	1
64	O	75.36487	75.10997	66.98289	321.70495	-185.26452	574.37218	1
65	N	77.63471	74.86031	66.73706	-447.05792	-446.53431	367.76425	1
66	H	78.40611	74.14296	66.67196	350.31316	1975.63644	-1843.31522	1
67	C	78.00539	76.22876	66.67813	-511.23061	374.03917	-471.51480	1
68	H	79.05436	76.13843	66.31500	2234.79579	-898.70890	-1273.45190	1
69	C	77.05587	76.98961	65.63621	529.53781	-159.34528	563.72604	1
70	H	77.63158	77.83142	65.16138	654.59388	2347.94251	1217.51488	1
71	H	76.85219	76.24633	64.81940	-1526.55661	2103.42026	817.87394	1
72	O	75.84251	77.53801	66.15657	-554.84278	14.12789	399.58769	1
73	H	75.42216	76.66724	66.52353	1297.06236	2061.84854	1220.68812	1
74	C	77.95152	76.86556	68.17369	-662.15484	-412.13544	123.62687	1
75	O	77.90801	76.19450	69.18866	-540.01537	-317.05804	274.91456	1
76	N	78.11074	78.17584	68.07500	-202.76299	-690.00100	-131.49145	1
77	H	78.16084	78.60365	67.15301	-702.62132	-2617.37191	281.70413	1
78	C	78.02729	78.96473	69.25920	-491.73914	576.34187	222.73509	1
79	H	77.33110	78.42218	69.93743	1977.17978	-1823.58850	-434.68928	1
80	C	79.49677	79.02812	69.86436	-649.50797	-328.66843	306.11224	1
81	H	80.21005	79.45570	69.12687	2075.07803	1452.16490	-1004.45904	1
82	C	79.44259	79.89452	71.16755	-615.18735	-489.99689	-70.96352	1
83	H	80.44350	79.97277	71.65358	-1226.32661	-1724.38906	-1716.47170	1
84	H	79.09479	80.93274	70.95171	2381.64273	-969.84735	900.46860	1
85	H	78.74058	79.46091	71.91747	2122.74991	1702.23946	-141.36228	1

86	C	79.92168	77.57438	70.27122	-501.86074	-479.61276	-376.42482	1
87	H	80.87630	77.56482	70.84897	993.79261	-2246.95401	-1177.81305	1
88	H	79.13860	77.08317	70.89823	42.71279	-626.15391	-2651.37258	1
89	H	80.06551	76.92621	69.37286	-2026.39012	-1590.33709	-887.82922	1
90	C	77.54921	80.46035	68.78815	-672.89153	382.57394	-156.34072	1
91	O	78.08948	81.03091	67.86998	410.04627	221.86223	500.35950	1
92	N	76.60496	80.89724	69.61026	-378.11782	-443.79414	-441.10984	1
93	H	76.30709	80.30083	70.38156	2404.15973	-568.14894	1149.30085	1
94	C	75.73768	81.97387	69.20343	-544.54484	466.16019	331.29119	1
95	H	76.37164	82.88541	69.27555	-1409.80988	-170.17955	2325.32679	1
96	C	75.26404	81.74887	67.70979	-184.48284	116.78282	-758.89137	1
97	H	76.14134	81.59992	67.03393	1893.78641	1861.14652	611.04528	1
98	H	74.64962	80.82495	67.61732	-2170.79665	-974.19311	1327.50117	1
99	C	74.43697	83.00527	67.29080	389.51668	672.81878	-138.49152	1
100	H	73.61257	83.18221	68.02070	510.64577	1933.03327	1851.02484	1
101	H	75.06062	83.92330	67.36820	-2302.30869	-1105.72939	-948.89774	1
102	C	73.83878	82.89234	65.83902	-559.93427	-126.34590	542.30857	1
103	O	73.16107	83.78968	65.40825	-670.36003	-111.83166	76.36448	1
104	N	74.15795	81.75106	65.19002	-216.06729	-537.07037	446.51379	1
105	H	74.72829	80.95237	65.49198	-1251.96487	1074.12894	-2168.52500	1
106	H	73.84338	81.53025	64.23888	-2451.83023	-720.73851	944.84612	1
107	C	74.46391	81.99057	70.20640	546.24052	-563.88337	-85.11809	1
108	O	73.84645	83.02146	70.28828	71.70702	-307.40463	606.69673	1
109	N	74.14075	80.78514	70.69176	479.90863	-504.50129	222.86849	1
110	C	73.50609	80.65824	71.97755	75.51268	-600.91904	506.73700	1
111	H	72.66257	81.38689	71.97521	-2033.61562	1795.30103	254.89480	1
112	C	73.05874	79.13861	72.02254	523.79067	517.99274	284.45581	1
113	H	73.17092	78.69512	73.03784	1599.61665	-1127.00911	1895.98173	1
114	H	71.98298	79.03179	71.75813	-1881.83093	1275.82488	-1501.55016	1
115	C	73.96864	78.45076	70.95642	-600.05639	-404.05026	316.64485	1
116	H	74.97296	78.21637	71.37444	-2597.05260	496.36221	657.73249	1
117	H	73.55413	77.49576	70.56251	-1666.24518	1294.38985	-1723.90591	1
118	C	74.04816	79.59591	69.85630	493.57570	-129.95376	-602.56394	1
119	H	74.92680	79.54396	69.17226	-1469.08415	-637.84797	2204.22581	1
120	H	73.11991	79.72106	69.24930	-1038.97840	1068.88701	-2280.71789	1
121	C	74.58316	81.00099	73.14855	188.88100	241.05089	-727.87821	1
122	O	75.77712	81.02177	72.98991	531.88613	-49.19943	427.07960	1
123	N	73.88321	81.23697	74.27361	708.14833	26.93417	-179.73509	1
124	H	72.88309	81.06005	74.17466	-2232.69501	-1179.09831	1023.94816	1
125	C	74.54579	81.22001	75.58257	-738.32412	259.92548	104.42456	1
126	H	75.41545	81.90766	75.46326	2028.89123	1260.02983	1311.33324	1
127	C	73.52703	81.63902	76.61973	-258.65678	-345.52513	661.28459	1
128	H	72.63919	80.97422	76.49697	-1826.06090	-1801.46097	-918.64554	1
129	C	74.04822	81.44839	78.03289	-541.23400	531.92970	-218.41428	1
130	H	73.25551	81.67196	78.79957	1311.73218	-2219.18200	882.19023	1
131	H	74.38355	80.38539	78.19770	-1048.71298	1223.58118	-2196.97971	1
132	H	74.92647	82.11623	78.25001	419.06414	1903.92898	1903.44670	1
133	C	73.05502	83.06897	76.42780	-423.86431	152.66566	-648.55262	1
134	H	72.22586	83.32862	77.14252	105.68386	-2342.50080	1387.51238	1
135	H	73.88659	83.80700	76.59542	-1695.63603	-1484.73621	-1531.02793	1
136	H	72.66596	83.23694	75.38594	-1853.57121	-487.39031	1936.59343	1
137	C	75.00675	79.64986	75.86750	539.71428	-510.58232	267.58633	1
138	O	74.19060	78.78372	76.16384	-15.93758	-278.34085	-624.49402	1
139	N	76.30684	79.55697	75.75045	-676.81886	12.05292	276.17960	1
140	H	76.79305	80.41156	75.49110	-1694.44250	-373.84189	-2100.66098	1
141	C	76.96695	78.29703	75.87508	412.33078	-664.70360	108.35451	1
142	H	76.24330	77.58571	75.41651	1765.77476	1294.44366	1621.76594	1
143	C	78.34310	78.45286	75.11860	-179.66635	-721.95667	-264.73915	1
144	H	78.18089	78.76588	74.06218	-607.34922	2587.87032	-598.10018	1
145	H	78.95226	79.26194	75.58122	-359.69332	-1479.13954	-2259.74260	1
146	C	79.09658	77.08341	75.19344	-240.01076	616.02425	431.85322	1
147	H	79.25831	76.79210	76.25853	-1359.17131	782.54425	2227.99181	1

148	H	78.49726	76.26597	74.73347	-820.36667	85.81767	-2596.78715	1
149	C	80.47401	77.27243	74.43954	-513.07015	236.18570	-551.87280	1
150	H	80.31195	77.53533	73.36841	1816.11944	-1183.11722	-1650.94321	1
151	H	81.05191	78.11939	74.87569	-1800.04429	-1361.53473	1526.34643	1
152	C	81.25731	75.94652	74.57750	726.08972	-253.19732	-179.64713	1
153	H	81.51157	75.67024	75.62049	1224.27271	-456.51798	-2390.90304	1
154	H	80.79741	75.08169	74.05917	1206.40339	-1150.93514	-2154.90344	1
155	N	82.64274	76.14498	73.87589	329.70796	-633.68968	-155.67358	1
156	H	83.29053	75.30542	73.89962	1348.31305	1938.76845	1359.00643	1
157	H	82.63519	76.37399	72.83938	2096.92035	1446.54551	-966.48890	1
158	H	83.27435	76.90433	74.26498	-1197.07217	-2303.53719	827.28733	1
159	C	77.16216	77.98843	77.47495	-378.01186	-556.17301	-413.96481	1
160	O	78.25096	77.90100	77.98601	-409.44433	-307.55053	-453.30833	1
161	N	75.96063	77.81861	78.01708	-429.02477	524.70884	274.08502	1
162	H	75.10422	77.95785	77.43197	1706.34263	-1425.96036	1574.38926	1
163	C	75.89909	77.64755	79.42559	-45.25864	-626.22952	478.93267	1
164	H	76.91835	77.88527	79.81265	1988.63164	570.90773	1772.87287	1
165	C	74.73441	78.58695	79.95407	551.77128	-20.49526	-564.54996	1
166	H	74.87597	79.63490	79.60367	1434.61535	-1753.10253	1513.99471	1
167	H	73.76040	78.25823	79.52435	-714.67738	1819.09770	1898.36494	1
168	C	74.69260	78.53094	81.51533	446.99263	-555.77305	338.97221	1
169	H	74.86276	77.48622	81.87935	1953.68466	1892.25957	-161.67766	1
170	H	75.50307	79.14822	81.96425	-403.03785	2688.07032	-188.43591	1
171	C	73.26319	79.03979	81.96256	567.86262	335.74681	434.04421	1
172	H	73.11031	80.10774	81.68321	-1080.02275	1568.26081	-1948.78900	1
173	H	72.46444	78.47259	81.43345	-919.54108	2111.34692	1456.13463	1
174	C	73.15498	78.83599	83.49160	195.81897	173.33862	-745.11536	1
175	H	73.15619	77.77680	83.81954	1405.67949	-2301.21089	-390.08113	1
176	H	73.88734	79.41602	84.08784	-940.37328	-1118.32446	2299.72133	1
177	N	71.76031	79.38994	83.93778	319.26422	656.36007	-42.02424	1
178	H	71.55907	79.32560	84.97718	1961.03633	619.91968	1787.09422	1
179	H	71.56525	80.41660	83.74994	854.14343	-2156.80752	1429.08711	1
180	H	70.89868	78.92314	83.53173	1237.02905	-1378.50857	-1998.28500	1
181	C	75.40231	76.12761	79.80346	532.53319	-268.57236	517.55729	1
182	O	75.53649	75.73518	80.96252	266.16714	-290.73804	-558.88002	1
183	N	74.79965	75.54221	78.79266	-226.25352	640.49678	-270.32839	1
184	H	74.85143	76.10199	77.94439	2007.69063	-1035.27229	1523.50231	1
185	C	74.06451	74.33240	78.81684	-540.76542	-573.33303	49.50000	1
186	H	73.88574	74.11360	77.74107	-2374.20950	-1036.76023	843.75774	1
187	C	74.93493	73.19923	79.53659	-77.09082	666.87422	-415.84136	1
188	H	75.27177	73.58827	80.54026	-985.81834	617.19825	2463.91927	1
189	O	76.12357	72.80477	78.82955	293.29899	-391.65602	-477.80926	1
190	H	76.80737	72.95283	79.52037	2528.72714	-681.76262	-751.27122	1
191	C	73.87487	72.06218	79.76439	252.47363	-605.14473	440.05134	1
192	H	74.29865	71.23274	80.37841	-2052.65063	1456.49051	-1043.51830	1
193	H	72.96421	72.44141	80.29643	-2152.98800	-1661.97574	-161.70652	1
194	H	73.53532	71.62300	78.79793	-473.12726	-1584.27339	2165.61725	1
195	C	72.64031	74.53488	79.60370	360.36307	488.46713	505.10056	1
196	O	71.67693	73.95262	79.16470	-200.08817	-528.03552	-385.82850	1
197	N	72.75715	75.31350	80.66563	-597.54095	-226.44775	355.20479	1
198	H	73.69806	75.65710	80.92821	2179.23655	-1300.70981	-991.33835	1
199	C	71.69794	75.44427	81.60620	-687.68921	297.39807	-249.45179	1
200	H	72.03214	76.29422	82.24291	-349.16256	-2467.37713	-1101.72831	1
201	C	70.32352	75.74515	80.83374	672.47345	361.54328	-201.62880	1
202	H	70.05731	74.86909	80.18948	1541.41502	582.18425	2169.97026	1
203	H	69.48988	75.88181	81.55999	-2534.67717	60.25153	997.72295	1
204	C	70.49597	77.00478	79.97461	574.26774	-389.43119	-377.02542	1
205	C	70.37358	78.30614	80.54792	688.82679	-287.33580	-257.96133	1
206	H	70.19103	78.43153	81.62993	331.14182	1470.38163	2269.80013	1
207	C	70.78391	76.85621	78.58378	-383.52382	-675.04808	144.24917	1
208	H	70.91832	75.84979	78.14364	4.09847	1517.59662	2262.86397	1
209	C	70.47820	79.41750	79.71047	-134.76730	428.45285	-649.50303	1

210	H	70.36902	80.42393	80.15055	-903.23433	1600.49020	2011.53387	1
211	C	70.88106	77.99740	77.78538	-335.53281	-615.00040	-364.39058	1
212	H	71.09756	77.86781	76.71026	1596.45398	-1369.33862	1732.02659	1
213	C	70.70734	79.31192	78.30831	585.48547	-340.24194	-406.23938	1
214	O	70.76828	80.47392	77.48947	-419.15649	-173.04408	-511.94141	1
215	H	70.87087	80.04010	76.60694	-1071.84350	1559.71507	-1960.13012	1
216	C	71.63726	74.05843	82.43864	291.41878	-183.13091	710.72246	1
217	O	72.52400	73.20150	82.34213	379.87695	523.47396	-222.23622	1
218	N	70.58408	74.07290	83.21954	564.30591	373.09380	277.24371	1
219	H	70.01161	74.91343	83.17068	-120.59931	-2436.07824	-1214.35098	1
220	C	70.16239	72.97721	84.02131	404.07514	-299.37480	608.84009	1
221	H	69.12154	73.24445	84.31389	-1071.07882	-841.69025	2359.66467	1
222	C	70.26096	71.65678	83.14234	-683.12807	68.71770	-390.13096	1
223	H	69.64698	71.74744	82.21794	2068.88918	1596.58590	770.89603	1
224	H	71.31013	71.50324	82.78830	1379.86429	2342.49779	-179.85638	1
225	C	69.79109	70.45959	84.02270	-176.39967	537.49466	550.97268	1
226	H	70.36428	70.42217	84.97596	-396.28051	1942.22168	1869.33314	1
227	H	68.72437	70.57073	84.31893	-94.44700	586.00678	-2659.20016	1
228	C	70.02027	69.13038	83.16625	-291.69381	-718.18079	-150.72929	1
229	H	69.40149	69.03632	82.23802	-2303.38776	1089.76242	964.62032	1
230	H	71.08384	68.90963	82.89373	884.16729	2568.80533	-207.74283	1
231	N	69.59823	68.14541	84.07157	-594.49522	-252.81478	342.29276	1
232	H	69.31329	68.46063	84.98595	-1735.17426	2084.05705	-263.71605	1
233	C	69.55623	66.89962	83.81778	595.23177	-271.52487	442.22352	1
234	N	69.95912	66.48341	82.54394	585.53813	-424.79750	-105.81303	1
235	H	70.29363	67.04070	81.75935	959.88797	1327.56823	-2177.11905	1
236	H	69.96830	65.51634	82.21952	1578.48647	16.27378	-2220.76233	1
237	N	69.09263	66.18138	84.92947	-452.17763	-390.33541	-421.51853	1
238	H	68.79591	66.49624	85.85157	470.26107	1974.25629	-1817.92087	1
239	H	68.97878	65.16747	84.93091	1856.67307	-1573.97321	-1224.35416	1
240	C	71.13050	72.82105	85.32651	-531.47271	-581.45780	-55.06206	1
241	O	70.64332	72.76139	86.42151	-243.00837	192.73507	609.52485	1
242	N	72.41342	72.64914	84.97672	343.49288	-644.25607	38.09164	1
243	H	72.66329	72.69658	83.94880	-1691.16043	-1535.97525	-1484.73099	1
244	C	73.44568	73.03321	85.95987	542.66492	350.14337	454.42563	1
245	H	72.87220	73.61454	86.71889	1209.57979	-2396.95920	463.86744	1
246	C	74.00874	71.73946	86.50973	-737.14309	145.93010	242.71942	1
247	H	74.28052	71.08970	85.64827	-1050.18303	159.36419	-2509.06125	1
248	C	75.24975	71.96254	87.35326	-706.77696	-252.88343	-245.16230	1
249	H	75.65103	70.99538	87.76467	-1624.64039	-1665.49085	1417.86935	1
250	H	76.07750	72.43978	86.75897	2566.10521	598.51109	693.22305	1
251	H	75.03951	72.63567	88.22974	-1972.69758	107.10018	-1876.34312	1
252	C	72.95790	70.99575	87.31631	412.85148	672.58832	-27.69222	1
253	H	73.27837	69.94572	87.55995	1447.02277	1762.76533	-1490.78944	1
254	H	72.73933	71.51573	88.28892	1320.77379	-145.20455	2378.68491	1
255	H	71.98226	70.93825	86.75385	-1512.10848	1470.52031	1724.75147	1
256	C	74.50054	73.96528	85.08846	-607.11113	499.56689	73.73769	1
257	O	74.33570	75.16049	85.04399	357.97126	460.81534	356.68785	1
258	N	75.43657	73.24289	84.49563	536.55407	-368.62270	332.76306	1
259	H	75.45166	72.22849	84.58607	524.38866	2297.69985	1367.20941	1
260	C	76.39133	73.91163	83.68745	46.50277	-774.29190	-147.97904	1
261	H	75.89353	74.86006	83.37606	1676.51875	1883.29066	1032.55549	1
262	C	77.74372	74.15996	84.54398	-559.41456	-34.19198	-556.30433	1
263	H	78.18561	73.16946	84.80582	-64.66664	395.18769	2695.05373	1
264	H	78.50723	74.67483	83.91381	-2703.44278	-60.40056	333.79418	1
265	C	77.46450	74.94608	85.79374	-519.76435	377.31045	459.42366	1
266	H	76.58818	74.49082	86.30820	-1746.74323	1667.50644	-1261.73691	1
267	C	78.66186	74.88520	86.73509	570.95554	16.46261	-545.27700	1
268	H	78.46855	75.44101	87.68833	2391.58273	28.05277	-1305.07271	1
269	H	78.91762	73.83009	87.01207	175.75588	917.63458	2559.43867	1
270	H	79.57544	75.33537	86.26861	-1063.97851	-2155.34650	1283.00462	1
271	C	77.13142	76.39748	85.47556	193.76014	2.62946	-765.53141	1

272	H	76.98204	77.00060	86.40814	507.39394	-846.55087	2539.60089	1
273	H	77.94708	76.89099	84.88668	1337.57841	1818.19054	1526.01994	1
274	H	76.18522	76.47643	84.87574	1100.88635	-1172.91350	-2199.08909	1
275	C	76.80098	72.88529	82.51796	-549.21115	475.64486	-309.38218	1
276	O	76.64066	71.69636	82.59518	556.06106	-390.37755	-78.24250	1
277	O	77.54464	73.44693	81.44383	-572.27940	-310.19032	-209.75862	1
278	H	77.27641	74.40084	81.56152	-1380.08193	2212.14486	790.85944	1

Listing 70: C00070.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.5878	0.0000	300.0000
3	H	67.86796	69.34608	69.51791	-2043.14101	-1757.64893	399.89339		1
4	N	68.05051	70.34421	69.41266	426.75047	490.45733	-334.42467		1
5	H	68.06388	70.71096	70.37677	442.25559	-1110.30854	-2448.52907		1
6	C	69.19287	70.63909	68.63437	415.32972	-666.39213	83.73172		1
7	H	68.90938	70.29183	67.61768	879.32219	2491.00447	667.35213		1
8	C	69.45866	72.22865	68.69826	31.35357	477.41777	628.23362		1
9	H	69.67214	72.53721	69.75077	1168.38489	2240.25337	-1019.71136		1
10	H	70.36575	72.50521	68.10886	-360.43770	2534.90498	931.67112		1
11	C	68.23119	72.93254	68.18244	463.18208	512.70242	-382.34388		1
12	H	67.33601	72.35781	68.51282	1725.29117	1863.52247	-987.07854		1
13	C	68.12932	74.33917	68.75808	710.42801	-144.27427	-313.15367		1
14	H	67.21207	74.86927	68.39252	364.20195	-1033.13725	2494.72524		1
15	H	68.08261	74.32641	69.87744	2567.61904	335.80679	847.48802		1
16	H	69.01201	74.96683	68.47175	-2587.99029	680.92867	-512.16411		1
17	C	68.24235	72.99521	66.66084	268.17616	741.64379	-40.42634		1
18	H	67.31259	73.47395	66.25857	1283.54314	-1945.37420	-1411.27812		1
19	H	69.11227	73.59059	66.28077	-1258.57796	1317.15249	-2026.02085		1
20	H	68.31549	71.97465	66.20442	-2502.84526	909.80597	575.92391		1
21	C	70.48417	69.82917	69.16417	619.36578	-458.64843	-172.09273		1
22	O	71.42176	69.70408	68.42147	-81.40433	433.87611	522.34594		1
23	N	70.31339	69.31273	70.40253	175.23996	-622.20190	341.55523		1
24	H	69.55378	69.75638	70.95734	-876.57256	-303.22879	-2561.90213		1
25	C	71.51371	68.98747	71.15706	-571.88214	-534.10783	-106.15033		1
26	H	71.82025	69.96152	71.58705	-2713.20841	-16.25800	-248.80809		1
27	C	71.03152	67.96610	72.26632	166.60354	288.16399	-716.09568		1
28	H	70.62698	67.04886	71.75776	-2097.85574	1636.78449	-586.18044		1
29	O	69.95940	68.41479	73.14172	-317.80580	-363.38227	484.43082		1
30	H	69.26645	67.76323	72.93216	1863.74748	-1451.84923	1357.29467		1
31	C	72.39224	67.61518	72.97068	503.80731	517.99032	318.51606		1
32	H	72.25214	66.84339	73.76277	640.61020	-2157.10410	-1536.29104		1
33	H	73.13755	67.21248	72.24244	1687.88455	465.60692	2087.56452		1
34	H	72.84910	68.50737	73.45752	-1293.07895	-1899.88581	-1463.57452		1
35	C	72.67475	68.31215	70.25498	-153.07550	-733.68902	248.70981		1
36	O	72.57068	67.15399	69.94153	186.15459	-480.78787	-449.34387		1
37	N	73.74486	69.13223	70.12714	-487.53139	543.18517	42.03850		1
38	C	74.84869	68.71143	69.33836	-699.35871	69.34393	360.10701		1
39	H	74.59121	67.69900	68.94379	2.81126	-221.99807	-2715.58072		1
40	C	74.87179	69.88766	68.26505	-507.46439	-592.59194	122.07761		1
41	H	75.81710	69.92266	67.67829	-1975.08116	525.87560	-1801.71556		1
42	H	74.03564	69.78001	67.53765	1588.27743	-1913.22100	1113.83566		1
43	C	74.65749	71.13206	69.17988	-613.62442	-457.55993	-194.14490		1
44	H	75.61985	71.46191	69.65990	1707.54637	-721.27992	1996.92523		1
45	H	74.26724	72.01827	68.62933	758.23357	2100.81767	1560.55011		1
46	C	73.62861	70.58098	70.25637	-352.41524	704.96076	49.21465		1
47	H	73.88173	70.84650	71.31029	1714.76886	-2070.42778	443.35792		1
48	H	72.56224	70.83711	70.04534	1224.15040	1801.50881	1636.97633		1
49	C	76.27009	68.77788	70.17921	566.85117	537.05831	117.62814		1
50	O	77.30768	68.82612	69.56364	-550.26779	-406.08867	4.21666		1
51	N	76.07265	68.79284	71.49659	566.34832	-425.77725	180.18749		1

52	H	75.08533	68.70082	71.73432	644.44502	2646.80550	-52.73430	1
53	C	77.09249	68.36020	72.40053	612.34801	-281.48662	411.56221	1
54	H	76.52071	68.21355	73.34352	1667.23498	-1490.75142	1556.16753	1
55	C	77.67997	66.97445	71.86332	-714.45746	-175.43074	286.98927	1
56	H	78.14908	67.15284	70.85660	-787.09484	1763.03619	-1922.46060	1
57	O	76.68242	65.94851	71.68336	-429.46514	516.51932	-128.40526	1
58	H	76.72679	65.81422	70.71724	1981.82785	436.16847	-1818.18182	1
59	C	78.81098	66.60109	72.88864	630.79189	-468.94448	76.03230	1
60	H	79.30588	65.64035	72.61273	-1775.71861	2062.30353	131.89849	1
61	H	79.61729	67.38835	72.93845	-1855.14608	88.94118	1993.53760	1
62	H	78.40273	66.47618	73.91866	-1504.82350	-780.94249	-2132.90992	1
63	C	78.17034	69.56045	72.54498	288.57638	618.62814	-397.00270	1
64	O	79.35090	69.33910	72.72664	321.70495	-185.26452	574.37218	1
65	N	77.54113	70.74467	72.64830	-447.05792	-446.53431	367.76425	1
66	H	76.56345	70.71854	72.35689	350.31316	1975.63644	-1843.31522	1
67	C	78.35827	71.89366	72.39767	-511.23061	374.03917	-471.51480	1
68	H	79.37344	71.57205	72.73055	2234.79579	-898.70890	-1273.45190	1
69	C	78.30239	72.14610	70.81947	529.53781	-159.34528	563.72604	1
70	H	79.17769	72.79585	70.55987	654.59388	2347.94251	1217.51488	1
71	H	78.45471	71.15522	70.31090	-1526.55661	2103.42026	817.87394	1
72	O	77.05466	72.70639	70.29477	-554.84278	14.12789	399.58769	1
73	H	77.20466	73.64313	70.52054	1297.06236	2061.84854	1220.68812	1
74	C	77.78560	73.19168	73.18306	-662.15484	-412.13544	123.62687	1
75	O	78.19270	74.29202	72.89367	-540.01537	-317.05804	274.91456	1
76	N	76.88086	72.86539	74.11988	-202.76299	-690.00100	-131.49145	1
77	H	76.76449	71.85601	74.21288	-702.62132	-2617.37191	281.70413	1
78	C	76.46251	73.79164	75.17769	-491.73914	576.34187	222.73509	1
79	H	75.90261	73.13205	75.88313	1977.17978	-1823.58850	-434.68928	1
80	C	77.68627	74.41077	75.82483	-649.50797	-328.66843	306.11224	1
81	H	78.28106	74.90077	75.01728	2075.07803	1452.16490	-1004.45904	1
82	C	77.33212	75.46371	76.85742	-615.18735	-489.99689	-70.96352	1
83	H	78.25057	75.96217	77.27238	-1226.32661	-1724.38906	-1716.47170	1
84	H	76.67802	76.27964	76.41420	2381.64273	-969.84735	900.46860	1
85	H	76.76811	75.02041	77.72394	2122.74991	1702.23946	-141.36228	1
86	C	78.56157	73.35380	76.47748	-501.86074	-479.61276	-376.42482	1
87	H	79.48892	73.79972	76.92977	993.79261	-2246.95401	-1177.81305	1
88	H	78.01483	72.81841	77.30136	42.71279	-626.15391	-2651.37258	1
89	H	78.88845	72.57462	75.73587	-2026.39012	-1590.33709	-887.82922	1
90	C	75.45897	74.89842	74.47220	-672.89153	382.57394	-156.34072	1
91	O	75.35480	76.02586	74.90834	410.04627	221.86223	500.35950	1
92	N	74.75699	74.34493	73.49999	-378.11782	-443.79414	-441.10984	1
93	H	75.00875	73.39753	73.23130	2404.15973	-568.14894	1149.30085	1
94	C	73.71741	75.13536	72.90143	-544.54484	466.16019	331.29119	1
95	H	73.23891	75.56496	73.81043	-1409.80988	-170.17955	2325.32679	1
96	C	74.48236	76.25465	72.08012	-184.48284	116.78282	-758.89137	1
97	H	75.22907	76.75267	72.74487	1893.78641	1861.14652	611.04528	1
98	H	75.06718	75.80277	71.24649	-2170.79665	-974.19311	1327.50117	1
99	C	73.43779	77.27702	71.53708	389.51668	672.81878	-138.49152	1
100	H	72.74677	76.76112	70.83063	510.64577	1933.03327	1851.02484	1
101	H	72.77950	77.63290	72.35828	-2302.30869	-1105.72939	-948.89774	1
102	C	74.09179	78.53323	70.84657	-559.93427	-126.34590	542.30857	1
103	O	73.37763	79.38733	70.38783	-670.36003	-111.83166	76.36448	1
104	N	75.44190	78.54052	70.86205	-216.06729	-537.07037	446.51379	1
105	H	76.10099	77.84522	71.23171	-1251.96487	1074.12894	-2168.52500	1
106	H	76.01421	79.29018	70.45864	-2451.83023	-720.73851	944.84612	1
107	C	72.74190	74.17603	72.02457	546.24052	-563.88337	-85.11809	1
108	O	72.58069	74.42570	70.85935	71.70702	-307.40463	606.69673	1
109	N	72.13980	73.23972	72.78217	479.90863	-504.50129	222.86849	1
110	C	71.47689	72.10425	72.23882	75.51268	-600.91904	506.73700	1
111	H	71.93233	71.89426	71.24362	-2033.61562	1795.30103	254.89480	1
112	C	71.74509	71.03499	73.39185	523.79067	517.99274	284.45581	1
113	H	71.05024	70.15656	73.34263	1599.61665	-1127.00911	1895.98173	1

114	H	72.78295	70.63626	73.34052	-1881.83093	1275.82488	-1501.55016	1
115	C	71.54058	71.88631	74.68167	-600.05639	-404.05026	316.64485	1
116	H	70.46673	71.93804	74.96891	-2597.05260	496.36221	657.73249	1
117	H	72.07612	71.47745	75.56779	-1666.24518	1294.38985	-1723.90591	1
118	C	72.07821	73.31481	74.23835	493.57570	-129.95376	-602.56394	1
119	H	71.36683	74.15913	74.45601	-1469.08415	-637.84797	2204.22581	1
120	H	73.09322	73.58136	74.61967	-1038.97840	1068.88701	-2280.71789	1
121	C	69.85732	72.32036	72.14911	188.88100	241.05089	-727.87821	1
122	O	69.15146	71.42985	71.66872	531.88613	-49.19943	427.07960	1
123	N	69.49258	73.47800	72.63743	708.14833	26.93417	-179.73509	1
124	H	70.29719	73.99338	72.98363	-2232.69501	-1179.09831	1023.94816	1
125	C	68.12473	73.90763	72.87851	-738.32412	259.92548	104.42456	1
126	H	67.62179	73.70380	71.90336	2028.89123	1260.02983	1311.33324	1
127	C	67.48004	73.12167	74.01152	-258.65678	-345.52513	661.28459	1
128	H	67.99799	73.40421	74.95538	-1826.06090	-1801.46097	-918.64554	1
129	C	66.01247	73.48246	74.15322	-541.23400	531.92970	-218.41428	1
130	H	65.52778	72.93898	75.00988	1311.73218	-2219.18200	882.19023	1
131	H	65.88023	74.59242	74.33773	-1048.71298	1223.58118	-2196.97971	1
132	H	65.43067	73.22588	73.22555	419.06414	1903.92898	1903.44670	1
133	C	67.61195	71.61725	73.85291	-423.86431	152.66566	-648.55262	1
134	H	67.05400	71.06049	74.65553	105.68386	-2342.50080	1387.51238	1
135	H	67.20837	71.27191	72.85953	-1695.63603	-1484.73621	-1531.02793	1
136	H	68.68626	71.28378	73.90069	-1853.57121	-487.39031	1936.59343	1
137	C	68.23015	75.51993	73.28271	539.71428	-510.58232	267.58633	1
138	O	67.35748	75.99830	73.97711	-15.93758	-278.34085	-624.49402	1
139	N	69.26301	76.11813	72.72331	-676.81886	12.05292	276.17960	1
140	H	69.81329	75.52635	72.10499	-1694.44250	-373.84189	-2100.66098	1
141	C	69.51606	77.50734	72.86922	412.33078	-664.70360	108.35451	1
142	H	70.14736	77.72861	71.97968	1765.77476	1294.44366	1621.76594	1
143	C	68.13692	78.27235	72.91845	-179.66635	-721.95667	-264.73915	1
144	H	67.45173	77.89407	72.12547	-607.34922	2587.87032	-598.10018	1
145	H	67.61823	78.06679	73.89215	-359.69332	-1479.13954	-2259.74260	1
146	C	68.38988	79.81056	72.76075	-240.01076	616.02425	431.85322	1
147	H	69.05867	80.17804	73.57407	-1359.17131	782.54425	2227.99181	1
148	H	68.90514	80.04257	71.80186	-820.36667	85.81767	-2596.78715	1
149	C	66.97285	80.50799	72.83384	-513.07015	236.18570	-551.87280	1
150	H	66.31897	80.16399	71.99964	1816.11944	-1183.11722	-1650.94321	1
151	H	66.44258	80.21975	73.77077	-1800.04429	-1361.53473	1526.34643	1
152	C	67.17391	82.04024	72.77692	726.08972	-253.19732	-179.64713	1
153	H	67.73404	82.46357	73.63448	1224.27271	-456.51798	-2390.90304	1
154	H	67.59743	82.41689	71.82454	1206.40339	-1150.93514	-2154.90344	1
155	N	65.75545	82.69617	72.87079	329.70796	-633.68968	-155.67358	1
156	H	65.73346	83.75675	72.86343	1348.31305	1938.76845	1359.00643	1
157	H	65.06145	82.46664	72.10099	2096.92035	1446.54551	-966.48890	1
158	H	65.19297	82.48183	73.74416	-1197.07217	-2303.53719	827.28733	1
159	C	70.30288	77.84818	74.28197	-378.01186	-556.17301	-413.96481	1
160	O	69.81495	78.62665	75.07315	-409.44433	-307.55053	-453.30833	1
161	N	71.48370	77.25714	74.30607	-429.02477	524.70884	274.08502	1
162	H	71.63594	76.63226	73.51727	1706.34263	-1425.96036	1574.38926	1
163	C	72.49613	77.54024	75.28011	-45.25864	-626.22952	478.93267	1
164	H	73.42291	77.47974	74.66222	1988.63164	570.90773	1772.87287	1
165	C	72.25198	78.97969	75.89105	551.77128	-20.49526	-564.54996	1
166	H	71.84814	79.67037	75.11448	1434.61535	-1753.10253	1513.99471	1
167	H	71.44101	78.91397	76.65428	-714.67738	1819.09770	1898.36494	1
168	C	73.57060	79.55520	76.50618	446.99263	-555.77305	338.97221	1
169	H	74.21106	78.74640	76.93507	1953.68466	1892.25957	-161.67766	1
170	H	74.20227	80.04667	75.73256	-403.03785	2688.07032	-188.43591	1
171	C	73.14014	80.57608	77.63460	567.86262	335.74681	434.04421	1
172	H	72.81061	81.54535	77.19470	-1080.02275	1568.26081	-1948.78900	1
173	H	72.26621	80.19334	78.21036	-919.54108	2111.34692	1456.13463	1
174	C	74.35564	80.75905	78.57500	195.81897	173.33862	-745.11536	1
175	H	74.58938	79.87033	79.19775	1405.67949	-2301.21089	-390.08113	1

176	H	75.28061	81.11520	78.07502	-940.37328	-1118.32446	2299.72133	1
177	N	73.98285	81.87961	79.60127	319.26422	656.36007	-42.02424	1
178	H	74.72156	82.11100	80.32639	1961.03633	619.91968	1787.09422	1
179	H	73.76112	82.84252	79.21280	854.14343	-2156.80752	1429.08711	1
180	H	73.13901	81.69299	80.21631	1237.02905	-1378.50857	-1998.28500	1
181	C	72.48146	76.33296	76.35522	532.53319	-268.57236	517.55729	1
182	O	72.19925	75.18590	75.97668	266.16714	-290.73804	-558.88002	1
183	N	72.93529	76.69272	77.52127	-226.25352	640.49678	-270.32839	1
184	H	73.11793	77.68176	77.67251	2007.69063	-1035.27229	1523.50231	1
185	C	72.97218	75.81143	78.65301	-540.76542	-573.33303	49.50000	1
186	H	71.94071	75.80579	79.06645	-2374.20950	-1036.76023	843.75774	1
187	C	73.41088	74.36369	78.15578	-77.09082	666.87422	-415.84136	1
188	H	73.99842	74.51692	77.20604	-985.81834	617.19825	2463.91927	1
189	O	72.33022	73.48526	77.82222	293.29899	-391.65602	-477.80926	1
190	H	72.11168	73.84613	76.88507	2528.72714	-681.76262	-751.27122	1
191	C	74.36942	73.83239	79.27974	252.47363	-605.14473	440.05134	1
192	H	74.80404	72.84151	79.01112	-2052.65063	1456.49051	-1043.51830	1
193	H	75.22472	74.52672	79.46583	-2152.98800	-1661.97574	-161.70652	1
194	H	73.83294	73.70506	80.24943	-473.12726	-1584.27339	2165.61725	1
195	C	74.01990	76.54597	79.66638	360.36307	488.46713	505.10056	1
196	O	73.71252	76.73705	80.82116	-200.08817	-528.03552	-385.82850	1
197	N	75.16740	76.81363	79.04283	-597.54095	-226.44775	355.20479	1
198	H	75.22422	76.60100	78.04704	2179.23655	-1300.70981	-991.33835	1
199	C	76.22196	77.44136	79.75100	-687.68921	297.39807	-249.45179	1
200	H	75.68765	77.87166	80.62918	-349.16256	-2467.37713	-1101.72831	1
201	C	77.34691	76.38315	80.19207	672.47345	361.54328	-201.62880	1
202	H	77.87914	75.99057	79.29860	1541.41502	582.18425	2169.97026	1
203	H	78.11561	76.90881	80.80653	-2534.67717	60.25153	997.72295	1
204	C	76.76293	75.21447	80.99498	574.26774	-389.43119	-377.02542	1
205	C	76.05587	75.45169	82.21197	688.82679	-287.33580	-257.96133	1
206	H	75.90512	76.48072	82.58528	331.14182	1470.38163	2269.80013	1
207	C	76.94498	73.88081	80.51421	-383.52382	-675.04808	144.24917	1
208	H	77.49755	73.69005	79.57635	4.09847	1517.59662	2262.86397	1
209	C	75.53695	74.36097	82.90798	-134.76730	428.45285	-649.50303	1
210	H	74.97945	74.54791	83.84253	-903.23433	1600.49020	2011.53387	1
211	C	76.40934	72.82037	81.25107	-335.53281	-615.00040	-364.39058	1
212	H	76.55096	71.79482	80.86835	1596.45398	-1369.33862	1732.02659	1
213	C	75.68762	73.01501	82.46465	585.48547	-340.24194	-406.23938	1
214	O	75.13659	71.94621	83.21860	-419.15649	-173.04408	-511.94141	1
215	H	75.39418	71.18719	82.64424	-1071.84350	1559.71507	-1960.13012	1
216	C	76.88550	78.51930	78.73629	291.41878	-183.13091	710.72246	1
217	O	76.24814	79.05596	77.85175	379.87695	523.47396	-222.23622	1
218	N	78.14470	78.76222	79.09403	564.30591	373.09380	277.24371	1
219	H	78.54606	78.28997	79.90439	-120.59931	-2436.07824	-1214.35098	1
220	C	78.91923	79.63162	78.28256	404.07514	-299.37480	608.84009	1
221	H	78.24438	79.91635	77.43962	-1071.07882	-841.69025	2359.66467	1
222	C	79.30072	80.85591	79.22097	-683.12807	68.71770	-390.13096	1
223	H	78.40169	81.20668	79.77568	2068.88918	1596.58590	770.89603	1
224	H	80.02807	80.53688	80.00053	1379.86429	2342.49779	-179.85638	1
225	C	79.89377	82.00510	78.35188	-176.39967	537.49466	550.97268	1
226	H	80.80716	81.66586	77.80584	-396.28051	1942.22168	1869.33314	1
227	H	79.17466	82.33642	77.56937	-94.44700	586.00678	-2659.20016	1
228	C	80.22584	83.18449	79.37849	-291.69381	-718.18079	-150.72929	1
229	H	79.35456	83.58659	79.95546	-2303.38776	1089.76242	964.62032	1
230	H	81.04256	82.95436	80.10941	884.16729	2568.80533	-207.74283	1
231	N	80.69003	84.20766	78.54114	-594.49522	-252.81478	342.29276	1
232	H	80.84929	83.96607	77.57536	-1735.17426	2084.05705	-263.71605	1
233	C	80.93413	85.39461	78.92440	595.23177	-271.52487	442.22352	1
234	N	80.71644	85.70087	80.27233	585.53813	-424.79750	-105.81303	1
235	H	80.40088	85.09715	81.03060	959.88797	1327.56823	-2177.11905	1
236	H	80.88847	86.61118	80.70024	1578.48647	16.27378	-2220.76233	1
237	N	81.39228	86.18448	77.86121	-452.17763	-390.33541	-421.51853	1

238	H	81.55833	85.95666	76.88189	470.26107	1974.25629	-1817.92087	1
239	H	81.64963	87.16677	77.96668	1856.67307	-1573.97321	-1224.35416	1
240	C	80.30678	78.89196	77.81248	-531.47271	-581.45780	-55.06206	1
241	O	81.16833	79.55670	77.27062	-243.00837	192.73507	609.52485	1
242	N	80.31233	77.59817	78.09025	343.49288	-644.25607	38.09164	1
243	H	79.43400	77.29437	78.50547	-1691.16043	-1535.97525	-1484.73099	1
244	C	81.38163	76.66326	77.80385	542.66492	350.14337	454.42563	1
245	H	80.86397	75.67514	77.81653	1209.57979	-2396.95920	463.86744	1
246	C	81.98139	76.98741	76.44632	-737.14309	145.93010	242.71942	1
247	H	82.19224	78.09427	76.42181	-1050.18303	159.36419	-2509.06125	1
248	C	83.28596	76.26020	76.18755	-706.77696	-252.88343	-245.16230	1
249	H	83.68152	76.46811	75.15465	-1624.64039	-1665.49085	1417.86935	1
250	H	84.08563	76.57272	76.91904	2566.10521	598.51109	693.22305	1
251	H	83.16657	75.14554	76.28363	-1972.69758	107.10018	-1876.34312	1
252	C	80.99183	76.68096	75.33602	412.85148	672.58832	-27.69222	1
253	H	81.38511	76.98816	74.32844	1447.02277	1762.76533	-1490.78944	1
254	H	80.75556	75.58263	75.28118	1320.77379	-145.20455	2378.68491	1
255	H	80.01824	77.22150	75.49590	-1512.10848	1470.52031	1724.75147	1
256	C	82.52302	76.70465	79.03332	-607.11113	499.56689	73.73769	1
257	O	83.42484	75.89690	78.99887	357.97126	460.81534	356.68785	1
258	N	82.23119	77.58932	79.96609	536.55407	-368.62270	332.76306	1
259	H	81.39647	78.12525	79.73925	524.38866	2297.69985	1367.20941	1
260	C	83.07813	77.91774	81.05305	46.50277	-774.29190	-147.97904	1
261	H	82.38978	78.40725	81.77567	1676.51875	1883.29066	1032.55549	1
262	C	83.81905	76.61292	81.64164	-559.41456	-34.19198	-556.30433	1
263	H	84.41351	76.13076	80.81857	-64.66664	395.18769	2695.05373	1
264	H	84.55778	76.90099	82.42836	-2703.44278	-60.40056	333.79418	1
265	C	82.81346	75.63618	82.19142	-519.76435	377.31045	459.42366	1
266	H	82.04417	75.45211	81.40768	-1746.74323	1667.50644	-1261.73691	1
267	C	83.49612	74.31397	82.52101	570.95554	16.46261	-545.27700	1
268	H	82.76828	73.55710	82.91191	2391.58273	28.05277	-1305.07271	1
269	H	83.98832	73.86755	81.61842	175.75588	917.63458	2559.43867	1
270	H	84.29003	74.44336	83.30121	-1063.97851	-2155.34650	1283.00462	1
271	C	82.12802	76.17865	83.43790	193.76014	2.62946	-765.53141	1
272	H	81.40876	75.43541	83.86934	507.39394	-846.55087	2539.60089	1
273	H	82.86971	76.42578	84.24084	1337.57841	1818.19054	1526.01994	1
274	H	81.54887	77.11261	83.22125	1100.88635	-1172.91350	-2199.08909	1
275	C	84.22542	78.93798	80.57192	-549.21115	475.64486	-309.38218	1
276	O	84.44449	79.24276	79.42942	556.06106	-390.37755	-78.24250	1
277	O	85.02194	79.47048	81.61934	-572.27940	-310.19032	-209.75862	1
278	H	84.56361	79.04120	82.39133	-1380.08193	2212.14486	790.85944	1

Listing 71: C00071.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.5846	0.0000	300.0000
3	H	70.98780	76.29341	64.63402	-2043.14101	-1757.64893	399.89339		1
4	N	71.34539	77.14752	65.05520	426.75047	490.45733	-334.42467		1
5	H	71.65383	76.82109	65.96787	442.25559	-1110.30854	-2448.52907		1
6	C	72.34935	77.81718	64.31655	415.32972	-666.39213	83.73172		1
7	H	72.11617	77.68635	63.23580	879.32219	2491.00447	667.35213		1
8	C	72.33001	79.36200	64.81388	31.35357	477.41777	628.23362		1
9	H	72.41254	79.38452	65.92659	1168.38489	2240.25337	-1019.71136		1
10	H	73.22141	79.91187	64.42882	-360.43770	2534.90498	931.67112		1
11	C	71.05564	80.02195	64.36833	463.18208	512.70242	-382.34388		1
12	H	70.21382	79.31369	64.54202	1725.29117	1863.52247	-987.07854		1
13	C	70.80817	81.28205	65.19013	710.42801	-144.27427	-313.15367		1
14	H	69.87269	81.81206	64.87417	364.20195	-1033.13725	2494.72524		1
15	H	70.71101	81.04959	66.28378	2567.61904	335.80679	847.48802		1
16	H	71.65817	82.00933	65.09324	-2587.99029	680.92867	-512.16411		1
17	C	71.10746	80.37763	62.88856	268.17616	741.64379	-40.42634		1

18	H	70.16082	80.87171	62.54870	1283.54314	-1945.37420	-1411.27812	1
19	H	71.94838	81.08428	62.66569	-1258.57796	1317.15249	-2026.02085	1
20	H	71.25800	79.47077	62.24811	-2502.84526	909.80597	575.92391	1
21	C	73.75441	77.20763	64.77144	619.36578	-458.64843	-172.09273	1
22	O	74.14010	77.09688	65.98904	-81.40433	433.87611	522.34594	1
23	N	74.50868	76.92023	63.74922	175.23996	-622.20190	341.55523	1
24	H	74.12569	76.99460	62.80879	-876.57256	-303.22879	-2561.90213	1
25	C	75.58037	76.03161	64.10757	-571.88214	-534.10783	-106.15033	1
26	H	75.13509	75.02385	63.99863	-2713.20841	-16.25800	-248.80809	1
27	C	76.75098	76.27197	63.08410	166.60354	288.16399	-716.09568	1
28	H	77.00519	77.36766	63.06775	-2097.85574	1636.78449	-586.18044	1
29	O	76.47163	75.92053	61.70598	-317.80580	-363.38227	484.43082	1
30	H	76.61962	76.77073	61.25329	1863.74748	-1451.84923	1357.29467	1
31	C	77.90695	75.47675	63.80093	503.80731	517.99032	318.51606	1
32	H	78.87910	75.59659	63.26866	640.61020	-2157.10410	-1536.29104	1
33	H	78.04923	75.83437	64.85257	1687.88455	465.60692	2087.56452	1
34	H	77.69052	74.38392	63.84709	-1293.07895	-1899.88581	-1463.57452	1
35	C	75.97843	76.44125	65.70320	-153.07550	-733.68902	248.70981	1
36	O	76.73967	77.39963	65.88605	186.15459	-480.78787	-449.34387	1
37	N	76.05560	75.26566	66.44108	-487.53139	543.18517	42.03850	1
38	C	76.52869	75.31001	67.76540	-699.35871	69.34393	360.10701	1
39	H	76.42532	76.37907	68.06716	2.81126	-221.99807	-2715.58072	1
40	C	75.58502	74.27502	68.53054	-507.46439	-592.59194	122.07761	1
41	H	76.07673	73.82601	69.42275	-1975.08116	525.87560	-1801.71556	1
42	H	74.66890	74.78285	68.90525	1588.27743	-1913.22100	1113.83566	1
43	C	75.22413	73.22846	67.43596	-613.62442	-457.55993	-194.14490	1
44	H	75.96502	72.39780	67.39655	1707.54637	-721.27992	1996.92523	1
45	H	74.23677	72.74378	67.60387	758.23357	2100.81767	1560.55011	1
46	C	75.25792	74.11062	66.10313	-352.41524	704.96076	49.21465	1
47	H	75.74085	73.60715	65.23028	1714.76886	-2070.42778	443.35792	1
48	H	74.26599	74.51834	65.78820	1224.15040	1801.50881	1636.97633	1
49	C	78.13133	74.86876	67.80239	566.85117	537.05831	117.62814	1
50	O	78.92782	75.72425	68.09704	-550.26779	-406.08867	4.21666	1
51	N	78.33493	73.59944	67.49447	566.34832	-425.77725	180.18749	1
52	H	77.51885	73.06418	67.20351	644.44502	2646.80550	-52.73430	1
53	C	79.60600	72.98914	67.68317	612.34801	-281.48662	411.56221	1
54	H	79.43143	71.93205	67.38160	1667.23498	-1490.75142	1556.16753	1
55	C	80.64684	73.73710	66.72685	-714.45746	-175.43074	286.98927	1
56	H	80.75771	74.79425	67.09877	-787.09484	1763.03619	-1922.46060	1
57	O	80.25589	73.83110	65.34279	-429.46514	516.51932	-128.40526	1
58	H	80.14085	74.79781	65.25160	1981.82785	436.16847	-1818.18182	1
59	C	81.98295	72.94596	66.97321	630.79189	-468.94448	76.03230	1
60	H	82.82741	73.38642	66.39353	-1775.71861	2062.30353	131.89849	1
61	H	82.28064	72.95621	68.05529	-1855.14608	88.94118	1993.53760	1
62	H	81.89073	71.87999	66.65937	-1504.82350	-780.94249	-2132.90992	1
63	C	79.95888	73.14827	69.26910	288.57638	618.62814	-397.00270	1
64	O	81.08932	73.47359	69.65452	321.70495	-185.26452	574.37218	1
65	N	78.90644	72.82049	69.96516	-447.05792	-446.53431	367.76425	1
66	H	78.09977	72.58555	69.38891	350.31316	1975.63644	-1843.31522	1
67	C	78.81480	72.74628	71.38587	-511.23061	374.03917	-471.51480	1
68	H	78.45253	71.70803	71.54813	2234.79579	-898.70890	-1273.45190	1
69	C	80.22445	73.02635	72.07101	529.53781	-159.34528	563.72604	1
70	H	80.12525	72.75431	73.15802	654.59388	2347.94251	1217.51488	1
71	H	80.95561	72.30476	71.60945	-1526.55661	2103.42026	817.87394	1
72	O	80.74599	74.36383	71.99355	-554.84278	14.12789	399.58769	1
73	H	81.17017	74.29965	71.05937	1297.06236	2061.84854	1220.68812	1
74	C	77.62132	73.76924	71.82521	-662.15484	-412.13544	123.62687	1
75	O	76.61020	73.29552	72.28677	-540.01537	-317.05804	274.91456	1
76	N	77.89797	75.05556	71.59707	-202.76299	-690.00100	-131.49145	1
77	H	78.83516	75.26130	71.24341	-702.62132	-2617.37191	281.70413	1
78	C	76.95669	76.09825	71.98675	-491.73914	576.34187	222.73509	1
79	H	75.94803	75.64560	71.83682	1977.17978	-1823.58850	-434.68928	1

80	C	77.21675	76.48421	73.43385	-649.50797	-328.66843	306.11224	1
81	H	78.30615	76.69807	73.54561	2075.07803	1452.16490	-1004.45904	1
82	C	76.44303	77.73506	73.80628	-615.18735	-489.99689	-70.96352	1
83	H	76.61842	78.03238	74.87943	-1226.32661	-1724.38906	-1716.47170	1
84	H	76.74617	78.60768	73.16095	2381.64273	-969.84735	900.46860	1
85	H	75.33430	77.59378	73.67776	2122.74991	1702.23946	-141.36228	1
86	C	76.86911	75.35727	74.38796	-501.86074	-479.61276	-376.42482	1
87	H	77.13349	75.61278	75.45164	993.79261	-2246.95401	-1177.81305	1
88	H	75.77003	75.11943	74.36364	42.71279	-626.15391	-2651.37258	1
89	H	77.41320	74.40745	74.11635	-2026.39012	-1590.33709	-887.82922	1
90	C	77.28705	77.42224	71.02495	-672.89153	382.57394	-156.34072	1
91	O	78.40530	77.85949	70.92052	410.04627	221.86223	500.35950	1
92	N	76.14598	77.91156	70.57422	-378.11782	-443.79414	-441.10984	1
93	H	75.30951	77.37689	70.79896	2404.15973	-568.14894	1149.30085	1
94	C	76.15252	78.97701	69.61205	-544.54484	466.16019	331.29119	1
95	H	76.87900	78.64716	68.83342	-1409.80988	-170.17955	2325.32679	1
96	C	74.65872	79.07065	69.09808	-184.48284	116.78282	-758.89137	1
97	H	74.32041	78.09547	68.67853	1893.78641	1861.14652	611.04528	1
98	H	73.97648	79.28144	69.95149	-2170.79665	-974.19311	1327.50117	1
99	C	74.54680	80.19758	68.02361	389.51668	672.81878	-138.49152	1
100	H	75.10694	81.10485	68.34815	510.64577	1933.03327	1851.02484	1
101	H	75.05925	79.88261	67.08647	-2302.30869	-1105.72939	-948.89774	1
102	C	73.05449	80.59956	67.72191	-559.93427	-126.34590	542.30857	1
103	O	72.82528	81.53843	67.00146	-670.36003	-111.83166	76.36448	1
104	N	72.13608	79.80138	68.30557	-216.06729	-537.07037	446.51379	1
105	H	72.27779	78.96839	68.88820	-1251.96487	1074.12894	-2168.52500	1
106	H	71.12139	79.90967	68.20405	-2451.83023	-720.73851	944.84612	1
107	C	76.65777	80.37602	70.27223	546.24052	-563.88337	-85.11809	1
108	O	77.08878	81.17740	69.48262	71.70702	-307.40463	606.69673	1
109	N	76.36502	80.57172	71.56627	479.90863	-504.50129	222.86849	1
110	C	77.07337	81.60359	72.27288	75.51268	-600.91904	506.73700	1
111	H	77.26258	82.35360	71.46960	-2033.61562	1795.30103	254.89480	1
112	C	76.05990	82.05524	73.39790	523.79067	517.99274	284.45581	1
113	H	76.57264	82.34073	74.34428	1599.61665	-1127.00911	1895.98173	1
114	H	75.49393	82.95789	73.07523	-1881.83093	1275.82488	-1501.55016	1
115	C	75.09696	80.83605	73.57485	-600.05639	-404.05026	316.64485	1
116	H	75.50682	80.08665	74.28770	-2597.05260	496.36221	657.73249	1
117	H	74.09778	81.12199	73.97277	-1666.24518	1294.38985	-1723.90591	1
118	C	75.03585	80.27422	72.09210	493.57570	-129.95376	-602.56394	1
119	H	74.86530	79.17641	72.00812	-1469.08415	-637.84797	2204.22581	1
120	H	74.32405	80.81025	71.42069	-1038.97840	1068.88701	-2280.71789	1
121	C	78.49506	81.02819	72.85275	188.88100	241.05089	-727.87821	1
122	O	79.51859	81.29191	72.25904	531.88613	-49.19943	427.07960	1
123	N	78.36800	80.35182	73.98528	708.14833	26.93417	-179.73509	1
124	H	77.45020	80.22534	74.40553	-2232.69501	-1179.09831	1023.94816	1
125	C	79.56498	79.76216	74.49662	-738.32412	259.92548	104.42456	1
126	H	80.14840	79.50898	73.58080	2028.89123	1260.02983	1311.33324	1
127	C	80.29310	80.86452	75.38325	-258.65678	-345.52513	661.28459	1
128	H	79.59893	81.28194	76.14355	-1826.06090	-1801.46097	-918.64554	1
129	C	81.52463	80.18761	76.07387	-541.23400	531.92970	-218.41428	1
130	H	82.09506	80.91194	76.70167	1311.73218	-2219.18200	882.19023	1
131	H	81.20637	79.34959	76.73889	-1048.71298	1223.58118	-2196.97971	1
132	H	82.23321	79.76358	75.32421	419.06414	1903.92898	1903.44670	1
133	C	80.82294	82.00622	74.44817	-423.86431	152.66566	-648.55262	1
134	H	81.52057	82.69059	74.98678	105.68386	-2342.50080	1387.51238	1
135	H	81.37027	81.59190	73.56615	-1695.63603	-1484.73621	-1531.02793	1
136	H	79.98614	82.63125	74.05265	-1853.57121	-487.39031	1936.59343	1
137	C	79.16652	78.49159	75.45121	539.71428	-510.58232	267.58633	1
138	O	79.65268	77.40249	75.25222	-15.93758	-278.34085	-624.49402	1
139	N	78.36389	78.87007	76.44047	-676.81886	12.05292	276.17960	1
140	H	78.02259	79.83027	76.44616	-1694.44250	-373.84189	-2100.66098	1
141	C	77.80288	77.86433	77.27733	412.33078	-664.70360	108.35451	1

142	H	78.29152	76.90377	76.98424	1765.77476	1294.44366	1621.76594	1
143	C	78.06906	78.29205	78.77340	-179.66635	-721.95667	-264.73915	1
144	H	79.15350	78.47352	78.93622	-607.34922	2587.87032	-598.10018	1
145	H	77.57205	79.25894	79.00438	-359.69332	-1479.13954	-2259.74260	1
146	C	77.53964	77.13539	79.72767	-240.01076	616.02425	431.85322	1
147	H	76.42859	77.03521	79.63273	-1359.17131	782.54425	2227.99181	1
148	H	77.96010	76.14896	79.40947	-820.36667	85.81767	-2596.78715	1
149	C	77.92986	77.44576	81.15730	-513.07015	236.18570	-551.87280	1
150	H	79.03891	77.50277	81.24025	1816.11944	-1183.11722	-1650.94321	1
151	H	77.57027	78.46378	81.43026	-1800.04429	-1361.53473	1526.34643	1
152	C	77.40815	76.46860	82.11233	726.08972	-253.19732	-179.64713	1
153	H	76.29513	76.45041	82.18222	1224.27271	-456.51798	-2390.90304	1
154	H	77.79072	75.43711	81.97046	1206.40339	-1150.93514	-2154.90344	1
155	N	77.88807	76.86109	83.54661	329.70796	-633.68968	-155.67358	1
156	H	77.56750	76.22612	84.33625	1348.31305	1938.76845	1359.00643	1
157	H	78.93716	76.89067	83.71708	2096.92035	1446.54551	-966.48890	1
158	H	77.58151	77.81066	83.91216	-1197.07217	-2303.53719	827.28733	1
159	C	76.17309	77.90607	77.03990	-378.01186	-556.17301	-413.96481	1
160	O	75.55796	78.88878	76.71570	-409.44433	-307.55053	-453.30833	1
161	N	75.74705	76.67967	77.29500	-429.02477	524.70884	274.08502	1
162	H	76.36278	75.90065	77.60380	1706.34263	-1425.96036	1574.38926	1
163	C	74.35617	76.45730	77.53811	-45.25864	-626.22952	478.93267	1
164	H	73.88433	77.41940	77.84069	1988.63164	570.90773	1772.87287	1
165	C	73.82338	75.90841	76.15030	551.77128	-20.49526	-564.54996	1
166	H	74.20678	76.55241	75.32769	1434.61535	-1753.10253	1513.99471	1
167	H	74.24478	74.89715	75.95529	-714.67738	1819.09770	1898.36494	1
168	C	72.26197	75.86715	76.11303	446.99263	-555.77305	338.97221	1
169	H	71.85594	75.18519	76.89298	1953.68466	1892.25957	-161.67766	1
170	H	71.82348	76.87101	76.30993	-403.03785	2688.07032	-188.43591	1
171	C	71.90107	75.35962	74.65712	567.86262	335.74681	434.04421	1
172	H	72.33642	76.03705	73.88687	-1080.02275	1568.26081	-1948.78900	1
173	H	72.35668	74.36038	74.46885	-919.54108	2111.34692	1456.13463	1
174	C	70.36476	75.28850	74.50946	195.81897	173.33862	-745.11536	1
175	H	69.86689	74.57770	75.19860	1405.67949	-2301.21089	-390.08113	1
176	H	69.84935	76.26916	74.53881	-940.37328	-1118.32446	2299.72133	1
177	N	70.07137	74.72123	73.07760	319.26422	656.36007	-42.02424	1
178	H	69.04726	74.59901	72.83046	1961.03633	619.91968	1787.09422	1
179	H	70.42112	75.28462	72.24879	854.14343	-2156.80752	1429.08711	1
180	H	70.45364	73.75518	72.86026	1237.02905	-1378.50857	-1998.28500	1
181	C	74.51219	75.30913	78.69010	532.53319	-268.57236	517.55729	1
182	O	75.55809	74.67046	78.72699	266.16714	-290.73804	-558.88002	1
183	N	73.43361	75.19770	79.44307	-226.25352	640.49678	-270.32839	1
184	H	72.66022	75.83804	79.26484	2007.69063	-1035.27229	1523.50231	1
185	C	73.51734	74.45521	80.65710	-540.76542	-573.33303	49.50000	1
186	H	74.51473	73.96815	80.54322	-2374.20950	-1036.76023	843.75774	1
187	C	73.47729	75.48772	81.86972	-77.09082	666.87422	-415.84136	1
188	H	72.42154	75.85080	82.00259	-985.81834	617.19825	2463.91927	1
189	O	74.26606	76.69558	81.71688	293.29899	-391.65602	-477.80926	1
190	H	73.56294	77.37104	81.73247	2528.72714	-681.76262	-751.27122	1
191	C	73.90492	74.58393	83.08198	252.47363	-605.14473	440.05134	1
192	H	73.79692	75.12492	84.05137	-2052.65063	1456.49051	-1043.51830	1
193	H	73.29270	73.64938	83.16198	-2152.98800	-1661.97574	-161.70652	1
194	H	74.97068	74.26996	82.99762	-473.12726	-1584.27339	2165.61725	1
195	C	72.27435	73.38561	80.59616	360.36307	488.46713	505.10056	1
196	O	72.16759	72.66295	79.63219	-200.08817	-528.03552	-385.82850	1
197	N	71.55254	73.38717	81.70755	-597.54095	-226.44775	355.20479	1
198	H	71.78551	74.05693	82.44027	2179.23655	-1300.70981	-991.33835	1
199	C	70.31465	72.70536	81.84201	-687.68921	297.39807	-249.45179	1
200	H	69.86617	73.15739	82.75510	-349.16256	-2467.37713	-1101.72831	1
201	C	69.42108	72.93528	80.52596	672.47345	361.54328	-201.62880	1
202	H	69.89546	72.41238	79.66243	1541.41502	582.18425	2169.97026	1
203	H	68.41452	72.48114	80.67267	-2534.67717	60.25153	997.72295	1

204	C	69.31297	74.43748	80.23727	574.26774	-389.43119	-377.02542	1
205	C	68.38005	75.25954	80.93865	688.82679	-287.33580	-257.96133	1
206	H	67.69036	74.82315	81.68364	331.14182	1470.38163	2269.80013	1
207	C	70.20007	75.01226	79.27713	-383.52382	-675.04808	144.24917	1
208	H	70.93469	74.37312	78.74911	4.09847	1517.59662	2262.86397	1
209	C	68.36600	76.62780	80.66919	-134.76730	428.45285	-649.50303	1
210	H	67.64615	77.26486	81.21206	-903.23433	1600.49020	2011.53387	1
211	C	70.14961	76.38784	79.04275	-335.53281	-615.00040	-364.39058	1
212	H	70.84578	76.82223	78.30455	1596.45398	-1369.33862	1732.02659	1
213	C	69.23909	77.24533	79.72674	585.48547	-340.24194	-406.23938	1
214	O	69.18518	78.64591	79.50358	-419.15649	-173.04408	-511.94141	1
215	H	69.88229	78.73048	78.81047	-1071.84350	1559.71507	-1960.13012	1
216	C	70.52000	71.10713	81.99138	291.41878	-183.13091	710.72246	1
217	O	69.57275	70.39317	82.31204	379.87695	523.47396	-222.23622	1
218	N	71.75985	70.72652	81.72571	564.30591	373.09380	277.24371	1
219	H	72.40162	71.45871	81.41830	-120.59931	-2436.07824	-1214.35098	1
220	C	71.92580	69.35363	81.31664	404.07514	-299.37480	608.84009	1
221	H	70.91936	69.10582	80.90590	-1071.07882	-841.69025	2359.66467	1
222	C	73.11694	69.27496	80.27985	-683.12807	68.71770	-390.13096	1
223	H	72.92804	69.93254	79.40049	2068.88918	1596.58590	770.89603	1
224	H	74.06222	69.64418	80.73777	1379.86429	2342.49779	-179.85638	1
225	C	73.24647	67.77613	79.86134	-176.39967	537.49466	550.97268	1
226	H	73.38933	67.13632	80.76281	-396.28051	1942.22168	1869.33314	1
227	H	72.31079	67.41349	79.38032	-94.44700	586.00678	-2659.20016	1
228	C	74.49262	67.63465	78.87394	-291.69381	-718.18079	-150.72929	1
229	H	74.35986	68.08689	77.85803	-2303.38776	1089.76242	964.62032	1
230	H	75.47892	67.97650	79.27938	884.16729	2568.80533	-207.74283	1
231	N	74.54922	66.23872	78.73329	-594.49522	-252.81478	342.29276	1
232	H	73.82085	65.70437	79.18123	-1735.17426	2084.05705	-263.71605	1
233	C	75.44724	65.60867	78.08963	595.23177	-271.52487	442.22352	1
234	N	76.45119	66.35930	77.46765	585.53813	-424.79750	-105.81303	1
235	H	76.57779	67.36994	77.44117	959.88797	1327.56823	-2177.11905	1
236	H	77.21983	65.96897	76.92213	1578.48647	16.27378	-2220.76233	1
237	N	75.22628	64.22446	78.14395	-452.17763	-390.33541	-421.51853	1
238	H	74.49963	63.68182	78.60758	470.26107	1974.25629	-1817.92087	1
239	H	75.84088	63.54306	77.69786	1856.67307	-1573.97321	-1224.35416	1
240	C	72.25886	68.49635	82.65886	-531.47271	-581.45780	-55.06206	1
241	O	73.34079	68.01497	82.87212	-243.00837	192.73507	609.52485	1
242	N	71.13516	68.42339	83.37696	343.49288	-644.25607	38.09164	1
243	H	70.29915	68.96636	83.04693	-1691.16043	-1535.97525	-1484.73099	1
244	C	71.13963	67.84274	84.72386	542.66492	350.14337	454.42563	1
245	H	70.06288	67.84260	85.01555	1209.57979	-2396.95920	463.86744	1
246	C	71.71602	66.44053	84.61814	-737.14309	145.93010	242.71942	1
247	H	72.76751	66.53885	84.24471	-1050.18303	159.36419	-2509.06125	1
248	C	71.75236	65.71996	85.95159	-706.77696	-252.88343	-245.16230	1
249	H	72.20891	64.69568	85.85779	-1624.64039	-1665.49085	1417.86935	1
250	H	72.35713	66.29131	86.71614	2566.10521	598.51109	693.22305	1
251	H	70.72015	65.58666	86.37830	-1972.69758	107.10018	-1876.34312	1
252	C	70.95308	65.60150	83.60791	412.85148	672.58832	-27.69222	1
253	H	71.41988	64.58842	83.46721	1447.02277	1762.76533	-1490.78944	1
254	H	69.88765	65.43721	83.92740	1320.77379	-145.20455	2378.68491	1
255	H	70.92387	66.10141	82.60087	-1512.10848	1470.52031	1724.75147	1
256	C	72.03147	68.82721	85.71016	-607.11113	499.56689	73.73769	1
257	O	72.35504	68.42772	86.80993	357.97126	460.81534	356.68785	1
258	N	72.23720	70.02602	85.19147	536.55407	-368.62270	332.76306	1
259	H	71.88519	70.19060	84.24843	524.38866	2297.69985	1367.20941	1
260	C	73.13324	70.90979	85.83818	46.50277	-774.29190	-147.97904	1
261	H	73.16066	70.56505	86.89761	1676.51875	1883.29066	1032.55549	1
262	C	74.58030	70.84020	85.12020	-559.41456	-34.19198	-556.30433	1
263	H	74.47305	71.17117	84.05975	-64.66664	395.18769	2695.05373	1
264	H	75.27354	71.57209	85.59949	-2703.44278	-60.40056	333.79418	1
265	C	75.16447	69.45457	85.16759	-519.76435	377.31045	459.42366	1

266	H	74.46476	68.75898	84.64315	-1746.74323	1667.50644	-1261.73691	1
267	C	76.50720	69.42836	84.44494	570.95554	16.46261	-545.27700	1
268	H	76.95942	68.40330	84.45152	2391.58273	28.05277	-1305.07271	1
269	H	76.40488	69.73934	83.37354	175.75588	917.63458	2559.43867	1
270	H	77.24695	70.12017	84.92416	-1063.97851	-2155.34650	1283.00462	1
271	C	75.35483	68.96967	86.59742	193.76014	2.62946	-765.53141	1
272	H	75.92893	68.00777	86.63460	507.39394	-846.55087	2539.60089	1
273	H	75.91538	69.71477	87.21935	1337.57841	1818.19054	1526.01994	1
274	H	74.36018	68.78185	87.10008	1100.88635	-1172.91350	-2199.08909	1
275	C	72.62444	72.42035	85.60590	-549.21115	475.64486	-309.38218	1
276	O	71.88027	72.75057	84.71884	556.06106	-390.37755	-78.24250	1
277	O	73.24872	73.40157	86.41574	-572.27940	-310.19032	-209.75862	1
278	H	73.75663	72.79431	87.02282	-1380.08193	2212.14486	790.85944	1

Listing 72: C00072.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.5749	0.0000	300.0000
3	H	68.66714	81.15212	64.89523	-2043.14101	-1757.64893	399.89339		1
4	N	69.57019	80.79999	65.20851	426.75047	490.45733	-334.42467		1
5	H	69.63235	79.89153	64.74438	442.25559	-1110.30854	-2448.52907		1
6	C	70.66804	81.62300	64.87644	415.32972	-666.39213	83.73172		1
7	H	70.31647	82.67763	64.84612	879.32219	2491.00447	667.35213		1
8	C	71.82668	81.36129	65.97109	31.35357	477.41777	628.23362		1
9	H	72.11397	80.25793	65.94740	1168.38489	2240.25337	-1019.71136		1
10	H	72.74768	81.93459	65.70815	-360.43770	2534.90498	931.67112		1
11	C	71.36148	81.73223	67.35208	463.18208	512.70242	-382.34388		1
12	H	70.39258	81.21837	67.54487	1725.29117	1863.52247	-987.07854		1
13	C	72.38247	81.25723	68.37976	710.42801	-144.27427	-313.15367		1
14	H	72.05282	81.47943	69.42718	364.20195	-1033.13725	2494.72524		1
15	H	72.55409	80.15166	68.30882	2567.61904	335.80679	847.48802		1
16	H	73.37541	81.75530	68.23215	-2587.99029	680.92867	-512.16411		1
17	C	71.15713	83.23448	67.49092	268.17616	741.64379	-40.42634		1
18	H	70.86146	83.51619	68.53459	1283.54314	-1945.37420	-1411.27812		1
19	H	72.09206	83.80210	67.24665	-1258.57796	1317.15249	-2026.02085		1
20	H	70.35266	83.60806	66.80635	-2502.84526	909.80597	575.92391		1
21	C	71.21423	81.04400	63.46114	619.36578	-458.64843	-172.09273		1
22	O	71.08796	79.86458	63.14191	-81.40433	433.87611	522.34594		1
23	N	71.90943	81.99242	62.86926	175.23996	-622.20190	341.55523		1
24	H	71.86104	82.92800	63.27093	-876.57256	-303.22879	-2561.90213		1
25	C	72.37845	81.82556	61.52108	-571.88214	-534.10783	-106.15033		1
26	H	71.44983	81.56337	60.96666	-2713.20841	-16.25800	-248.80809		1
27	C	72.97335	83.24524	61.10582	166.60354	288.16399	-716.09568		1
28	H	73.92447	83.42864	61.67631	-2097.85574	1636.78449	-586.18044		1
29	O	72.12012	84.37255	61.39477	-317.80580	-363.38227	484.43082		1
30	H	72.71227	84.92075	61.94573	1863.74748	-1451.84923	1357.29467		1
31	C	73.33095	83.02970	59.58969	503.80731	517.99032	318.51606		1
32	H	73.81074	83.93572	59.15178	640.61020	-2157.10410	-1536.29104		1
33	H	74.03747	82.17783	59.44278	1687.88455	465.60692	2087.56452		1
34	H	72.42047	82.81270	58.98399	-1293.07895	-1899.88581	-1463.57452		1
35	C	73.47091	80.62848	61.38763	-153.07550	-733.68902	248.70981		1
36	O	73.52949	80.12861	60.29338	186.15459	-480.78787	-449.34387		1
37	N	74.26290	80.40113	62.44515	-487.53139	543.18517	42.03850		1
38	C	75.16408	79.28968	62.48007	-699.35871	69.34393	360.10701		1
39	H	75.53650	79.14076	61.44035	2.81126	-221.99807	-2715.58072		1
40	C	76.24343	79.76368	63.54652	-507.46439	-592.59194	122.07761		1
41	H	76.81092	78.91536	63.99046	-1975.08116	525.87560	-1801.71556		1
42	H	76.99312	80.45208	63.09656	1588.27743	-1913.22100	1113.83566		1
43	C	75.33582	80.50676	64.57452	-613.62442	-457.55993	-194.14490		1
44	H	74.75959	79.78602	65.19874	1707.54637	-721.27992	1996.92523		1
45	H	75.89415	81.16689	65.27574	758.23357	2100.81767	1560.55011		1

46	C	74.38262	81.30390	63.58360	-352.41524	704.96076	49.21465	1
47	H	73.35358	81.49050	63.96513	1714.76886	-2070.42778	443.35792	1
48	H	74.80611	82.25646	63.18778	1224.15040	1801.50881	1636.97633	1
49	C	74.43657	77.95044	63.08102	566.85117	537.05831	117.62814	1
50	O	75.12399	76.98474	63.29670	-550.26779	-406.08867	4.21666	1
51	N	73.13325	78.11348	63.23451	566.34832	-425.77725	180.18749	1
52	H	72.66633	79.00897	62.97835	644.44502	2646.80550	-52.73430	1
53	C	72.34690	77.14616	63.93041	612.34801	-281.48662	411.56221	1
54	H	71.33471	77.55022	63.69570	1667.23498	-1490.75142	1556.16753	1
55	C	72.60722	75.70199	63.30311	-714.45746	-175.43074	286.98927	1
56	H	73.61937	75.35008	63.65445	-787.09484	1763.03619	-1922.46060	1
57	O	72.67463	75.64066	61.86018	-429.46514	516.51932	-128.40526	1
58	H	73.64340	75.71140	61.73297	1981.82785	436.16847	-1818.18182	1
59	C	71.46962	74.82373	63.94086	630.79189	-468.94448	76.03230	1
60	H	71.62290	73.74208	63.71857	-1775.71861	2062.30353	131.89849	1
61	H	71.41532	74.92889	65.04938	-1855.14608	88.94118	1993.53760	1
62	H	70.47025	75.10360	63.53451	-1504.82350	-780.94249	-2132.90992	1
63	C	72.70223	77.31819	65.51041	288.57638	618.62814	-397.00270	1
64	O	72.58277	78.40925	66.03105	321.70495	-185.26452	574.37218	1
65	N	73.05081	76.18185	66.07682	-447.05792	-446.53431	367.76425	1
66	H	73.18590	75.26414	65.61401	350.31316	1975.63644	-1843.31522	1
67	C	73.14593	76.13122	67.51110	-511.23061	374.03917	-471.51480	1
68	H	73.87303	76.92105	67.80737	2234.79579	-898.70890	-1273.45190	1
69	C	71.68749	76.42989	68.11318	529.53781	-159.34528	563.72604	1
70	H	71.81268	76.57833	69.22068	654.59388	2347.94251	1217.51488	1
71	H	71.36114	77.41614	67.68503	-1526.55661	2103.42026	817.87394	1
72	O	70.68181	75.40586	67.92306	-554.84278	14.12789	399.58769	1
73	H	70.39215	75.63178	67.01847	1297.06236	2061.84854	1220.68812	1
74	C	73.64525	74.61472	67.70135	-662.15484	-412.13544	123.62687	1
75	O	73.74878	73.89693	66.71546	-540.01537	-317.05804	274.91456	1
76	N	73.88905	74.30602	68.97736	-202.76299	-690.00100	-131.49145	1
77	H	73.81955	75.08991	69.62757	-702.62132	-2617.37191	281.70413	1
78	C	74.49953	73.02577	69.31580	-491.73914	576.34187	222.73509	1
79	H	74.16162	72.37783	68.47126	1977.17978	-1823.58850	-434.68928	1
80	C	76.00783	73.22007	69.30466	-649.50797	-328.66843	306.11224	1
81	H	76.23349	74.13773	69.89202	2075.07803	1452.16490	-1004.45904	1
82	C	76.74784	72.06087	69.94346	-615.18735	-489.99689	-70.96352	1
83	H	77.86406	72.19377	69.88671	-1226.32661	-1724.38906	-1716.47170	1
84	H	76.47845	71.94582	71.03319	2381.64273	-969.84735	900.46860	1
85	H	76.49983	71.08535	69.43917	2122.74991	1702.23946	-141.36228	1
86	C	76.52265	73.43606	67.89300	-501.86074	-479.61276	-376.42482	1
87	H	77.59962	73.76119	67.88207	993.79261	-2246.95401	-1177.81305	1
88	H	76.45171	72.49481	67.28063	42.71279	-626.15391	-2651.37258	1
89	H	75.92171	74.22091	67.34988	-2026.39012	-1590.33709	-887.82922	1
90	C	73.98923	72.46715	70.80329	-672.89153	382.57394	-156.34072	1
91	O	74.27936	71.32429	71.08480	410.04627	221.86223	500.35950	1
92	N	73.29055	73.33620	71.50246	-378.11782	-443.79414	-441.10984	1
93	H	73.11084	74.20185	71.00230	2404.15973	-568.14894	1149.30085	1
94	C	73.08024	73.24410	72.91435	-544.54484	466.16019	331.29119	1
95	H	72.09792	73.73746	73.07232	-1409.80988	-170.17955	2325.32679	1
96	C	73.13146	71.72148	73.32253	-184.48284	116.78282	-758.89137	1
97	H	72.56187	71.11624	72.57825	1893.78641	1861.14652	611.04528	1
98	H	74.18951	71.36146	73.26096	-2170.79665	-974.19311	1327.50117	1
99	C	72.58497	71.48298	74.76980	389.51668	672.81878	-138.49152	1
100	H	73.09076	72.15663	75.49828	510.64577	1933.03327	1851.02484	1
101	H	71.51223	71.77138	74.83334	-2302.30869	-1105.72939	-948.89774	1
102	C	72.78235	69.98528	75.19653	-559.93427	-126.34590	542.30857	1
103	O	72.59620	69.63719	76.34475	-670.36003	-111.83166	76.36448	1
104	N	73.13440	69.17888	74.17929	-216.06729	-537.07037	446.51379	1
105	H	73.34582	69.40397	73.19936	-1251.96487	1074.12894	-2168.52500	1
106	H	73.33878	68.17863	74.28516	-2451.83023	-720.73851	944.84612	1
107	C	74.30972	74.02202	73.66155	546.24052	-563.88337	-85.11809	1

108	O	75.41339	73.53983	73.65216	71.70702	-307.40463	606.69673	1
109	N	73.90734	75.17886	74.21742	479.90863	-504.50129	222.86849	1
110	C	74.86475	76.00061	74.88828	75.51268	-600.91904	506.73700	1
111	H	75.85527	75.73380	74.45109	-2033.61562	1795.30103	254.89480	1
112	C	74.32465	77.45864	74.55385	523.79067	517.99274	284.45581	1
113	H	74.67489	78.22331	75.28249	1599.61665	-1127.00911	1895.98173	1
114	H	74.66848	77.79565	73.55105	-1881.83093	1275.82488	-1501.55016	1
115	C	72.77826	77.25266	74.57623	-600.05639	-404.05026	316.64485	1
116	H	72.38908	77.25679	75.61899	-2597.05260	496.36221	657.73249	1
117	H	72.21763	78.04437	74.03075	-1666.24518	1294.38985	-1723.90591	1
118	C	72.63456	75.81744	73.91039	493.57570	-129.95376	-602.56394	1
119	H	71.81908	75.18694	74.33742	-1469.08415	-637.84797	2204.22581	1
120	H	72.55293	75.82225	72.79775	-1038.97840	1068.88701	-2280.71789	1
121	C	74.84375	75.77800	76.51221	188.88100	241.05089	-727.87821	1
122	O	75.83546	76.03344	77.14480	531.88613	-49.19943	427.07960	1
123	N	73.62607	75.47625	76.95145	708.14833	26.93417	-179.73509	1
124	H	72.86070	75.25969	76.28107	-2232.69501	-1179.09831	1023.94816	1
125	C	73.50359	74.82502	78.22399	-738.32412	259.92548	104.42456	1
126	H	74.48393	74.35771	78.46323	2028.89123	1260.02983	1311.33324	1
127	C	73.07743	75.91477	79.30108	-258.65678	-345.52513	661.28459	1
128	H	72.32336	76.60495	78.86542	-1826.06090	-1801.46097	-918.64554	1
129	C	72.53065	75.22659	80.59805	-541.23400	531.92970	-218.41428	1
130	H	72.25695	75.97729	81.37645	1311.73218	-2219.18200	882.19023	1
131	H	71.61803	74.62026	80.38812	-1048.71298	1223.58118	-2196.97971	1
132	H	73.28743	74.54473	81.05281	419.06414	1903.92898	1903.44670	1
133	C	74.35795	76.69628	79.75351	-423.86431	152.66566	-648.55262	1
134	H	74.11175	77.51079	80.47513	105.68386	-2342.50080	1387.51238	1
135	H	75.09408	76.02397	80.25499	-1695.63603	-1484.73621	-1531.02793	1
136	H	74.87813	77.16381	78.88204	-1853.57121	-487.39031	1936.59343	1
137	C	72.28399	73.80977	77.87065	539.71428	-510.58232	267.58633	1
138	O	71.62941	74.02028	76.85032	-15.93758	-278.34085	-624.49402	1
139	N	72.22057	72.81606	78.73393	-676.81886	12.05292	276.17960	1
140	H	72.86444	72.89156	79.52271	-1694.44250	-373.84189	-2100.66098	1
141	C	71.01807	72.03823	78.89353	412.33078	-664.70360	108.35451	1
142	H	70.28163	72.72122	79.37114	1765.77476	1294.44366	1621.76594	1
143	C	70.55346	71.56998	77.46637	-179.66635	-721.95667	-264.73915	1
144	H	70.42575	72.45386	76.77973	-607.34922	2587.87032	-598.10018	1
145	H	71.37464	70.93562	77.00824	-359.69332	-1479.13954	-2259.74260	1
146	C	69.22366	70.74465	77.52715	-240.01076	616.02425	431.85322	1
147	H	69.34984	69.81642	78.12994	-1359.17131	782.54425	2227.99181	1
148	H	68.40173	71.32080	78.00756	-820.36667	85.81767	-2596.78715	1
149	C	68.90486	70.42854	76.01012	-513.07015	236.18570	-551.87280	1
150	H	68.78585	71.37490	75.43398	1816.11944	-1183.11722	-1650.94321	1
151	H	69.76158	69.89502	75.53645	-1800.04429	-1361.53473	1526.34643	1
152	C	67.61917	69.57675	75.91169	726.08972	-253.19732	-179.64713	1
153	H	67.72641	68.53327	76.26918	1224.27271	-456.51798	-2390.90304	1
154	H	66.71880	70.04145	76.36048	1206.40339	-1150.93514	-2154.90344	1
155	N	67.27834	69.45103	74.38681	329.70796	-633.68968	-155.67358	1
156	H	66.42833	68.86268	74.15017	1348.31305	1938.76845	1359.00643	1
157	H	67.05846	70.35061	73.86782	2096.92035	1446.54551	-966.48890	1
158	H	68.01599	69.01352	73.76156	-1197.07217	-2303.53719	827.28733	1
159	C	71.36028	70.73988	79.81594	-378.01186	-556.17301	-413.96481	1
160	O	70.46523	70.17821	80.40664	-409.44433	-307.55053	-453.30833	1
161	N	72.65518	70.41298	79.77737	-429.02477	524.70884	274.08502	1
162	H	73.23945	70.97409	79.15941	1706.34263	-1425.96036	1574.38926	1
163	C	73.06363	69.13737	80.24232	-45.25864	-626.22952	478.93267	1
164	H	72.17930	68.75868	80.80682	1988.63164	570.90773	1772.87287	1
165	C	73.40016	68.26855	78.95907	551.77128	-20.49526	-564.54996	1
166	H	72.62211	68.39859	78.16757	1434.61535	-1753.10253	1513.99471	1
167	H	74.35527	68.60088	78.49221	-714.67738	1819.09770	1898.36494	1
168	C	73.49602	66.78583	79.44611	446.99263	-555.77305	338.97221	1
169	H	74.25792	66.71163	80.26568	1953.68466	1892.25957	-161.67766	1

170	H	72.53110	66.45459	79.89233	-403.03785	2688.07032	-188.43591	1
171	C	73.89651	65.84721	78.23820	567.86262	335.74681	434.04421	1
172	H	73.08353	65.79823	77.47752	-1080.02275	1568.26081	-1948.78900	1
173	H	74.79182	66.24092	77.70372	-919.54108	2111.34692	1456.13463	1
174	C	74.18543	64.45598	78.84969	195.81897	173.33862	-745.11536	1
175	H	75.08368	64.41923	79.49816	1405.67949	-2301.21089	-390.08113	1
176	H	73.32452	63.99314	79.37213	-940.37328	-1118.32446	2299.72133	1
177	N	74.50906	63.46755	77.67988	319.26422	656.36007	-42.02424	1
178	H	74.77181	62.48296	77.97526	1961.03633	619.91968	1787.09422	1
179	H	73.73510	63.27449	76.97957	854.14343	-2156.80752	1429.08711	1
180	H	75.32297	63.71903	77.04676	1237.02905	-1378.50857	-1998.28500	1
181	C	74.43800	69.26177	81.14068	532.53319	-268.57236	517.55729	1
182	O	75.03346	68.24520	81.43520	266.16714	-290.73804	-558.88002	1
183	N	74.68158	70.51259	81.48225	-226.25352	640.49678	-270.32839	1
184	H	73.97273	71.16634	81.15371	2007.69063	-1035.27229	1523.50231	1
185	C	75.75827	70.97345	82.28050	-540.76542	-573.33303	49.50000	1
186	H	75.37355	71.91365	82.73389	-2374.20950	-1036.76023	843.75774	1
187	C	76.18845	69.85636	83.33487	-77.09082	666.87422	-415.84136	1
188	H	76.57523	68.96792	82.75399	-985.81834	617.19825	2463.91927	1
189	O	75.13515	69.35772	84.18773	293.29899	-391.65602	-477.80926	1
190	H	74.88621	68.54773	83.69049	2528.72714	-681.76262	-751.27122	1
191	C	77.38537	70.56780	84.06700	252.47363	-605.14473	440.05134	1
192	H	77.88189	69.88349	84.79343	-2052.65063	1456.49051	-1043.51830	1
193	H	78.16713	70.91518	83.34992	-2152.98800	-1661.97574	-161.70652	1
194	H	77.04051	71.46184	84.63668	-473.12726	-1584.27339	2165.61725	1
195	C	77.05998	71.23568	81.30924	360.36307	488.46713	505.10056	1
196	O	77.64224	70.35453	80.72726	-200.08817	-528.03552	-385.82850	1
197	N	77.35438	72.52506	81.40972	-597.54095	-226.44775	355.20479	1
198	H	76.77154	73.18115	81.94330	2179.23655	-1300.70981	-991.33835	1
199	C	78.47741	73.01267	80.69226	-687.68921	297.39807	-249.45179	1
200	H	78.98226	72.07554	80.35777	-349.16256	-2467.37713	-1101.72831	1
201	C	77.89344	73.85266	79.45410	672.47345	361.54328	-201.62880	1
202	H	77.14180	74.59747	79.80237	1541.41502	582.18425	2169.97026	1
203	H	78.70696	74.41732	78.94380	-2534.67717	60.25153	997.72295	1
204	C	77.26661	72.83733	78.48935	574.26774	-389.43119	-377.02542	1
205	C	78.13848	72.15251	77.59010	688.82679	-287.33580	-257.96133	1
206	H	79.21986	72.37916	77.57030	331.14182	1470.38163	2269.80013	1
207	C	75.87454	72.51933	78.51126	-383.52382	-675.04808	144.24917	1
208	H	75.19936	73.02434	79.22762	4.09847	1517.59662	2262.86397	1
209	C	77.60296	71.17826	76.75117	-134.76730	428.45285	-649.50303	1
210	H	78.28387	70.64386	76.06610	-903.23433	1600.49020	2011.53387	1
211	C	75.38076	71.55224	77.62846	-335.53281	-615.00040	-364.39058	1
212	H	74.29811	71.33618	77.63424	1596.45398	-1369.33862	1732.02659	1
213	C	76.22071	70.83242	76.72946	585.48547	-340.24194	-406.23938	1
214	O	75.76789	69.81881	75.84928	-419.15649	-173.04408	-511.94141	1
215	H	74.79710	69.84673	76.02934	-1071.84350	1559.71507	-1960.13012	1
216	C	79.36423	73.87969	81.74750	291.41878	-183.13091	710.72246	1
217	O	79.49789	73.54298	82.90446	379.87695	523.47396	-222.23622	1
218	N	79.98542	74.88242	81.13151	564.30591	373.09380	277.24371	1
219	H	79.77134	75.11992	80.16541	-120.59931	-2436.07824	-1214.35098	1
220	C	80.95450	75.59699	81.89977	404.07514	-299.37480	608.84009	1
221	H	81.37863	74.84762	82.60792	-1071.07882	-841.69025	2359.66467	1
222	C	81.96004	76.22600	80.85462	-683.12807	68.71770	-390.13096	1
223	H	82.31131	75.45860	80.12867	2068.88918	1596.58590	770.89603	1
224	H	81.42762	76.99116	80.24537	1379.86429	2342.49779	-179.85638	1
225	C	83.16824	76.87123	81.60246	-176.39967	537.49466	550.97268	1
226	H	82.83471	77.45079	82.49053	-396.28051	1942.22168	1869.33314	1
227	H	83.86986	76.10088	81.99232	-94.44700	586.00678	-2659.20016	1
228	C	83.86383	77.81869	80.51921	-291.69381	-718.18079	-150.72929	1
229	H	84.29917	77.28981	79.63341	-2303.38776	1089.76242	964.62032	1
230	H	83.22622	78.65214	80.13242	884.16729	2568.80533	-207.74283	1
231	N	84.92079	78.42116	81.21221	-594.49522	-252.81478	342.29276	1

232	H	85.06120	78.13189	82.16744	-1735.17426	2084.05705	-263.71605	1
233	C	85.70148	79.29118	80.71333	595.23177	-271.52487	442.22352	1
234	N	85.48693	79.67364	79.38425	585.53813	-424.79750	-105.81303	1
235	H	84.78007	79.35220	78.72393	959.88797	1327.56823	-2177.11905	1
236	H	86.04783	80.35767	78.87538	1578.48647	16.27378	-2220.76233	1
237	N	86.66310	79.70729	81.64448	-452.17763	-390.33541	-421.51853	1
238	H	86.82619	79.42692	82.61049	470.26107	1974.25629	-1817.92087	1
239	H	87.38373	80.39772	81.42906	1856.67307	-1573.97321	-1224.35416	1
240	C	80.19174	76.83711	82.66754	-531.47271	-581.45780	-55.06206	1
241	O	79.49356	77.63675	82.09190	-243.00837	192.73507	609.52485	1
242	N	80.60326	76.84421	83.93283	343.49288	-644.25607	38.09164	1
243	H	81.23394	76.08282	84.18292	-1691.16043	-1535.97525	-1484.73099	1
244	C	80.02672	77.70690	84.95207	542.66492	350.14337	454.42563	1
245	H	80.68624	77.53638	85.83653	1209.57979	-2396.95920	463.86744	1
246	C	80.04272	79.14730	84.46958	-737.14309	145.93010	242.71942	1
247	H	79.35137	79.21012	83.59291	-1050.18303	159.36419	-2509.06125	1
248	C	79.55395	80.10588	85.53861	-706.77696	-252.88343	-245.16230	1
249	H	79.50335	81.16361	85.15976	-1624.64039	-1665.49085	1417.86935	1
250	H	78.51639	79.82312	85.89827	2566.10521	598.51109	693.22305	1
251	H	80.23111	80.10751	86.43665	-1972.69758	107.10018	-1876.34312	1
252	C	81.41790	79.58158	83.99377	412.85148	672.58832	-27.69222	1
253	H	81.42517	80.65566	83.66178	1447.02277	1762.76533	-1490.78944	1
254	H	82.19060	79.47696	84.80373	1320.77379	-145.20455	2378.68491	1
255	H	81.76115	78.96233	83.12167	-1512.10848	1470.52031	1724.75147	1
256	C	78.46617	77.18215	85.24483	-607.11113	499.56689	73.73769	1
257	O	77.64425	77.97973	85.64753	357.97126	460.81534	356.68785	1
258	N	78.35319	75.87874	85.09316	536.55407	-368.62270	332.76306	1
259	H	79.21175	75.44533	84.76056	524.38866	2297.69985	1367.20941	1
260	C	77.22197	75.13111	85.52053	46.50277	-774.29190	-147.97904	1
261	H	77.65086	74.11633	85.67777	1676.51875	1883.29066	1032.55549	1
262	C	76.53425	75.75636	86.84095	-559.41456	-34.19198	-556.30433	1
263	H	76.21912	76.81281	86.62520	-64.66664	395.18769	2695.05373	1
264	H	75.59620	75.20019	87.08180	-2703.44278	-60.40056	333.79418	1
265	C	77.48831	75.71988	88.00239	-519.76435	377.31045	459.42366	1
266	H	78.45009	76.17967	87.68049	-1746.74323	1667.50644	-1261.73691	1
267	C	76.93094	76.52954	89.16756	570.95554	16.46261	-545.27700	1
268	H	77.62777	76.52811	90.04480	2391.58273	28.05277	-1305.07271	1
269	H	76.75765	77.59903	88.88156	175.75588	917.63458	2559.43867	1
270	H	75.95100	76.11881	89.52288	-1063.97851	-2155.34650	1283.00462	1
271	C	77.75263	74.29100	88.45894	193.76014	2.62946	-765.53141	1
272	H	78.42805	74.26071	89.35232	507.39394	-846.55087	2539.60089	1
273	H	76.80339	73.76829	88.74379	1337.57841	1818.19054	1526.01994	1
274	H	78.23881	73.68074	87.65543	1100.88635	-1172.91350	-2199.08909	1
275	C	76.13854	75.12422	84.34631	-549.21115	475.64486	-309.38218	1
276	O	74.95973	75.25429	84.53639	556.06106	-390.37755	-78.24250	1
277	O	76.62613	74.75909	83.04663	-572.27940	-310.19032	-209.75862	1
278	H	77.59974	74.75724	83.25697	-1380.08193	2212.14486	790.85944	1

Listing 73: C00073.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.5588	0.0000	300.0000
3	H	79.75613	61.21994	84.47265	-2043.14101	-1757.64893	399.89339	1	
4	N	80.09836	61.17527	83.51549	426.75047	490.45733	-334.42467	1	
5	H	79.24356	61.32853	82.98166	442.25559	-1110.30854	-2448.52907	1	
6	C	81.13097	62.09573	83.20085	415.32972	-666.39213	83.73172	1	
7	H	81.60806	62.35867	84.17376	879.32219	2491.00447	667.35213	1	
8	C	82.18023	61.36810	82.19465	31.35357	477.41777	628.23362	1	
9	H	81.65730	61.10729	81.24503	1168.38489	2240.25337	-1019.71136	1	
10	H	82.99827	62.07047	81.91120	-360.43770	2534.90498	931.67112	1	
11	C	82.73275	60.13568	82.84384	463.18208	512.70242	-382.34388	1	

12	H	81.87642	59.50382	83.17366	1725.29117	1863.52247	-987.07854	1
13	C	83.57284	59.34212	81.84835	710.42801	-144.27427	-313.15367	1
14	H	83.97527	58.40143	82.30419	364.20195	-1033.13725	2494.72524	1
15	H	82.97797	59.04658	80.94653	2567.61904	335.80679	847.48802	1
16	H	84.45095	59.93588	81.48640	-2587.99029	680.92867	-512.16411	1
17	C	83.58773	60.47108	84.06005	268.17616	741.64379	-40.42634	1
18	H	84.03976	59.55132	84.51242	1283.54314	-1945.37420	-1411.27812	1
19	H	84.43112	61.15871	83.79457	-1258.57796	1317.15249	-2026.02085	1
20	H	82.98929	60.97256	84.86269	-2502.84526	909.80597	575.92391	1
21	C	80.42916	63.32653	82.48721	619.36578	-458.64843	-172.09273	1
22	O	79.16296	63.45391	82.30490	-81.40433	433.87611	522.34594	1
23	N	81.29636	64.21967	82.12290	175.23996	-622.20190	341.55523	1
24	H	82.28598	64.08714	82.31663	-876.57256	-303.22879	-2561.90213	1
25	C	80.74377	65.38753	81.51002	-571.88214	-534.10783	-106.15033	1
26	H	81.09219	66.21203	82.16257	-2713.20841	-16.25800	-248.80809	1
27	C	81.39692	65.49014	80.08183	166.60354	288.16399	-716.09568	1
28	H	81.03301	64.63265	79.45297	-2097.85574	1636.78449	-586.18044	1
29	O	82.84502	65.43382	80.03919	-317.80580	-363.38227	484.43082	1
30	H	82.99068	64.64052	79.49295	1863.74748	-1451.84923	1357.29467	1
31	C	80.75494	66.83693	79.57361	503.80731	517.99032	318.51606	1
32	H	81.04503	67.05325	78.51962	640.61020	-2157.10410	-1536.29104	1
33	H	79.63827	66.80710	79.61168	1687.88455	465.60692	2087.56452	1
34	H	81.08508	67.70422	80.19083	-1293.07895	-1899.88581	-1463.57452	1
35	C	79.06319	65.20009	81.42682	-153.07550	-733.68902	248.70981	1
36	O	78.51039	65.02243	80.33169	186.15459	-480.78787	-449.34387	1
37	N	78.52848	66.04362	82.39911	-487.53139	543.18517	42.03850	1
38	C	77.13133	66.17842	82.47204	-699.35871	69.34393	360.10701	1
39	H	76.73392	65.40801	81.76666	2.81126	-221.99807	-2715.58072	1
40	C	76.87627	65.93667	84.03863	-507.46439	-592.59194	122.07761	1
41	H	75.89028	66.32038	84.38126	-1975.08116	525.87560	-1801.71556	1
42	H	76.90749	64.85375	84.29082	1588.27743	-1913.22100	1113.83566	1
43	C	78.08037	66.69531	84.66078	-613.62442	-457.55993	-194.14490	1
44	H	77.88921	67.79404	84.68766	1707.54637	-721.27992	1996.92523	1
45	H	78.31439	66.38616	85.70387	758.23357	2100.81767	1560.55011	1
46	C	79.24215	66.33542	83.61943	-352.41524	704.96076	49.21465	1
47	H	79.95081	67.17435	83.41550	1714.76886	-2070.42778	443.35792	1
48	H	79.82263	65.41091	83.85947	1224.15040	1801.50881	1636.97633	1
49	C	76.68104	67.72653	82.08988	566.85117	537.05831	117.62814	1
50	O	76.87120	68.63608	82.89740	-550.26779	-406.08867	4.21666	1
51	N	76.19729	67.76101	80.88416	566.34832	-425.77725	180.18749	1
52	H	76.17151	66.84768	80.43046	644.44502	2646.80550	-52.73430	1
53	C	75.33491	68.79095	80.37691	612.34801	-281.48662	411.56221	1
54	H	74.32021	68.34242	80.44857	1667.23498	-1490.75142	1556.16753	1
55	C	75.46896	70.13228	81.21699	-714.45746	-175.43074	286.98927	1
56	H	76.56849	70.31847	81.38889	-787.09484	1763.03619	-1922.46060	1
57	O	74.88927	70.10769	82.52503	-429.46514	516.51932	-128.40526	1
58	H	75.70082	69.77421	83.05497	1981.82785	436.16847	-1818.18182	1
59	C	74.88477	71.21648	80.23941	630.79189	-468.94448	76.03230	1
60	H	74.95012	72.23798	80.67976	-1775.71861	2062.30353	131.89849	1
61	H	75.43054	71.24232	79.26783	-1855.14608	88.94118	1993.53760	1
62	H	73.81084	71.02210	80.01252	-1504.82350	-780.94249	-2132.90992	1
63	C	75.73719	68.97102	78.80512	288.57638	618.62814	-397.00270	1
64	O	74.91499	68.60400	77.96083	321.70495	-185.26452	574.37218	1
65	N	76.90605	69.53380	78.64653	-447.05792	-446.53431	367.76425	1
66	H	77.40075	69.71562	79.51937	350.31316	1975.63644	-1843.31522	1
67	C	77.49045	69.88643	77.40316	-511.23061	374.03917	-471.51480	1
68	H	78.56693	69.70231	77.61213	2234.79579	-898.70890	-1273.45190	1
69	C	76.91091	68.96273	76.24341	529.53781	-159.34528	563.72604	1
70	H	77.66170	68.97148	75.40246	654.59388	2347.94251	1217.51488	1
71	H	76.88110	67.92200	76.66787	-1526.55661	2103.42026	817.87394	1
72	O	75.64805	69.29900	75.64978	-554.84278	14.12789	399.58769	1
73	H	75.02974	68.92566	76.39121	1297.06236	2061.84854	1220.68812	1

74	C	77.28613	71.50113	77.16199	-662.15484	-412.13544	123.62687	1
75	O	78.28976	72.18105	77.18052	-540.01537	-317.05804	274.91456	1
76	N	76.01948	71.87354	77.05136	-202.76299	-690.00100	-131.49145	1
77	H	75.38599	71.07216	77.05731	-702.62132	-2617.37191	281.70413	1
78	C	75.53611	73.22540	76.81432	-491.73914	576.34187	222.73509	1
79	H	74.59275	73.27681	77.40741	1977.17978	-1823.58850	-434.68928	1
80	C	76.57022	74.25286	77.22751	-649.50797	-328.66843	306.11224	1
81	H	77.51753	74.03403	76.66744	2075.07803	1452.16490	-1004.45904	1
82	C	76.14416	75.66957	76.89852	-615.18735	-489.99689	-70.96352	1
83	H	76.87879	76.42157	77.29793	-1226.32661	-1724.38906	-1716.47170	1
84	H	76.06548	75.85170	75.76433	2381.64273	-969.84735	900.46860	1
85	H	75.14445	75.91679	77.34804	2122.74991	1702.23946	-141.36228	1
86	C	76.88393	74.16264	78.71203	-501.86074	-479.61276	-376.42482	1
87	H	77.67674	74.89959	79.01489	993.79261	-2246.95401	-1177.81305	1
88	H	75.97719	74.36615	79.34368	42.71279	-626.15391	-2651.37258	1
89	H	77.26131	73.13754	78.98434	-2026.39012	-1590.33709	-887.82922	1
90	C	75.22030	73.34260	75.17631	-672.89153	382.57394	-156.34072	1
91	O	76.09201	73.23348	74.35111	410.04627	221.86223	500.35950	1
92	N	73.94260	73.63012	74.99831	-378.11782	-443.79414	-441.10984	1
93	H	73.32925	73.64794	75.80910	2404.15973	-568.14894	1149.30085	1
94	C	73.46095	73.79959	73.66091	-544.54484	466.16019	331.29119	1
95	H	74.26433	74.40327	73.18230	-1409.80988	-170.17955	2325.32679	1
96	C	73.37792	72.35157	73.02524	-184.48284	116.78282	-758.89137	1
97	H	74.34580	71.81318	73.15424	1893.78641	1861.14652	611.04528	1
98	H	72.60973	71.73494	73.54555	-2170.79665	-974.19311	1327.50117	1
99	C	73.02530	72.53871	71.51642	389.51668	672.81878	-138.49152	1
100	H	72.06825	73.09796	71.41874	510.64577	1933.03327	1851.02484	1
101	H	73.77603	73.19751	71.02647	-2302.30869	-1105.72939	-948.89774	1
102	C	72.92201	71.18301	70.72115	-559.93427	-126.34590	542.30857	1
103	O	72.60747	71.20505	69.55907	-670.36003	-111.83166	76.36448	1
104	N	73.21830	70.08538	71.44969	-216.06729	-537.07037	446.51379	1
105	H	73.50511	70.00261	72.43232	-1251.96487	1074.12894	-2168.52500	1
106	H	73.21116	69.13079	71.07448	-2451.83023	-720.73851	944.84612	1
107	C	71.98981	74.50860	73.72498	546.24052	-563.88337	-85.11809	1
108	O	71.00334	73.82194	73.75381	71.70702	-307.40463	606.69673	1
109	N	72.09181	75.85318	73.78036	479.90863	-504.50129	222.86849	1
110	C	70.96124	76.71187	73.74716	75.51268	-600.91904	506.73700	1
111	H	70.07406	76.12693	74.07969	-2033.61562	1795.30103	254.89480	1
112	C	71.38540	77.96892	74.61683	523.79067	517.99274	284.45581	1
113	H	71.00920	78.92115	74.17841	1599.61665	-1127.00911	1895.98173	1
114	H	70.95614	77.92939	75.64198	-1881.83093	1275.82488	-1501.55016	1
115	C	72.94611	77.90869	74.63113	-600.05639	-404.05026	316.64485	1
116	H	73.40030	78.75328	74.06423	-2597.05260	496.36221	657.73249	1
117	H	73.33816	77.99755	75.66926	-1666.24518	1294.38985	-1723.90591	1
118	C	73.37074	76.51422	74.00682	493.57570	-129.95376	-602.56394	1
119	H	73.87389	76.59226	73.01297	-1469.08415	-637.84797	2204.22581	1
120	H	73.97218	75.85673	74.68062	-1038.97840	1068.88701	-2280.71789	1
121	C	70.79303	77.44728	72.27987	188.88100	241.05089	-727.87821	1
122	O	71.71658	78.01700	71.74281	531.88613	-49.19943	427.07960	1
123	N	69.52019	77.36035	71.91548	708.14833	26.93417	-179.73509	1
124	H	68.88345	76.85410	72.52997	-2232.69501	-1179.09831	1023.94816	1
125	C	69.02156	78.05983	70.78405	-738.32412	259.92548	104.42456	1
126	H	67.96111	77.73276	70.70501	2028.89123	1260.02983	1311.33324	1
127	C	69.11408	79.61084	71.14420	-258.65678	-345.52513	661.28459	1
128	H	70.16206	79.86214	71.40987	-1826.06090	-1801.46097	-918.64554	1
129	C	68.58711	80.50544	69.97274	-541.23400	531.92970	-218.41428	1
130	H	68.55525	81.58369	70.25952	1311.73218	-2219.18200	882.19023	1
131	H	69.23462	80.42208	69.06420	-1048.71298	1223.58118	-2196.97971	1
132	H	67.55451	80.21331	69.66912	419.06414	1903.92898	1903.44670	1
133	C	68.16791	79.91871	72.35423	-423.86431	152.66566	-648.55262	1
134	H	68.20322	80.99669	72.63932	105.68386	-2342.50080	1387.51238	1
135	H	67.10628	79.67415	72.11570	-1695.63603	-1484.73621	-1531.02793	1

136	H	68.45221	79.32602	73.25504	-1853.57121	-487.39031	1936.59343	1
137	C	69.88921	77.69581	69.45365	539.71428	-510.58232	267.58633	1
138	O	69.74764	78.38310	68.44152	-15.93758	-278.34085	-624.49402	1
139	N	70.61535	76.61602	69.62477	-676.81886	12.05292	276.17960	1
140	H	70.57363	76.24545	70.57653	-1694.44250	-373.84189	-2100.66098	1
141	C	71.42557	75.98295	68.65086	412.33078	-664.70360	108.35451	1
142	H	71.75315	75.04635	69.15604	1765.77476	1294.44366	1621.76594	1
143	C	70.49245	75.73334	67.39511	-179.66635	-721.95667	-264.73915	1
144	H	69.56818	75.19035	67.69561	-607.34922	2587.87032	-598.10018	1
145	H	70.14243	76.69797	66.95905	-359.69332	-1479.13954	-2259.74260	1
146	C	71.32639	74.90752	66.36241	-240.01076	616.02425	431.85322	1
147	H	72.19917	75.49699	66.00127	-1359.17131	782.54425	2227.99181	1
148	H	71.74824	73.99230	66.83584	-820.36667	85.81767	-2596.78715	1
149	C	70.36224	74.52428	65.16830	-513.07015	236.18570	-551.87280	1
150	H	69.50870	73.90475	65.52837	1816.11944	-1183.11722	-1650.94321	1
151	H	69.90674	75.43346	64.71264	-1800.04429	-1361.53473	1526.34643	1
152	C	71.21109	73.74912	64.13417	726.08972	-253.19732	-179.64713	1
153	H	72.00300	74.35080	63.64520	1224.27271	-456.51798	-2390.90304	1
154	H	71.63712	72.79698	64.50894	1206.40339	-1150.93514	-2154.90344	1
155	N	70.25634	73.32173	62.96937	329.70796	-633.68968	-155.67358	1
156	H	70.71501	72.79590	62.17049	1348.31305	1938.76845	1359.00643	1
157	H	69.45910	72.66665	63.21836	2096.92035	1446.54551	-966.48890	1
158	H	69.75013	74.09545	62.44799	-1197.07217	-2303.53719	827.28733	1
159	C	72.71405	76.91166	68.21998	-378.01186	-556.17301	-413.96481	1
160	O	73.82097	76.44123	68.30039	-409.44433	-307.55053	-453.30833	1
161	N	72.34307	78.10154	67.77192	-429.02477	524.70884	274.08502	1
162	H	71.33044	78.38416	67.77467	1706.34263	-1425.96036	1574.38926	1
163	C	73.34917	78.92465	67.18790	-45.25864	-626.22952	478.93267	1
164	H	74.15943	78.21478	66.89740	1988.63164	570.90773	1772.87287	1
165	C	72.65111	79.67227	65.97834	551.77128	-20.49526	-564.54996	1
166	H	72.13564	78.94324	65.31366	1434.61535	-1753.10253	1513.99471	1
167	H	71.84815	80.34387	66.35714	-714.67738	1819.09770	1898.36494	1
168	C	73.71729	80.49121	65.17969	446.99263	-555.77305	338.97221	1
169	H	74.26679	81.18450	65.86482	1953.68466	1892.25957	-161.67766	1
170	H	74.48929	79.82188	64.73739	-403.03785	2688.07032	-188.43591	1
171	C	72.95731	81.30442	64.05499	567.86262	335.74681	434.04421	1
172	H	72.53009	80.61907	63.28734	-1080.02275	1568.26081	-1948.78900	1
173	H	72.08947	81.85640	64.48369	-919.54108	2111.34692	1456.13463	1
174	C	73.96367	82.29227	63.42148	195.81897	173.33862	-745.11536	1
175	H	74.32812	83.08119	64.10950	1405.67949	-2301.21089	-390.08113	1
176	H	74.82042	81.81408	62.90645	-940.37328	-1118.32446	2299.72133	1
177	N	73.21064	83.07666	62.29356	319.26422	656.36007	-42.02424	1
178	H	73.78157	83.81542	61.79015	1961.03633	619.91968	1787.09422	1
179	H	72.83640	82.51122	61.47699	854.14343	-2156.80752	1429.08711	1
180	H	72.35654	83.63647	62.58299	1237.02905	-1378.50857	-1998.28500	1
181	C	73.88122	80.03611	68.26802	532.53319	-268.57236	517.55729	1
182	O	74.67565	80.88208	67.91383	266.16714	-290.73804	-558.88002	1
183	N	73.34900	79.87347	69.47064	-226.25352	640.49678	-270.32839	1
184	H	72.68933	79.10545	69.59282	2007.69063	-1035.27229	1523.50231	1
185	C	73.74752	80.77243	70.50209	-540.76542	-573.33303	49.50000	1
186	H	74.16713	81.66234	69.97616	-2374.20950	-1036.76023	843.75774	1
187	C	72.41108	81.08031	71.33635	-77.09082	666.87422	-415.84136	1
188	H	71.87749	80.09116	71.44884	-985.81834	617.19825	2463.91927	1
189	O	71.53002	82.01230	70.68531	293.29899	-391.65602	-477.80926	1
190	H	70.80370	81.42297	70.40990	2528.72714	-681.76262	-751.27122	1
191	C	72.92685	81.51832	72.75341	252.47363	-605.14473	440.05134	1
192	H	72.08300	81.70369	73.45830	-2052.65063	1456.49051	-1043.51830	1
193	H	73.57787	80.73757	73.22018	-2152.98800	-1661.97574	-161.70652	1
194	H	73.52822	82.45557	72.69779	-473.12726	-1584.27339	2165.61725	1
195	C	74.86949	80.07385	71.45459	360.36307	488.46713	505.10056	1
196	O	75.57888	80.82644	72.12361	-200.08817	-528.03552	-385.82850	1
197	N	74.79755	78.76193	71.46687	-597.54095	-226.44775	355.20479	1

198	H	74.06947	78.38963	70.85649	2179.23655	-1300.70981	-991.33835	1
199	C	75.83063	77.91602	71.93903	-687.68921	297.39807	-249.45179	1
200	H	75.58061	76.92808	71.49344	-349.16256	-2467.37713	-1101.72831	1
201	C	77.25755	78.47564	71.47390	672.47345	361.54328	-201.62880	1
202	H	77.38239	79.53094	71.81491	1541.41502	582.18425	2169.97026	1
203	H	78.06272	77.87548	71.95684	-2534.67717	60.25153	997.72295	1
204	C	77.37114	78.38723	69.94594	574.26774	-389.43119	-377.02542	1
205	C	77.70162	77.14729	69.32039	688.82679	-287.33580	-257.96133	1
206	H	77.85305	76.23394	69.92391	331.14182	1470.38163	2269.80013	1
207	C	77.14798	79.55382	69.15435	-383.52382	-675.04808	144.24917	1
208	H	76.85510	80.50836	69.62910	4.09847	1517.59662	2262.86397	1
209	C	77.83459	77.11243	67.93230	-134.76730	428.45285	-649.50303	1
210	H	78.09563	76.15373	67.45103	-903.23433	1600.49020	2011.53387	1
211	C	77.29594	79.46867	67.76845	-335.53281	-615.00040	-364.39058	1
212	H	77.11709	80.38067	67.17202	1596.45398	-1369.33862	1732.02659	1
213	C	77.65069	78.25834	67.10468	585.48547	-340.24194	-406.23938	1
214	O	77.81047	78.16987	65.69726	-419.15649	-173.04408	-511.94141	1
215	H	77.64441	79.11096	65.45163	-1071.84350	1559.71507	-1960.13012	1
216	C	75.88467	77.85771	73.56784	291.41878	-183.13091	710.72246	1
217	O	75.97234	76.76351	74.09517	379.87695	523.47396	-222.23622	1
218	N	75.87354	79.04374	74.14155	564.30591	373.09380	277.24371	1
219	H	75.83057	79.91853	73.56084	-120.59931	-2436.07824	-1214.35098	1
220	C	75.83446	79.09797	75.56157	404.07514	-299.37480	608.84009	1
221	H	76.00983	78.05947	75.92751	-1071.07882	-841.69025	2359.66467	1
222	C	76.93808	80.16183	75.98357	-683.12807	68.71770	-390.13096	1
223	H	77.90773	79.94887	75.48075	2068.88918	1596.58590	770.89603	1
224	H	76.64084	81.18111	75.64821	1379.86429	2342.49779	-179.85638	1
225	C	77.08114	80.10175	77.53322	-176.39967	537.49466	550.97268	1
226	H	76.09206	80.23980	78.02940	-396.28051	1942.22168	1869.33314	1
227	H	77.45186	79.10742	77.86847	-94.44700	586.00678	-2659.20016	1
228	C	78.09297	81.27400	77.93636	-291.69381	-718.18079	-150.72929	1
229	H	79.11973	81.21903	77.49435	-2303.38776	1089.76242	964.62032	1
230	H	77.68095	82.30165	77.77233	884.16729	2568.80533	-207.74283	1
231	N	78.18336	81.11950	79.32467	-594.49522	-252.81478	342.29276	1
232	H	77.40918	80.64378	79.76363	-1735.17426	2084.05705	-263.71605	1
233	C	79.11578	81.58042	80.05657	595.23177	-271.52487	442.22352	1
234	N	80.15583	82.27538	79.43137	585.53813	-424.79750	-105.81303	1
235	H	80.25687	82.53960	78.45232	959.88797	1327.56823	-2177.11905	1
236	H	80.92534	82.73507	79.91881	1578.48647	16.27378	-2220.76233	1
237	N	78.88255	81.27161	81.40274	-452.17763	-390.33541	-421.51853	1
238	H	78.09483	80.80263	81.84766	470.26107	1974.25629	-1817.92087	1
239	H	79.48722	81.58521	82.16283	1856.67307	-1573.97321	-1224.35416	1
240	C	74.41198	79.75496	76.04130	-531.47271	-581.45780	-55.06206	1
241	O	73.90849	80.72138	75.47679	-243.00837	192.73507	609.52485	1
242	N	73.96096	79.08508	77.08034	343.49288	-644.25607	38.09164	1
243	H	74.53285	78.33551	77.46276	-1691.16043	-1535.97525	-1484.73099	1
244	C	72.62369	79.33878	77.51603	542.66492	350.14337	454.42563	1
245	H	72.09497	79.57640	76.56554	1209.57979	-2396.95920	463.86744	1
246	C	72.04817	78.11641	78.34092	-737.14309	145.93010	242.71942	1
247	H	72.62715	78.01437	79.28401	-1050.18303	159.36419	-2509.06125	1
248	C	70.54726	78.46334	78.63809	-706.77696	-252.88343	-245.16230	1
249	H	70.03553	77.64276	79.19291	-1624.64039	-1665.49085	1417.86935	1
250	H	70.46283	79.38827	79.25968	2566.10521	598.51109	693.22305	1
251	H	69.96993	78.64014	77.70036	-1972.69758	107.10018	-1876.34312	1
252	C	72.04668	76.74151	77.58559	412.85148	672.58832	-27.69222	1
253	H	71.80724	75.90013	78.27699	1447.02277	1762.76533	-1490.78944	1
254	H	71.28664	76.70938	76.77028	1320.77379	-145.20455	2378.68491	1
255	H	73.03547	76.51862	77.12297	-1512.10848	1470.52031	1724.75147	1
256	C	72.65989	80.64166	78.51889	-607.11113	499.56689	73.73769	1
257	O	72.39779	80.52662	79.69026	357.97126	460.81534	356.68785	1
258	N	72.87270	81.71620	77.77655	536.55407	-368.62270	332.76306	1
259	H	73.07634	81.58747	76.75523	524.38866	2297.69985	1367.20941	1

260	C	73.16286	82.96912	78.36959	46.50277	-774.29190	-147.97904	1
261	H	72.99766	83.68396	77.53433	1676.51875	1883.29066	1032.55549	1
262	C	72.23148	83.24251	79.65450	-559.41456	-34.19198	-556.30433	1
263	H	72.48461	82.49392	80.45227	-64.66664	395.18769	2695.05373	1
264	H	72.45263	84.24625	80.09192	-2703.44278	-60.40056	333.79418	1
265	C	70.77677	83.12327	79.27916	-519.76435	377.31045	459.42366	1
266	H	70.64322	82.16869	78.72119	-1746.74323	1667.50644	-1261.73691	1
267	C	69.91396	83.06803	80.53377	570.95554	16.46261	-545.27700	1
268	H	68.82740	82.95305	80.28566	2391.58273	28.05277	-1305.07271	1
269	H	70.19886	82.20488	81.18983	175.75588	917.63458	2559.43867	1
270	H	70.01761	83.99993	81.14718	-1063.97851	-2155.34650	1283.00462	1
271	C	70.32777	84.27596	78.39248	193.76014	2.62946	-765.53141	1
272	H	69.24189	84.19408	78.12773	507.39394	-846.55087	2539.60089	1
273	H	70.47130	85.26539	78.89844	1337.57841	1818.19054	1526.01994	1
274	H	70.90192	84.30737	77.43093	1100.88635	-1172.91350	-2199.08909	1
275	C	74.70442	82.98316	78.85400	-549.21115	475.64486	-309.38218	1
276	O	75.31162	82.01785	79.23644	556.06106	-390.37755	-78.24250	1
277	O	75.29615	84.26831	78.91178	-572.27940	-310.19032	-209.75862	1
278	H	74.52408	84.80659	78.58213	-1380.08193	2212.14486	790.85944	1

Listing 74: C00074.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.5562	0.0000	300.0000
3	H	79.43042	79.80407	82.18581	-2043.14101	-1757.64893	399.89339		1
4	N	80.26650	79.38661	81.78143	426.75047	490.45733	-334.42467		1
5	H	79.90413	78.93429	80.94196	442.25559	-1110.30854	-2448.52907		1
6	C	81.30797	80.29430	81.49116	415.32972	-666.39213	83.73172		1
7	H	81.24935	81.12174	82.23039	879.32219	2491.00447	667.35213		1
8	C	82.69400	79.47212	81.55588	31.35357	477.41777	628.23362		1
9	H	82.68350	78.67332	80.77600	1168.38489	2240.25337	-1019.71136		1
10	H	83.55386	80.13860	81.30431	-360.43770	2534.90498	931.67112		1
11	C	82.85990	78.86376	82.92471	463.18208	512.70242	-382.34388		1
12	H	81.94590	78.26892	83.15119	1725.29117	1863.52247	-987.07854		1
13	C	84.06452	77.93187	82.95511	710.42801	-144.27427	-313.15367		1
14	H	84.19266	77.45453	83.96106	364.20195	-1033.13725	2494.72524		1
15	H	83.96934	77.10468	82.20501	2567.61904	335.80679	847.48802		1
16	H	85.01480	78.47993	82.72595	-2587.99029	680.92867	-512.16411		1
17	C	83.01880	79.93348	83.99628	268.17616	741.64379	-40.42634		1
18	H	83.19137	79.48242	85.00772	1283.54314	-1945.37420	-1411.27812		1
19	H	83.88771	80.60752	83.78029	-1258.57796	1317.15249	-2026.02085		1
20	H	82.10685	80.57972	84.07428	-2502.84526	909.80597	575.92391		1
21	C	81.05263	80.74878	79.94941	619.36578	-458.64843	-172.09273		1
22	O	80.68275	79.92695	79.10840	-81.40433	433.87611	522.34594		1
23	N	81.30237	82.03184	79.82100	175.23996	-622.20190	341.55523		1
24	H	81.62246	82.51181	80.66221	-876.57256	-303.22879	-2561.90213		1
25	C	81.24324	82.74736	78.60124	-571.88214	-534.10783	-106.15033		1
26	H	81.34104	83.79476	78.96188	-2713.20841	-16.25800	-248.80809		1
27	C	82.50487	82.29904	77.73648	166.60354	288.16399	-716.09568		1
28	H	82.39760	81.20911	77.48762	-2097.85574	1636.78449	-586.18044		1
29	O	83.77645	82.44873	78.40333	-317.80580	-363.38227	484.43082		1
30	H	84.07392	81.52105	78.45321	1863.74748	-1451.84923	1357.29467		1
31	C	82.34209	83.16092	76.43103	503.80731	517.99032	318.51606		1
32	H	83.18156	82.98169	75.71968	640.61020	-2157.10410	-1536.29104		1
33	H	81.39201	82.92384	75.88838	1687.88455	465.60692	2087.56452		1
34	H	82.33234	84.25228	76.65960	-1293.07895	-1899.88581	-1463.57452		1
35	C	79.81008	82.48902	77.82833	-153.07550	-733.68902	248.70981		1
36	O	79.75397	81.86289	76.74434	186.15459	-480.78787	-449.34387		1
37	N	78.85080	83.06507	78.49313	-487.53139	543.18517	42.03850		1
38	C	77.06835	80.51926	77.75918	-699.35871	69.34393	360.10701		1
39	H	76.93050	79.44883	77.49281	2.81126	-221.99807	-2715.58072		1

40	C	76.54539	80.74655	79.21764	-507.46439	-592.59194	122.07761	1
41	H	75.44570	80.56559	79.25980	-1975.08116	525.87560	-1801.71556	1
42	H	77.01233	80.01071	79.91370	1588.27743	-1913.22100	1113.83566	1
43	C	76.87831	82.20063	79.66767	-613.62442	-457.55993	-194.14490	1
44	H	76.40520	82.94273	78.98951	1707.54637	-721.27992	1996.92523	1
45	H	76.45718	82.38694	80.67820	758.23357	2100.81767	1560.55011	1
46	C	78.49328	82.39621	79.68196	-352.41524	704.96076	49.21465	1
47	H	78.82778	83.09133	80.49635	1714.76886	-2070.42778	443.35792	1
48	H	79.08108	81.43401	79.72575	1224.15040	1801.50881	1636.97633	1
49	C	76.29413	81.43799	76.71439	566.85117	537.05831	117.62814	1
50	O	75.09111	81.56553	76.69783	-550.26779	-406.08867	4.21666	1
51	N	77.19850	81.94790	75.85510	566.34832	-425.77725	180.18749	1
52	H	78.23677	81.78047	75.96937	644.44502	2646.80550	-52.73430	1
53	C	76.67762	82.83065	74.85258	612.34801	-281.48662	411.56221	1
54	H	75.76246	83.26215	75.31983	1667.23498	-1490.75142	1556.16753	1
55	C	77.83089	83.89382	74.61047	-714.45746	-175.43074	286.98927	1
56	H	78.73767	83.33583	74.24823	-787.09484	1763.03619	-1922.46060	1
57	O	78.30242	84.56060	75.82271	-429.46514	516.51932	-128.40526	1
58	H	78.62776	83.79217	76.32721	1981.82785	436.16847	-1818.18182	1
59	C	77.31108	84.86636	73.49788	630.79189	-468.94448	76.03230	1
60	H	78.06113	85.66060	73.27143	-1775.71861	2062.30353	131.89849	1
61	H	77.09284	84.33551	72.53680	-1855.14608	88.94118	1993.53760	1
62	H	76.37289	85.38048	73.81488	-1504.82350	-780.94249	-2132.90992	1
63	C	76.29197	81.99315	73.50599	288.57638	618.62814	-397.00270	1
64	O	75.81011	82.62093	72.55137	321.70495	-185.26452	574.37218	1
65	N	76.52947	80.71281	73.60509	-447.05792	-446.53431	367.76425	1
66	H	76.91472	80.49758	74.52308	350.31316	1975.63644	-1843.31522	1
67	C	76.43218	79.71433	72.60070	-511.23061	374.03917	-471.51480	1
68	H	76.04569	78.83578	73.16232	2234.79579	-898.70890	-1273.45190	1
69	C	75.44795	80.16074	71.42590	529.53781	-159.34528	563.72604	1
70	H	75.17531	79.23540	70.82834	654.59388	2347.94251	1217.51488	1
71	H	74.51249	80.51553	71.93866	-1526.55661	2103.42026	817.87394	1
72	O	75.91286	81.13359	70.48768	-554.84278	14.12789	399.58769	1
73	H	75.82994	81.97590	71.08579	1297.06236	2061.84854	1220.68812	1
74	C	77.95192	79.40692	72.09031	-662.15484	-412.13544	123.62687	1
75	O	78.89301	80.16105	72.19530	-540.01537	-317.05804	274.91456	1
76	N	77.92273	78.17943	71.57869	-202.76299	-690.00100	-131.49145	1
77	H	77.03790	77.67291	71.57259	-702.62132	-2617.37191	281.70413	1
78	C	79.10642	77.62388	71.02613	-491.73914	576.34187	222.73509	1
79	H	79.83715	78.46675	71.03065	1977.17978	-1823.58850	-434.68928	1
80	C	79.54173	76.45252	72.01980	-649.50797	-328.66843	306.11224	1
81	H	78.67978	75.78091	72.22341	2075.07803	1452.16490	-1004.45904	1
82	C	80.77566	75.63731	71.50912	-615.18735	-489.99689	-70.96352	1
83	H	81.13509	74.91489	72.28016	-1226.32661	-1724.38906	-1716.47170	1
84	H	80.53097	75.04636	70.59201	2381.64273	-969.84735	900.46860	1
85	H	81.63082	76.30695	71.25414	2122.74991	1702.23946	-141.36228	1
86	C	80.03826	77.14824	73.33208	-501.86074	-479.61276	-376.42482	1
87	H	80.21523	76.41099	74.15028	993.79261	-2246.95401	-1177.81305	1
88	H	80.99191	77.70255	73.16845	42.71279	-626.15391	-2651.37258	1
89	H	79.28923	77.89104	73.69766	-2026.39012	-1590.33709	-887.82922	1
90	C	78.81158	77.02559	69.53595	-672.89153	382.57394	-156.34072	1
91	O	79.62884	76.31261	69.00544	410.04627	221.86223	500.35950	1
92	N	77.66179	77.44622	69.04478	-378.11782	-443.79414	-441.10984	1
93	H	77.00756	78.07135	69.56210	2404.15973	-568.14894	1149.30085	1
94	C	77.18030	76.98414	67.76648	-544.54484	466.16019	331.29119	1
95	H	77.92868	77.32845	67.01713	-1409.80988	-170.17955	2325.32679	1
96	C	77.15815	75.39618	67.85892	-184.48284	116.78282	-758.89137	1
97	H	77.67365	75.06778	68.79160	1893.78641	1861.14652	611.04528	1
98	H	76.11430	75.01351	67.92538	-2170.79665	-974.19311	1327.50117	1
99	C	77.89149	74.81887	66.60978	389.51668	672.81878	-138.49152	1
100	H	77.47739	75.23835	65.66827	510.64577	1933.03327	1851.02484	1
101	H	78.95131	75.15901	66.61323	-2302.30869	-1105.72939	-948.89774	1

102	C	77.84049	73.24458	66.53773	-559.93427	-126.34590	542.30857	1
103	O	78.18821	72.68599	65.52973	-670.36003	-111.83166	76.36448	1
104	N	77.42040	72.65355	67.67654	-216.06729	-537.07037	446.51379	1
105	H	77.14521	73.07308	68.57239	-1251.96487	1074.12894	-2168.52500	1
106	H	77.37159	71.63776	67.81054	-2451.83023	-720.73851	944.84612	1
107	C	75.77690	77.75995	67.72802	546.24052	-563.88337	-85.11809	1
108	O	75.44220	78.38934	68.72002	71.70702	-307.40463	606.69673	1
109	N	75.13017	77.63809	66.56614	479.90863	-504.50129	222.86849	1
110	C	73.95904	78.41927	66.30095	75.51268	-600.91904	506.73700	1
111	H	74.13515	79.40982	66.77747	-2033.61562	1795.30103	254.89480	1
112	C	73.91207	78.39797	64.71902	523.79067	517.99274	284.45581	1
113	H	72.90353	78.63553	64.31204	1599.61665	-1127.00911	1895.98173	1
114	H	74.61915	79.13564	64.27770	-1881.83093	1275.82488	-1501.55016	1
115	C	74.36424	76.93145	64.42792	-600.05639	-404.05026	316.64485	1
116	H	73.52768	76.21927	64.62112	-2597.05260	496.36221	657.73249	1
117	H	74.69384	76.76308	63.37784	-1666.24518	1294.38985	-1723.90591	1
118	C	75.52875	76.73941	65.48829	493.57570	-129.95376	-602.56394	1
119	H	75.60717	75.71403	65.91743	-1469.08415	-637.84797	2204.22581	1
120	H	76.53428	77.08395	65.15027	-1038.97840	1068.88701	-2280.71789	1
121	C	72.66966	77.62325	66.95393	188.88100	241.05089	-727.87821	1
122	O	72.13340	76.72780	66.34125	531.88613	-49.19943	427.07960	1
123	N	72.34540	78.18904	68.10020	708.14833	26.93417	-179.73509	1
124	H	72.96117	78.93401	68.42677	-2232.69501	-1179.09831	1023.94816	1
125	C	71.33641	77.69216	68.96693	-738.32412	259.92548	104.42456	1
126	H	70.96398	78.59473	69.49912	2028.89123	1260.02983	1311.33324	1
127	C	70.23188	76.90271	68.14903	-258.65678	-345.52513	661.28459	1
128	H	70.68010	75.99801	67.66550	-1826.06090	-1801.46097	-918.64554	1
129	C	69.10860	76.49546	69.16527	-541.23400	531.92970	-218.41428	1
130	H	68.29752	75.91284	68.66962	1311.73218	-2219.18200	882.19023	1
131	H	69.51541	75.86389	69.99001	-1048.71298	1223.58118	-2196.97971	1
132	H	68.63681	77.38966	69.63514	419.06414	1903.92898	1903.44670	1
133	C	69.57763	77.82878	67.06541	-423.86431	152.66566	-648.55262	1
134	H	68.74892	77.31043	66.52832	105.68386	-2342.50080	1387.51238	1
135	H	69.15716	78.75866	67.51462	-1695.63603	-1484.73621	-1531.02793	1
136	H	70.33041	78.13388	66.29841	-1853.57121	-487.39031	1936.59343	1
137	C	72.00790	76.59866	70.00539	539.71428	-510.58232	267.58633	1
138	O	72.64298	75.63700	69.64098	-15.93758	-278.34085	-624.49402	1
139	N	71.55371	76.90941	71.21036	-676.81886	12.05292	276.17960	1
140	H	70.98494	77.75101	71.28704	-1694.44250	-373.84189	-2100.66098	1
141	C	72.02030	76.26582	72.38890	412.33078	-664.70360	108.35451	1
142	H	71.37336	76.68868	73.19064	1765.77476	1294.44366	1621.76594	1
143	C	71.79281	74.70857	72.17575	-179.66635	-721.95667	-264.73915	1
144	H	70.73091	74.52223	71.89901	-607.34922	2587.87032	-598.10018	1
145	H	72.39247	74.34745	71.30251	-359.69332	-1479.13954	-2259.74260	1
146	C	72.16465	73.91003	73.46725	-240.01076	616.02425	431.85322	1
147	H	73.27325	73.89262	73.59322	-1359.17131	782.54425	2227.99181	1
148	H	71.74509	74.41537	74.36697	-820.36667	85.81767	-2596.78715	1
149	C	71.65127	72.41467	73.42152	-513.07015	236.18570	-551.87280	1
150	H	70.53993	72.35428	73.35714	1816.11944	-1183.11722	-1650.94321	1
151	H	72.04564	71.87142	72.53234	-1800.04429	-1361.53473	1526.34643	1
152	C	72.18750	71.81370	74.74443	726.08972	-253.19732	-179.64713	1
153	H	73.28480	71.90295	74.88322	1224.27271	-456.51798	-2390.90304	1
154	H	71.66719	72.16697	75.66060	1206.40339	-1150.93514	-2154.90344	1
155	N	71.93043	70.27576	74.73034	329.70796	-633.68968	-155.67358	1
156	H	72.18556	69.82149	75.65429	1348.31305	1938.76845	1359.00643	1
157	H	70.93241	69.93894	74.60157	2096.92035	1446.54551	-966.48890	1
158	H	72.46661	69.67867	74.03520	-1197.07217	-2303.53719	827.28733	1
159	C	73.58362	76.68050	72.61243	-378.01186	-556.17301	-413.96481	1
160	O	74.18032	77.51396	71.97136	-409.44433	-307.55053	-453.30833	1
161	N	74.00891	76.04052	73.70299	-429.02477	524.70884	274.08502	1
162	H	73.35860	75.45708	74.22802	1706.34263	-1425.96036	1574.38926	1
163	C	75.41730	75.79428	73.78889	-45.25864	-626.22952	478.93267	1

164	H	75.81598	76.16465	72.81639	1988.63164	570.90773	1772.87287	1
165	C	75.85802	76.68985	75.01129	551.77128	-20.49526	-564.54996	1
166	H	75.39713	77.69996	74.93423	1434.61535	-1753.10253	1513.99471	1
167	H	75.49378	76.27732	75.97719	-714.67738	1819.09770	1898.36494	1
168	C	77.42502	76.78416	74.98435	446.99263	-555.77305	338.97221	1
169	H	77.89726	75.78633	75.13198	1953.68466	1892.25957	-161.67766	1
170	H	77.78655	77.16821	74.00211	-403.03785	2688.07032	-188.43591	1
171	C	77.75285	77.76886	76.15295	567.86262	335.74681	434.04421	1
172	H	77.25562	78.75057	75.98288	-1080.02275	1568.26081	-1948.78900	1
173	H	77.33201	77.38470	77.10784	-919.54108	2111.34692	1456.13463	1
174	C	79.33053	77.97237	76.29762	195.81897	173.33862	-745.11536	1
175	H	79.89077	77.01871	76.46130	1405.67949	-2301.21089	-390.08113	1
176	H	79.78998	78.55658	75.46321	-940.37328	-1118.32446	2299.72133	1
177	N	79.47842	78.76340	77.48120	319.26422	656.36007	-42.02424	1
178	H	79.89185	79.70482	77.39253	1961.03633	619.91968	1787.09422	1
179	H	78.16439	80.70846	77.69985	854.14343	-2156.80752	1429.08711	1
180	H	79.99288	78.35878	78.27457	1237.02905	-1378.50857	-1998.28500	1
181	C	75.66447	74.18550	74.02522	532.53319	-268.57236	517.55729	1
182	O	75.88616	73.51310	73.05142	266.16714	-290.73804	-558.88002	1
183	N	75.49742	73.80767	75.28247	-226.25352	640.49678	-270.32839	1
184	H	75.17331	74.42952	76.03671	2007.69063	-1035.27229	1523.50231	1
185	C	75.97865	72.54330	75.72102	-540.76542	-573.33303	49.50000	1
186	H	75.93360	71.82612	74.87149	-2374.20950	-1036.76023	843.75774	1
187	C	77.46711	72.75979	76.28225	-77.09082	666.87422	-415.84136	1
188	H	77.44663	73.62444	77.00158	-985.81834	617.19825	2463.91927	1
189	O	78.46709	73.09757	75.30597	293.29899	-391.65602	-477.80926	1
190	H	78.78206	73.95815	75.64799	2528.72714	-681.76262	-751.27122	1
191	C	77.74371	71.43835	77.08707	252.47363	-605.14473	440.05134	1
192	H	78.74362	71.46531	77.57908	-2052.65063	1456.49051	-1043.51830	1
193	H	76.98884	71.27331	77.89146	-2152.98800	-1661.97574	-161.70652	1
194	H	77.72849	70.54385	76.42216	-473.12726	-1584.27339	2165.61725	1
195	C	74.94936	72.30502	76.97250	360.36307	488.46713	505.10056	1
196	O	74.48816	73.31253	77.48467	-200.08817	-528.03552	-385.82850	1
197	N	74.83371	71.03004	77.28408	-597.54095	-226.44775	355.20479	1
198	H	75.36757	70.38184	76.70296	2179.23655	-1300.70981	-991.33835	1
199	C	74.13440	70.51678	78.39967	-687.68921	297.39807	-249.45179	1
200	H	74.62124	69.53908	78.60742	-349.16256	-2467.37713	-1101.72831	1
201	C	74.17392	71.55099	79.61779	672.47345	361.54328	-201.62880	1
202	H	73.79205	72.54949	79.27451	1541.41502	582.18425	2169.97026	1
203	H	73.48674	71.19640	80.42089	-2534.67717	60.25153	997.72295	1
204	C	75.60217	71.68081	80.16905	574.26774	-389.43119	-377.02542	1
205	C	76.14546	70.65776	81.00250	688.82679	-287.33580	-257.96133	1
206	H	75.55937	69.75101	81.23815	331.14182	1470.38163	2269.80013	1
207	C	76.37219	72.84328	79.86329	-383.52382	-675.04808	144.24917	1
208	H	75.95713	73.63082	79.20548	4.09847	1517.59662	2262.86397	1
209	C	77.42635	70.83403	81.52670	-134.76730	428.45285	-649.50303	1
210	H	77.84230	70.04843	82.18144	-903.23433	1600.49020	2011.53387	1
211	C	77.65033	72.97487	80.41176	-335.53281	-615.00040	-364.39058	1
212	H	78.23080	73.88364	80.17506	1596.45398	-1369.33862	1732.02659	1
213	C	78.22255	71.98668	81.26503	585.48547	-340.24194	-406.23938	1
214	O	79.51734	72.11236	81.83348	-419.15649	-173.04408	-511.94141	1
215	H	79.75950	73.00836	81.50053	-1071.84350	1559.71507	-1960.13012	1
216	C	72.55197	70.34502	78.00265	291.41878	-183.13091	710.72246	1
217	O	71.84181	71.29798	77.76591	379.87695	523.47396	-222.23622	1
218	N	72.22011	69.05698	78.02673	564.30591	373.09380	277.24371	1
219	H	72.92580	68.35742	78.25181	-120.59931	-2436.07824	-1214.35098	1
220	C	70.89992	68.73812	77.60985	404.07514	-299.37480	608.84009	1
221	H	70.47349	69.73237	77.32460	-1071.07882	-841.69025	2359.66467	1
222	C	71.01200	67.69837	76.41536	-683.12807	68.71770	-390.13096	1
223	H	71.86114	67.95367	75.74424	2068.88918	1596.58590	770.89603	1
224	H	71.22901	66.67160	76.78490	1379.86429	2342.49779	-179.85638	1
225	C	69.65569	67.73755	75.64728	-176.39967	537.49466	550.97268	1

226	H	68.84981	67.23302	76.22598	-396.28051	1942.22168	1869.33314	1
227	H	69.30608	68.78332	75.49821	-94.44700	586.00678	-2659.20016	1
228	C	69.92234	67.01912	74.24526	-291.69381	-718.18079	-150.72929	1
229	H	70.69904	67.50051	73.59743	-2303.38776	1089.76242	964.62032	1
230	H	70.15757	65.92595	74.30157	884.16729	2568.80533	-207.74283	1
231	N	68.68681	67.15985	73.59723	-594.49522	-252.81478	342.29276	1
232	H	67.95070	67.61392	74.11517	-1735.17426	2084.05705	-263.71605	1
233	C	68.44264	66.75335	72.41776	595.23177	-271.52487	442.22352	1
234	N	69.47904	66.12515	71.71808	585.53813	-424.79750	-105.81303	1
235	H	70.43307	65.92518	72.01570	959.88797	1327.56823	-2177.11905	1
236	H	69.40251	65.75205	70.77139	1578.48647	16.27378	-2220.76233	1
237	N	67.11970	67.03656	72.05030	-452.17763	-390.33541	-421.51853	1
238	H	66.36483	67.49282	72.56035	470.26107	1974.25629	-1817.92087	1
239	H	66.72954	66.78605	71.14086	1856.67307	-1573.97321	-1224.35416	1
240	C	70.02964	67.99167	78.79586	-531.47271	-581.45780	-55.06206	1
241	O	68.91640	68.41247	79.03078	-243.00837	192.73507	609.52485	1
242	N	70.60821	66.88405	79.25282	343.49288	-644.25607	38.09164	1
243	H	71.54945	66.81074	78.86762	-1691.16043	-1535.97525	-1484.73099	1
244	C	70.24203	66.22389	80.50873	542.66492	350.14337	454.42563	1
245	H	70.83862	65.28539	80.42705	1209.57979	-2396.95920	463.86744	1
246	C	70.68519	67.08545	81.67530	-737.14309	145.93010	242.71942	1
247	H	70.16317	68.06525	81.59408	-1050.18303	159.36419	-2509.06125	1
248	C	70.31440	66.45409	83.00502	-706.77696	-252.88343	-245.16230	1
249	H	70.68565	67.06088	83.87551	-1624.64039	-1665.49085	1417.86935	1
250	H	69.19291	66.35872	83.11518	2566.10521	598.51109	693.22305	1
251	H	70.74790	65.42159	83.10935	-1972.69758	107.10018	-1876.34312	1
252	C	72.18091	67.34844	81.64204	412.85148	672.58832	-27.69222	1
253	H	72.51389	67.97190	82.51596	1447.02277	1762.76533	-1490.78944	1
254	H	72.76773	66.38978	81.67582	1320.77379	-145.20455	2378.68491	1
255	H	72.48411	67.89293	80.70640	-1512.10848	1470.52031	1724.75147	1
256	C	68.61173	65.92091	80.53057	-607.11113	499.56689	73.73769	1
257	O	67.90969	66.29394	81.44454	357.97126	460.81534	356.68785	1
258	N	68.27252	65.17110	79.49534	536.55407	-368.62270	332.76306	1
259	H	69.00027	64.94679	78.81941	524.38866	2297.69985	1367.20941	1
260	C	66.93590	64.71700	79.39555	46.50277	-774.29190	-147.97904	1
261	H	66.47218	64.95166	80.38168	1676.51875	1883.29066	1032.55549	1
262	C	66.22111	65.48199	78.16284	-559.41456	-34.19198	-556.30433	1
263	H	66.74635	65.22309	77.21296	-64.66664	395.18769	2695.05373	1
264	H	65.17101	65.12458	78.03994	-2703.44278	-60.40056	333.79418	1
265	C	66.26252	66.96670	78.39835	-519.76435	377.31045	459.42366	1
266	H	67.32848	67.27922	78.59047	-1746.74323	1667.50644	-1261.73691	1
267	C	65.76057	67.70561	77.16446	570.95554	16.46261	-545.27700	1
268	H	65.81481	68.81666	77.29980	2391.58273	28.05277	-1305.07271	1
269	H	66.36642	67.45205	76.25626	175.75588	917.63458	2559.43867	1
270	H	64.69441	67.44914	76.93425	-1063.97851	-2155.34650	1283.00462	1
271	C	65.44431	67.36168	79.61912	193.76014	2.62946	-765.53141	1
272	H	65.37595	68.47541	79.72562	507.39394	-846.55087	2539.60089	1
273	H	64.39703	66.96564	79.56678	1337.57841	1818.19054	1526.01994	1
274	H	65.91162	66.97069	80.56457	1100.88635	-1172.91350	-2199.08909	1
275	C	66.97030	63.14873	79.01302	-549.21115	475.64486	-309.38218	1
276	O	67.91458	62.60906	78.49949	556.06106	-390.37755	-78.24250	1
277	O	65.75429	62.44972	79.20411	-572.27940	-310.19032	-209.75862	1
278	H	65.22067	63.18042	79.62310	-1380.08193	2212.14486	790.85944	1

Listing 75: C00075.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.5493	0.0000	300.0000
3	H	64.05977	78.49321	79.57454	-2043.14101	-1757.64893	399.89339		1
4	N	64.19204	78.57048	78.56809	426.75047	490.45733	-334.42467		1
5	H	63.23825	78.74533	78.25760	442.25559	-1110.30854	-2448.52907		1

6	C	65.10950	79.58213	78.19322	415.32972	-666.39213	83.73172	1
7	H	65.94767	79.39620	78.89930	879.32219	2491.00447	667.35213	1
8	C	65.54297	79.37197	76.65398	31.35357	477.41777	628.23362	1
9	H	64.67813	79.60721	75.98862	1168.38489	2240.25337	-1019.71136	1
10	H	66.35249	80.08583	76.36953	-360.43770	2534.90498	931.67112	1
11	C	65.99447	77.95149	76.44319	463.18208	512.70242	-382.34388	1
12	H	65.19541	77.27202	76.81777	1725.29117	1863.52247	-987.07854	1
13	C	66.20926	77.68478	74.95826	710.42801	-144.27427	-313.15367	1
14	H	66.53579	76.62964	74.76967	364.20195	-1033.13725	2494.72524	1
15	H	65.27229	77.85348	74.36731	2567.61904	335.80679	847.48802	1
16	H	66.99562	78.35869	74.52919	-2587.99029	680.92867	-512.16411	1
17	C	67.27890	77.65386	77.20513	268.17616	741.64379	-40.42634	1
18	H	67.63637	76.60837	77.01873	1283.54314	-1945.37420	-1411.27812	1
19	H	68.10680	78.34727	76.90615	-1258.57796	1317.15249	-2026.02085	1
20	H	67.13736	77.76138	78.31123	-2502.84526	909.80597	575.92391	1
21	C	64.36599	80.97893	78.50354	619.36578	-458.64843	-172.09273	1
22	O	63.66861	81.10847	79.51751	-81.40433	433.87611	522.34594	1
23	N	64.75409	81.91078	77.66518	175.23996	-622.20190	341.55523	1
24	H	65.34990	81.60214	76.89866	-876.57256	-303.22879	-2561.90213	1
25	C	63.96541	83.09142	77.42217	-571.88214	-534.10783	-106.15033	1
26	H	63.14439	82.74984	76.75381	-2713.20841	-16.25800	-248.80809	1
27	C	63.37291	83.63369	78.80279	166.60354	288.16399	-716.09568	1
28	H	64.10601	83.34400	79.61126	-2097.85574	1636.78449	-586.18044	1
29	O	62.13524	83.04931	79.21079	-317.80580	-363.38227	484.43082	1
30	H	62.49864	82.20776	79.69148	1863.74748	-1451.84923	1357.29467	1
31	C	63.35412	85.19314	78.61040	503.80731	517.99032	318.51606	1
32	H	63.04068	85.71598	79.54366	640.61020	-2157.10410	-1536.29104	1
33	H	64.35345	85.59481	78.32212	1687.88455	465.60692	2087.56452	1
34	H	62.63844	85.48982	77.80822	-1293.07895	-1899.88581	-1463.57452	1
35	C	64.94496	84.11118	76.62942	-153.07550	-733.68902	248.70981	1
36	O	64.41881	84.72306	75.73612	186.15459	-480.78787	-449.34387	1
37	N	66.18941	84.25087	77.11961	-487.53139	543.18517	42.03850	1
38	C	67.17076	84.98667	76.39111	-699.35871	69.34393	360.10701	1
39	H	66.62624	85.72994	75.76359	2.81126	-221.99807	-2715.58072	1
40	C	68.06986	85.57141	77.56268	-507.46439	-592.59194	122.07761	1
41	H	69.07950	85.88674	77.21561	-1975.08116	525.87560	-1801.71556	1
42	H	67.59917	86.46274	78.03464	1588.27743	-1913.22100	1113.83566	1
43	C	68.09767	84.35796	78.54346	-613.62442	-457.55993	-194.14490	1
44	H	68.78134	83.55386	78.17593	1707.54637	-721.27992	1996.92523	1
45	H	68.43714	84.62042	79.57066	758.23357	2100.81767	1560.55011	1
46	C	66.57579	83.90702	78.48404	-352.41524	704.96076	49.21465	1
47	H	66.39854	82.81738	78.63668	1714.76886	-2070.42778	443.35792	1
48	H	65.89481	84.48168	79.15343	1224.15040	1801.50881	1636.97633	1
49	C	68.14009	83.98951	75.50739	566.85117	537.05831	117.62814	1
50	O	68.92882	84.47716	74.73263	-550.26779	-406.08867	4.21666	1
51	N	67.93219	82.71271	75.80683	566.34832	-425.77725	180.18749	1
52	H	67.20051	82.56279	76.49934	644.44502	2646.80550	-52.73430	1
53	C	68.91440	81.71185	75.55604	612.34801	-281.48662	411.56221	1
54	H	68.43071	80.79271	75.95243	1667.23498	-1490.75142	1556.16753	1
55	C	69.13249	81.64719	73.97828	-714.45746	-175.43074	286.98927	1
56	H	69.48654	82.65521	73.61486	-787.09484	1763.03619	-1922.46060	1
57	O	67.94422	81.37933	73.19859	-429.46514	516.51932	-128.40526	1
58	H	67.80816	82.24602	72.77023	1981.82785	436.16847	-1818.18182	1
59	C	70.27667	80.58036	73.82884	630.79189	-468.94448	76.03230	1
60	H	70.64955	80.53370	72.77893	-1775.71861	2062.30353	131.89849	1
61	H	71.16966	80.78931	74.49289	-1855.14608	88.94118	1993.53760	1
62	H	69.90895	79.56080	74.08953	-1504.82350	-780.94249	-2132.90992	1
63	C	70.22118	82.10297	76.46031	288.57638	618.62814	-397.00270	1
64	O	70.18270	81.82503	77.66047	321.70495	-185.26452	574.37218	1
65	N	71.14327	82.73117	75.78010	-447.05792	-446.53431	367.76425	1
66	H	70.89332	82.94535	74.81619	350.31316	1975.63644	-1843.31522	1
67	C	72.49032	82.90826	76.19821	-511.23061	374.03917	-471.51480	1

68	H	72.86107	83.62165	75.42721	2234.79579	-898.70890	-1273.45190	1
69	C	72.49048	83.52624	77.67367	529.53781	-159.34528	563.72604	1
70	H	73.41508	84.15091	77.80427	654.59388	2347.94251	1217.51488	1
71	H	71.61954	84.23411	77.69659	-1526.55661	2103.42026	817.87394	1
72	O	72.42384	82.58602	78.75386	-554.84278	14.12789	399.58769	1
73	H	71.49006	82.18594	78.54397	1297.06236	2061.84854	1220.68812	1
74	C	73.27510	81.48967	76.11282	-662.15484	-412.13544	123.62687	1
75	O	72.86873	80.53260	75.48605	-540.01537	-317.05804	274.91456	1
76	N	74.45666	81.62243	76.71274	-202.76299	-690.00100	-131.49145	1
77	H	74.62382	82.51720	77.16696	-702.62132	-2617.37191	281.70413	1
78	C	75.40080	80.51399	76.79050	-491.73914	576.34187	222.73509	1
79	H	74.77996	79.65614	76.43175	1977.17978	-1823.58850	-434.68928	1
80	C	76.58959	80.80457	75.88027	-649.50797	-328.66843	306.11224	1
81	H	77.10086	81.70914	76.27949	2075.07803	1452.16490	-1004.45904	1
82	C	77.59430	79.67054	75.86694	-615.18735	-489.99689	-70.96352	1
83	H	78.51140	79.93385	75.27121	-1226.32661	-1724.38906	-1716.47170	1
84	H	77.93638	79.40830	76.91709	2381.64273	-969.84735	900.46860	1
85	H	77.17078	78.72456	75.41595	2122.74991	1702.23946	-141.36228	1
86	C	76.14110	81.11896	74.46560	-501.86074	-479.61276	-376.42482	1
87	H	77.00847	81.37563	73.79761	993.79261	-2246.95401	-1177.81305	1
88	H	75.60350	80.23860	73.99957	42.71279	-626.15391	-2651.37258	1
89	H	75.42800	81.98855	74.44514	-2026.39012	-1590.33709	-887.82922	1
90	C	75.88854	80.39021	78.36930	-672.89153	382.57394	-156.34072	1
91	O	76.92467	79.82517	78.64186	410.04627	221.86223	500.35950	1
92	N	74.98586	80.87087	79.20654	-378.11782	-443.79414	-441.10984	1
93	H	74.14375	81.31224	78.83189	2404.15973	-568.14894	1149.30085	1
94	C	75.18906	80.63819	80.60366	-544.54484	466.16019	331.29119	1
95	H	76.30229	80.66621	80.67473	-1409.80988	-170.17955	2325.32679	1
96	C	74.45541	81.83342	81.34637	-184.48284	116.78282	-758.89137	1
97	H	74.60123	82.78376	80.78433	1893.78641	1861.14652	611.04528	1
98	H	73.35444	81.66545	81.36683	-2170.79665	-974.19311	1327.50117	1
99	C	75.02407	81.95261	82.79421	389.51668	672.81878	-138.49152	1
100	H	74.84457	81.00682	83.35813	510.64577	1933.03327	1851.02484	1
101	H	76.13297	82.03756	82.76358	-2302.30869	-1105.72939	-948.89774	1
102	C	74.43462	83.16698	83.60670	-559.93427	-126.34590	542.30857	1
103	O	74.81349	83.36612	84.73220	-670.36003	-111.83166	76.36448	1
104	N	73.52685	83.90121	82.92814	-216.06729	-537.07037	446.51379	1
105	H	73.15260	83.77029	81.98106	-1251.96487	1074.12894	-2168.52500	1
106	H	73.04215	84.71620	83.32008	-2451.83023	-720.73851	944.84612	1
107	C	74.63247	79.21799	81.18250	546.24052	-563.88337	-85.11809	1
108	O	74.89403	79.02838	82.34701	71.70702	-307.40463	606.69673	1
109	N	73.95541	78.39255	80.36656	479.90863	-504.50129	222.86849	1
110	C	73.34692	77.21289	80.89918	75.51268	-600.91904	506.73700	1
111	H	73.03038	77.45445	81.94028	-2033.61562	1795.30103	254.89480	1
112	C	72.17584	76.94738	79.85686	523.79067	517.99274	284.45581	1
113	H	71.79090	75.90376	79.89745	1599.61665	-1127.00911	1895.98173	1
114	H	71.30734	77.62044	80.03371	-1881.83093	1275.82488	-1501.55016	1
115	C	72.89657	77.29036	78.51682	-600.05639	-404.05026	316.64485	1
116	H	73.56546	76.45874	78.19796	-2597.05260	496.36221	657.73249	1
117	H	72.20117	77.48375	77.66907	-1666.24518	1294.38985	-1723.90591	1
118	C	73.73734	78.57175	78.93816	493.57570	-129.95376	-602.56394	1
119	H	74.74047	78.64013	78.45622	-1469.08415	-637.84797	2204.22581	1
120	H	73.19953	79.54285	78.82652	-1038.97840	1068.88701	-2280.71789	1
121	C	74.36977	75.92969	80.84412	188.88100	241.05089	-727.87821	1
122	O	73.95597	74.84711	81.18980	531.88613	-49.19943	427.07960	1
123	N	75.60228	76.25310	80.45973	708.14833	26.93417	-179.73509	1
124	H	75.68763	77.24635	80.24642	-2232.69501	-1179.09831	1023.94816	1
125	C	76.58061	75.28018	79.97729	-738.32412	259.92548	104.42456	1
126	H	77.53093	75.86256	80.02485	2028.89123	1260.02983	1311.33324	1
127	C	76.56171	74.02875	80.83401	-258.65678	-345.52513	661.28459	1
128	H	75.58617	73.51245	80.64784	-1826.06090	-1801.46097	-918.64554	1
129	C	77.67813	73.07450	80.45035	-541.23400	531.92970	-218.41428	1

130	H	77.64333	72.12771	81.05548	1311.73218	-2219.18200	882.19023	1
131	H	77.60681	72.78019	79.36511	-1048.71298	1223.58118	-2196.97971	1
132	H	78.69209	73.53363	80.60730	419.06414	1903.92898	1903.44670	1
133	C	76.62183	74.34414	82.31739	-423.86431	152.66566	-648.55262	1
134	H	76.61588	73.41145	82.94498	105.68386	-2342.50080	1387.51238	1
135	H	77.54595	74.92562	82.58432	-1695.63603	-1484.73621	-1531.02793	1
136	H	75.73109	74.96286	82.62583	-1853.57121	-487.39031	1936.59343	1
137	C	76.16594	74.87248	78.42060	539.71428	-510.58232	267.58633	1
138	O	75.92835	73.72321	78.13222	-15.93758	-278.34085	-624.49402	1
139	N	76.15838	75.93273	77.62571	-676.81886	12.05292	276.17960	1
140	H	76.43846	76.82558	78.02829	-1694.44250	-373.84189	-2100.66098	1
141	C	76.07398	75.68627	76.22617	412.33078	-664.70360	108.35451	1
142	H	75.58493	74.68926	76.12098	1765.77476	1294.44366	1621.76594	1
143	C	75.29608	76.90249	75.58171	-179.66635	-721.95667	-264.73915	1
144	H	74.29071	77.03355	76.04116	-607.34922	2587.87032	-598.10018	1
145	H	75.84070	77.85864	75.76938	-359.69332	-1479.13954	-2259.74260	1
146	C	75.18785	76.60171	74.04941	-240.01076	616.02425	431.85322	1
147	H	76.18828	76.36139	73.62109	-1359.17131	782.54425	2227.99181	1
148	H	74.55442	75.70652	73.85939	-820.36667	85.81767	-2596.78715	1
149	C	74.58176	77.88816	73.36008	-513.07015	236.18570	-551.87280	1
150	H	73.56586	78.11754	73.75865	1816.11944	-1183.11722	-1650.94321	1
151	H	75.20750	78.79192	73.58533	-1800.04429	-1361.53473	1526.34643	1
152	C	74.53607	77.61065	71.83897	726.08972	-253.19732	-179.64713	1
153	H	75.52820	77.46618	71.36565	1224.27271	-456.51798	-2390.90304	1
154	H	73.85273	76.79154	71.53811	1206.40339	-1150.93514	-2154.90344	1
155	N	73.95154	78.89247	71.15865	329.70796	-633.68968	-155.67358	1
156	H	73.85533	78.84553	70.10333	1348.31305	1938.76845	1359.00643	1
157	H	72.97395	79.19018	71.44637	2096.92035	1446.54551	-966.48890	1
158	H	74.49958	79.79365	71.27839	-1197.07217	-2303.53719	827.28733	1
159	C	77.59862	75.74118	75.58877	-378.01186	-556.17301	-413.96481	1
160	O	78.33368	76.68539	75.74691	-409.44433	-307.55053	-453.30833	1
161	N	77.76864	74.65322	74.85359	-429.02477	524.70884	274.08502	1
162	H	77.02264	73.96039	74.82316	1706.34263	-1425.96036	1574.38926	1
163	C	78.91146	74.54362	74.01054	-45.25864	-626.22952	478.93267	1
164	H	79.26148	75.60140	73.96045	1988.63164	570.90773	1772.87287	1
165	C	79.94076	73.59967	74.75440	551.77128	-20.49526	-564.54996	1
166	H	79.90601	73.78087	75.85215	1434.61535	-1753.10253	1513.99471	1
167	H	79.63825	72.53728	74.61916	-714.67738	1819.09770	1898.36494	1
168	C	81.39459	73.81484	74.21801	446.99263	-555.77305	338.97221	1
169	H	81.43600	73.78833	73.10603	1953.68466	1892.25957	-161.67766	1
170	H	81.79556	74.80898	74.51719	-403.03785	2688.07032	-188.43591	1
171	C	82.23298	72.63176	74.85160	567.86262	335.74681	434.04421	1
172	H	82.20464	72.68423	75.96510	-1080.02275	1568.26081	-1948.78900	1
173	H	81.77956	71.64757	74.59071	-919.54108	2111.34692	1456.13463	1
174	C	83.68850	72.70557	74.33762	195.81897	173.33862	-745.11536	1
175	H	83.81354	72.46404	73.26318	1405.67949	-2301.21089	-390.08113	1
176	H	84.21967	73.64769	74.57951	-940.37328	-1118.32446	2299.72133	1
177	N	84.48734	71.59494	75.10210	319.26422	656.36007	-42.02424	1
178	H	85.51319	71.48823	74.85050	1961.03633	619.91968	1787.09422	1
179	H	84.54305	71.70866	76.15498	854.14343	-2156.80752	1429.08711	1
180	H	84.14006	70.59603	75.01185	1237.02905	-1378.50857	-1998.28500	1
181	C	78.36746	73.92110	72.59420	532.53319	-268.57236	517.55729	1
182	O	77.34764	74.34823	72.10401	266.16714	-290.73804	-558.88002	1
183	N	79.19524	73.00197	72.11109	-226.25352	640.49678	-270.32839	1
184	H	80.01762	72.73690	72.64764	2007.69063	-1035.27229	1523.50231	1
185	C	78.88488	72.37313	70.88184	-540.76542	-573.33303	49.50000	1
186	H	77.90039	72.80210	70.58185	-2374.20950	-1036.76023	843.75774	1
187	C	80.07354	72.71572	69.86544	-77.09082	666.87422	-415.84136	1
188	H	81.05005	72.37069	70.30473	-985.81834	617.19825	2463.91927	1
189	O	80.27093	74.11178	69.57525	293.29899	-391.65602	-477.80926	1
190	H	81.18106	74.24836	69.90583	2528.72714	-681.76262	-751.27122	1
191	C	79.70603	71.80542	68.63782	252.47363	-605.14473	440.05134	1

192	H	80.48284	71.86649	67.84044	-2052.65063	1456.49051	-1043.51830	1
193	H	79.61616	70.72994	68.92919	-2152.98800	-1661.97574	-161.70652	1
194	H	78.73643	72.11056	68.17976	-473.12726	-1584.27339	2165.61725	1
195	C	78.85893	70.74483	71.15458	360.36307	488.46713	505.10056	1
196	O	77.82312	70.14795	70.98584	-200.08817	-528.03552	-385.82850	1
197	N	80.04475	70.29186	71.53188	-597.54095	-226.44775	355.20479	1
198	H	80.79274	70.97393	71.64061	2179.23655	-1300.70981	-991.33835	1
199	C	80.29615	68.90155	71.68472	-687.68921	297.39807	-249.45179	1
200	H	81.35601	68.89846	72.02308	-349.16256	-2467.37713	-1101.72831	1
201	C	79.30085	68.34730	72.81198	672.47345	361.54328	-201.62880	1
202	H	78.23831	68.48577	72.49963	1541.41502	582.18425	2169.97026	1
203	H	79.46239	67.25593	72.97567	-2534.67717	60.25153	997.72295	1
204	C	79.59826	69.12790	74.10023	574.26774	-389.43119	-377.02542	1
205	C	80.80520	68.86131	74.81484	688.82679	-287.33580	-257.96133	1
206	H	81.49851	68.07115	74.47346	331.14182	1470.38163	2269.80013	1
207	C	78.69524	70.13269	74.56021	-383.52382	-675.04808	144.24917	1
208	H	77.76299	70.34604	74.00607	4.09847	1517.59662	2262.86397	1
209	C	81.09206	69.61765	75.95090	-134.76730	428.45285	-649.50303	1
210	H	82.02920	69.41349	76.49757	-903.23433	1600.49020	2011.53387	1
211	C	79.01514	70.84706	75.71790	-335.53281	-615.00040	-364.39058	1
212	H	78.30329	71.61450	76.07122	1596.45398	-1369.33862	1732.02659	1
213	C	80.22441	70.63563	76.44382	585.48547	-340.24194	-406.23938	1
214	O	80.57473	71.39307	77.59188	-419.15649	-173.04408	-511.94141	1
215	H	79.75761	71.93918	77.68457	-1071.84350	1559.71507	-1960.13012	1
216	C	80.14180	68.21058	70.22393	291.41878	-183.13091	710.72246	1
217	O	80.66236	68.73604	69.26364	379.87695	523.47396	-222.23622	1
218	N	79.60632	66.97643	70.28955	564.30591	373.09380	277.24371	1
219	H	79.23003	66.77488	71.21615	-120.59931	-2436.07824	-1214.35098	1
220	C	78.73639	66.59838	69.18306	404.07514	-299.37480	608.84009	1
221	H	77.82714	67.22008	69.33387	-1071.07882	-841.69025	2359.66467	1
222	C	79.48061	66.88434	67.82976	-683.12807	68.71770	-390.13096	1
223	H	79.55796	67.98576	67.64209	2068.88918	1596.58590	770.89603	1
224	H	80.52973	66.51637	67.90571	1379.86429	2342.49779	-179.85638	1
225	C	78.74498	66.20432	66.62631	-176.39967	537.49466	550.97268	1
226	H	78.63225	65.10737	66.78475	-396.28051	1942.22168	1869.33314	1
227	H	77.71391	66.60143	66.49745	-94.44700	586.00678	-2659.20016	1
228	C	79.66259	66.51226	65.35674	-291.69381	-718.18079	-150.72929	1
229	H	79.78721	67.59794	65.11164	-2303.38776	1089.76242	964.62032	1
230	H	80.68514	66.05620	65.38494	884.16729	2568.80533	-207.74283	1
231	N	78.97411	65.92211	64.28874	-594.49522	-252.81478	342.29276	1
232	H	78.09175	65.48369	64.50084	-1735.17426	2084.05705	-263.71605	1
233	C	79.38979	65.90993	63.08792	595.23177	-271.52487	442.22352	1
234	N	80.61778	66.52571	62.81812	585.53813	-424.79750	-105.81303	1
235	H	81.25958	66.99783	63.45367	959.88797	1327.56823	-2177.11905	1
236	H	81.05384	66.57815	61.89711	1578.48647	16.27378	-2220.76233	1
237	N	78.48756	65.25188	62.23994	-452.17763	-390.33541	-421.51853	1
238	H	77.59362	64.80217	62.43156	470.26107	1974.25629	-1817.92087	1
239	H	78.64630	65.14094	61.23760	1856.67307	-1573.97321	-1224.35416	1
240	C	78.45340	65.01166	69.37509	-531.47271	-581.45780	-55.06206	1
241	O	79.12932	64.17293	68.80987	-243.00837	192.73507	609.52485	1
242	N	77.41784	64.81327	70.18823	343.49288	-644.25607	38.09164	1
243	H	76.98323	65.65644	70.56434	-1691.16043	-1535.97525	-1484.73099	1
244	C	77.06627	63.48761	70.68756	542.66492	350.14337	454.42563	1
245	H	76.13701	63.65994	71.28140	1209.57979	-2396.95920	463.86744	1
246	C	76.85802	62.55663	69.50452	-737.14309	145.93010	242.71942	1
247	H	77.82622	62.51678	68.94231	-1050.18303	159.36419	-2509.06125	1
248	C	76.49724	61.15048	69.94105	-706.77696	-252.88343	-245.16230	1
249	H	76.41461	60.44878	69.06554	-1624.64039	-1665.49085	1417.86935	1
250	H	77.27985	60.72665	70.64571	2566.10521	598.51109	693.22305	1
251	H	75.51156	61.12347	70.48255	-1972.69758	107.10018	-1876.34312	1
252	C	75.79839	63.08367	68.55335	412.85148	672.58832	-27.69222	1
253	H	75.68611	62.42677	67.64768	1447.02277	1762.76533	-1490.78944	1

254	H	74.79078	63.14332	69.04898	1320.77379	-145.20455	2378.68491	1
255	H	76.05278	64.11732	68.19062	-1512.10848	1470.52031	1724.75147	1
256	C	78.33253	62.98603	71.63908	-607.11113	499.56689	73.73769	1
257	O	78.60352	61.80924	71.76204	357.97126	460.81534	356.68785	1
258	N	78.87253	64.01869	72.26219	536.55407	-368.62270	332.76306	1
259	H	78.48599	64.92962	72.02764	524.38866	2297.69985	1367.20941	1
260	C	80.03525	63.83602	73.04786	46.50277	-774.29190	-147.97904	1
261	H	80.09807	62.73675	73.21940	1676.51875	1883.29066	1032.55549	1
262	C	81.31281	64.43100	72.25435	-559.41456	-34.19198	-556.30433	1
263	H	81.19266	65.53434	72.13713	-64.66664	395.18769	2695.05373	1
264	H	82.23976	64.28744	72.85886	-2703.44278	-60.40056	333.79418	1
265	C	81.45013	63.78332	70.90389	-519.76435	377.31045	459.42366	1
266	H	80.50879	63.96601	70.31973	-1746.74323	1667.50644	-1261.73691	1
267	C	82.61180	64.40835	70.14134	570.95554	16.46261	-545.27700	1
268	H	82.72538	63.95845	69.12136	2391.58273	28.05277	-1305.07271	1
269	H	82.46537	65.51112	70.00257	175.75588	917.63458	2559.43867	1
270	H	83.58471	64.26532	70.67867	-1063.97851	-2155.34650	1283.00462	1
271	C	81.64941	62.27931	71.01785	193.76014	2.62946	-765.53141	1
272	H	81.86964	61.81595	70.02127	507.39394	-846.55087	2539.60089	1
273	H	82.49965	62.02118	71.70093	1337.57841	1818.19054	1526.01994	1
274	H	80.72398	61.77534	71.41808	1100.88635	-1172.91350	-2199.08909	1
275	C	79.88309	64.73622	74.37537	-549.21115	475.64486	-309.38218	1
276	O	79.05873	65.60400	74.50368	556.06106	-390.37755	-78.24250	1
277	O	80.87919	64.53908	75.36254	-572.27940	-310.19032	-209.75862	1
278	H	81.34123	63.75356	74.95758	-1380.08193	2212.14486	790.85944	1

Listing 76: C00076.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	1.7470	6988
		0.2500	300.00	0.00	0.00	0.00	-1293.5411	0.0000	300.0000
3	H	82.71846	80.50228	86.82710	-2043.14101	-1757.64893	399.89339		1
4	N	83.20327	80.18903	85.98727	426.75047	490.45733	-334.42467		1
5	H	82.46463	80.25172	85.28124	442.25559	-1110.30854	-2448.52907		1
6	C	84.32230	80.98340	85.63981	415.32972	-666.39213	83.73172		1
7	H	84.35508	81.74596	86.44761	879.32219	2491.00447	667.35213		1
8	C	85.65567	80.07852	85.63149	31.35357	477.41777	628.23362		1
9	H	85.57642	79.31052	84.82512	1168.38489	2240.25337	-1019.71136		1
10	H	86.55106	80.69688	85.38294	-360.43770	2534.90498	931.67112		1
11	C	85.82969	79.41976	86.97436	463.18208	512.70242	-382.34388		1
12	H	84.89645	78.86003	87.21005	1725.29117	1863.52247	-987.07854		1
13	C	86.99359	78.43673	86.93555	710.42801	-144.27427	-313.15367		1
14	H	87.12839	77.91616	87.91860	364.20195	-1033.13725	2494.72524		1
15	H	86.84217	77.64485	86.15753	2567.61904	335.80679	847.48802		1
16	H	87.95995	78.95260	86.69982	-2587.99029	680.92867	-512.16411		1
17	C	86.07546	80.44361	88.07467	268.17616	741.64379	-40.42634		1
18	H	86.25963	79.95046	89.06381	1283.54314	-1945.37420	-1411.27812		1
19	H	86.96857	81.08238	87.85160	-1258.57796	1317.15249	-2026.02085		1
20	H	85.20067	81.13041	88.20723	-2502.84526	909.80597	575.92391		1
21	C	83.92933	81.61237	84.20086	619.36578	-458.64843	-172.09273		1
22	O	82.76967	81.79074	83.88325	-81.40433	433.87611	522.34594		1
23	N	85.02193	81.98345	83.53277	175.23996	-622.20190	341.55523		1
24	H	85.94257	81.74182	83.89326	-876.57256	-303.22879	-2561.90213		1
25	C	84.83570	82.44999	82.19266	-571.88214	-534.10783	-106.15033		1
26	H	83.94294	83.10927	82.25891	-2713.20841	-16.25800	-248.80809		1
27	C	86.19571	83.17189	81.76776	166.60354	288.16399	-716.09568		1
28	H	87.02926	82.42146	81.85017	-2097.85574	1636.78449	-586.18044		1
29	O	86.58726	84.28871	82.58908	-317.80580	-363.38227	484.43082		1
30	H	87.43776	83.96939	82.94931	1863.74748	-1451.84923	1357.29467		1
31	C	85.95435	83.49548	80.24739	503.80731	517.99032	318.51606		1
32	H	86.88224	83.87848	79.76258	640.61020	-2157.10410	-1536.29104		1
33	H	85.62918	82.59541	79.67182	1687.88455	465.60692	2087.56452		1

34	H	85.17060	84.27659	80.11529	-1293.07895	-1899.88581	-1463.57452	1
35	C	84.59125	81.13902	81.25190	-153.07550	-733.68902	248.70981	1
36	O	85.38137	80.23152	81.27980	186.15459	-480.78787	-449.34387	1
37	N	83.53579	81.32552	80.44897	-487.53139	543.18517	42.03850	1
38	C	83.15750	80.33659	79.48375	-699.35871	69.34393	360.10701	1
39	H	83.21999	79.34548	79.98653	2.81126	-221.99807	-2715.58072	1
40	C	81.70983	80.80658	79.04439	-507.46439	-592.59194	122.07761	1
41	H	81.42327	80.43393	78.03465	-1975.08116	525.87560	-1801.71556	1
42	H	80.92588	80.45413	79.75186	1588.27743	-1913.22100	1113.83566	1
43	C	81.88329	82.35560	79.10608	-613.62442	-457.55993	-194.14490	1
44	H	82.49610	82.71371	78.24502	1707.54637	-721.27992	1996.92523	1
45	H	80.92404	82.92016	79.08676	758.23357	2100.81767	1560.55011	1
46	C	82.67874	82.50220	80.47489	-352.41524	704.96076	49.21465	1
47	H	83.30864	83.41762	80.55995	1714.76886	-2070.42778	443.35792	1
48	H	82.05116	82.39470	81.39267	1224.15040	1801.50881	1636.97633	1
49	C	84.21539	80.48292	78.23052	566.85117	537.05831	117.62814	1
50	O	84.30325	81.48804	77.56684	-550.26779	-406.08867	4.21666	1
51	N	84.85100	79.32741	78.10700	566.34832	-425.77725	180.18749	1
52	H	84.64010	78.56045	78.74529	644.44502	2646.80550	-52.73430	1
53	C	85.93172	79.23619	77.19238	612.34801	-281.48662	411.56221	1
54	H	85.91117	80.18092	76.59870	1667.23498	-1490.75142	1556.16753	1
55	C	87.21916	79.07488	78.13795	-714.45746	-175.43074	286.98927	1
56	H	87.00054	78.23550	78.85443	-787.09484	1763.03619	-1922.46060	1
57	O	87.51401	80.21158	78.97382	-429.46514	516.51932	-128.40526	1
58	H	86.94787	80.02233	79.75468	1981.82785	436.16847	-1818.18182	1
59	C	88.33608	78.63944	77.12672	630.79189	-468.94448	76.03230	1
60	H	89.28860	78.39577	77.65289	-1775.71861	2062.30353	131.89849	1
61	H	88.03651	77.73585	76.54431	-1855.14608	88.94118	1993.53760	1
62	H	88.56107	79.44982	76.39450	-1504.82350	-780.94249	-2132.90992	1
63	C	85.63978	77.85813	76.35790	288.57638	618.62814	-397.00270	1
64	O	85.68334	76.76710	76.92373	321.70495	-185.26452	574.37218	1
65	N	85.47961	78.15195	75.08911	-447.05792	-446.53431	367.76425	1
66	H	85.54078	79.15131	74.88378	350.31316	1975.63644	-1843.31522	1
67	C	84.67403	77.37111	74.20896	-511.23061	374.03917	-471.51480	1
68	H	84.87347	77.84491	73.22153	2234.79579	-898.70890	-1273.45190	1
69	C	85.15340	75.84719	74.26481	529.53781	-159.34528	563.72604	1
70	H	84.88059	75.34756	73.29296	654.59388	2347.94251	1217.51488	1
71	H	86.27497	75.88794	74.30959	-1526.55661	2103.42026	817.87394	1
72	O	84.62643	75.02506	75.30976	-554.84278	14.12789	399.58769	1
73	H	85.03772	75.51833	76.12212	1297.06236	2061.84854	1220.68812	1
74	C	83.11402	77.54014	74.63051	-662.15484	-412.13544	123.62687	1
75	O	82.71840	78.11662	75.61432	-540.01537	-317.05804	274.91456	1
76	N	82.38447	77.00162	73.65002	-202.76299	-690.00100	-131.49145	1
77	H	82.88339	76.55389	72.88112	-702.62132	-2617.37191	281.70413	1
78	C	80.92580	76.96985	73.69906	-491.73914	576.34187	222.73509	1
79	H	80.65302	76.85436	74.77457	1977.17978	-1823.58850	-434.68928	1
80	C	80.39607	78.25533	73.08515	-649.50797	-328.66843	306.11224	1
81	H	80.83556	78.34443	72.06652	2075.07803	1452.16490	-1004.45904	1
82	C	78.88504	78.23022	72.95172	-615.18735	-489.99689	-70.96352	1
83	H	78.49333	79.17719	72.48784	-1226.32661	-1724.38906	-1716.47170	1
84	H	78.53621	77.36899	72.30362	2381.64273	-969.84735	900.46860	1
85	H	78.38327	78.11845	73.95221	2122.74991	1702.23946	-141.36228	1
86	C	80.81749	79.48046	73.87562	-501.86074	-479.61276	-376.42482	1
87	H	80.48748	80.43507	73.38052	993.79261	-2246.95401	-1177.81305	1
88	H	80.38171	79.47130	74.91261	42.71279	-626.15391	-2651.37258	1
89	H	81.93688	79.52907	73.99513	-2026.39012	-1590.33709	-887.82922	1
90	C	80.52407	75.69031	72.71646	-672.89153	382.57394	-156.34072	1
91	O	81.06557	75.52743	71.64944	410.04627	221.86223	500.35950	1
92	N	79.50687	75.02675	73.24090	-378.11782	-443.79414	-441.10984	1
93	H	79.15316	75.32523	74.14759	2404.15973	-568.14894	1149.30085	1
94	C	79.03467	73.86245	72.57621	-544.54484	466.16019	331.29119	1
95	H	79.59373	73.84387	71.61155	-1409.80988	-170.17955	2325.32679	1

96	C	79.34158	72.62961	73.53187	-184.48284	116.78282	-758.89137	1
97	H	80.43779	72.52819	73.69917	1893.78641	1861.14652	611.04528	1
98	H	78.89102	72.78788	74.53766	-2170.79665	-974.19311	1327.50117	1
99	C	78.74965	71.35892	72.85057	389.51668	672.81878	-138.49152	1
100	H	77.64650	71.47957	72.74868	510.64577	1933.03327	1851.02484	1
101	H	79.11565	71.27575	71.80339	-2302.30869	-1105.72939	-948.89774	1
102	C	79.06181	70.02119	73.62239	-559.93427	-126.34590	542.30857	1
103	O	78.64857	68.98030	73.18087	-670.36003	-111.83166	76.36448	1
104	N	79.79422	70.18348	74.74467	-216.06729	-537.07037	446.51379	1
105	H	80.16815	71.04199	75.16628	-1251.96487	1074.12894	-2168.52500	1
106	H	80.08248	69.41242	75.35667	-2451.83023	-720.73851	944.84612	1
107	C	77.40726	74.00102	72.43341	546.24052	-563.88337	-85.11809	1
108	O	76.70091	73.49548	73.26534	71.70702	-307.40463	606.69673	1
109	N	77.06918	74.72791	71.35615	479.90863	-504.50129	222.86849	1
110	C	75.70453	74.85771	70.95954	75.51268	-600.91904	506.73700	1
111	H	75.09061	74.76506	71.88423	-2033.61562	1795.30103	254.89480	1
112	C	75.72257	76.28137	70.25961	523.79067	517.99274	284.45581	1
113	H	74.85771	76.43964	69.57708	1599.61665	-1127.00911	1895.98173	1
114	H	75.69343	77.10339	71.00933	-1881.83093	1275.82488	-1501.55016	1
115	C	77.09436	76.24308	69.51528	-600.05639	-404.05026	316.64485	1
116	H	77.01370	75.65147	68.57322	-2597.05260	496.36221	657.73249	1
117	H	77.47562	77.24908	69.22751	-1666.24518	1294.38985	-1723.90591	1
118	C	78.02071	75.50341	70.57044	493.57570	-129.95376	-602.56394	1
119	H	78.76404	74.80103	70.12587	-1469.08415	-637.84797	2204.22581	1
120	H	78.54278	76.17542	71.30238	-1038.97840	1068.88701	-2280.71789	1
121	C	75.41040	73.65888	69.86928	188.88100	241.05089	-727.87821	1
122	O	75.90956	73.67457	68.76894	531.88613	-49.19943	427.07960	1
123	N	74.61510	72.74743	70.41054	708.14833	26.93417	-179.73509	1
124	H	74.26637	72.87959	71.35935	-2232.69501	-1179.09831	1023.94816	1
125	C	74.16127	71.68446	69.57609	-738.32412	259.92548	104.42456	1
126	H	74.82955	71.68754	68.68184	2028.89123	1260.02983	1311.33324	1
127	C	74.24285	70.35121	70.45099	-258.65678	-345.52513	661.28459	1
128	H	73.60944	70.44383	71.36987	-1826.06090	-1801.46097	-918.64554	1
129	C	73.78998	69.12926	69.58592	-541.23400	531.92970	-218.41428	1
130	H	73.87625	68.17411	70.15650	1311.73218	-2219.18200	882.19023	1
131	H	72.71150	69.22135	69.25011	-1048.71298	1223.58118	-2196.97971	1
132	H	74.41610	69.02363	68.66850	419.06414	1903.92898	1903.44670	1
133	C	75.74556	70.14083	70.83804	-423.86431	152.66566	-648.55262	1
134	H	75.88679	69.25398	71.50042	105.68386	-2342.50080	1387.51238	1
135	H	76.38500	69.98979	69.93668	-1695.63603	-1484.73621	-1531.02793	1
136	H	76.14559	71.02985	71.38020	-1853.57121	-487.39031	1936.59343	1
137	C	72.60825	72.01786	69.21855	539.71428	-510.58232	267.58633	1
138	O	71.82052	72.58918	69.97973	-15.93758	-278.34085	-624.49402	1
139	N	72.35468	71.47698	68.05513	-676.81886	12.05292	276.17960	1
140	H	73.10152	70.97533	67.57493	-1694.44250	-373.84189	-2100.66098	1
141	C	70.99630	71.43328	67.61299	412.33078	-664.70360	108.35451	1
142	H	70.56134	72.41954	67.89357	1765.77476	1294.44366	1621.76594	1
143	C	71.07301	71.14318	66.06297	-179.66635	-721.95667	-264.73915	1
144	H	71.80724	71.82610	65.57905	-607.34922	2587.87032	-598.10018	1
145	H	71.45423	70.11424	65.87467	-359.69332	-1479.13954	-2259.74260	1
146	C	69.65064	71.33277	65.43811	-240.01076	616.02425	431.85322	1
147	H	68.92589	70.60140	65.86118	-1359.17131	782.54425	2227.99181	1
148	H	69.24434	72.34247	65.67019	-820.36667	85.81767	-2596.78715	1
149	C	69.82237	71.13855	63.87753	-513.07015	236.18570	-551.87280	1
150	H	70.58965	71.84024	63.47686	1816.11944	-1183.11722	-1650.94321	1
151	H	70.19968	70.11603	63.64609	-1800.04429	-1361.53473	1526.34643	1
152	C	68.45682	71.38631	63.19673	726.08972	-253.19732	-179.64713	1
153	H	67.67237	70.64561	63.44962	1224.27271	-456.51798	-2390.90304	1
154	H	68.06050	72.41432	63.31664	1206.40339	-1150.93514	-2154.90344	1
155	N	68.67590	71.22680	61.65361	329.70796	-633.68968	-155.67358	1
156	H	67.81600	71.37097	61.04974	1348.31305	1938.76845	1359.00643	1
157	H	69.36619	71.88934	61.19396	2096.92035	1446.54551	-966.48890	1

158	H	69.01685	70.28240	61.30953	-1197.07217	-2303.53719	827.28733	1
159	C	70.25761	70.19058	68.40037	-378.01186	-556.17301	-413.96481	1
160	O	70.81183	69.13903	68.64626	-409.44433	-307.55053	-453.30833	1
161	N	69.00482	70.55417	68.60850	-429.02477	524.70884	274.08502	1
162	H	68.74154	71.47727	68.26639	1706.34263	-1425.96036	1574.38926	1
163	C	68.06640	69.72279	69.27365	-45.25864	-626.22952	478.93267	1
164	H	67.09310	70.22199	69.06569	1988.63164	570.90773	1772.87287	1
165	C	68.16289	68.26722	68.65787	551.77128	-20.49526	-564.54996	1
166	H	68.21695	68.31181	67.54671	1434.61535	-1753.10253	1513.99471	1
167	H	69.10739	67.76876	68.98383	-714.67738	1819.09770	1898.36494	1
168	C	66.90645	67.46391	69.13082	446.99263	-555.77305	338.97221	1
169	H	66.86541	67.43421	70.24836	1953.68466	1892.25957	-161.67766	1
170	H	65.96849	67.96500	68.80132	-403.03785	2688.07032	-188.43591	1
171	C	66.99814	66.00396	68.52943	567.86262	335.74681	434.04421	1
172	H	67.05330	66.03486	67.41691	-1080.02275	1568.26081	-1948.78900	1
173	H	67.93128	65.49546	68.86448	-919.54108	2111.34692	1456.13463	1
174	C	65.74805	65.22190	68.99531	195.81897	173.33862	-745.11536	1
175	H	65.68354	65.06524	70.09055	1405.67949	-2301.21089	-390.08113	1
176	H	64.78599	65.61864	68.61399	-940.37328	-1118.32446	2299.72133	1
177	N	65.84367	63.77864	68.39459	319.26422	656.36007	-42.02424	1
178	H	65.04269	63.12759	68.63921	1961.03633	619.91968	1787.09422	1
179	H	65.86356	63.69474	67.33662	854.14343	-2156.80752	1429.08711	1
180	H	66.68235	63.19245	68.67683	1237.02905	-1378.50857	-1998.28500	1
181	C	68.38232	69.66161	70.88425	532.53319	-268.57236	517.55729	1
182	O	67.90354	68.78199	71.56453	266.16714	-290.73804	-558.88002	1
183	N	69.07247	70.72275	71.27631	-226.25352	640.49678	-270.32839	1
184	H	69.40227	71.34352	70.53935	2007.69063	-1035.27229	1523.50231	1
185	C	69.42065	70.87555	72.65537	-540.76542	-573.33303	49.50000	1
186	H	69.61698	69.84244	73.02269	-2374.20950	-1036.76023	843.75774	1
187	C	70.70417	71.83184	72.67648	-77.09082	666.87422	-415.84136	1
188	H	70.55082	72.66234	71.92443	-985.81834	617.19825	2463.91927	1
189	O	71.91834	71.21509	72.24172	293.29899	-391.65602	-477.80926	1
190	H	72.03580	71.70008	71.33518	2528.72714	-681.76262	-751.27122	1
191	C	70.70844	72.43811	74.12365	252.47363	-605.14473	440.05134	1
192	H	71.65788	72.98559	74.33294	-2052.65063	1456.49051	-1043.51830	1
193	H	69.87333	73.16416	74.27782	-2152.98800	-1661.97574	-161.70652	1
194	H	70.60267	71.63868	74.89299	-473.12726	-1584.27339	2165.61725	1
195	C	68.19804	71.53908	73.48445	360.36307	488.46713	505.10056	1
196	O	68.29365	71.58657	74.71883	-200.08817	-528.03552	-385.82850	1
197	N	67.24762	71.99853	72.70900	-597.54095	-226.44775	355.20479	1
198	H	67.39629	71.82733	71.71480	2179.23655	-1300.70981	-991.33835	1
199	C	66.13516	72.74409	73.16223	-687.68921	297.39807	-249.45179	1
200	H	65.47005	72.80395	72.27330	-349.16256	-2467.37713	-1101.72831	1
201	C	65.46132	72.04435	74.43563	672.47345	361.54328	-201.62880	1
202	H	66.23389	71.86155	75.22338	1541.41502	582.18425	2169.97026	1
203	H	64.69843	72.72918	74.87256	-2534.67717	60.25153	997.72295	1
204	C	64.81047	70.71874	74.01993	574.26774	-389.43119	-377.02542	1
205	C	63.48989	70.70348	73.47829	688.82679	-287.33580	-257.96133	1
206	H	62.93142	71.64436	73.32259	331.14182	1470.38163	2269.80013	1
207	C	65.53667	69.50289	74.19973	-383.52382	-675.04808	144.24917	1
208	H	66.56986	69.52001	74.59313	4.09847	1517.59662	2262.86397	1
209	C	62.91729	69.47225	73.16103	-134.76730	428.45285	-649.50303	1
210	H	61.89284	69.45695	72.75006	-903.23433	1600.49020	2011.53387	1
211	C	64.91648	68.29556	73.87145	-335.53281	-615.00040	-364.39058	1
212	H	65.48301	67.36031	74.02411	1596.45398	-1369.33862	1732.02659	1
213	C	63.59182	68.23066	73.34852	585.48547	-340.24194	-406.23938	1
214	O	62.95396	67.00730	73.01562	-419.15649	-173.04408	-511.94141	1
215	H	63.66100	66.37359	73.28397	-1071.84350	1559.71507	-1960.13012	1
216	C	66.63754	74.22088	73.65485	291.41878	-183.13091	710.72246	1
217	O	66.24245	75.19805	73.06927	379.87695	523.47396	-222.23622	1
218	N	67.38176	74.14008	74.75977	564.30591	373.09380	277.24371	1
219	H	67.71238	73.19964	75.08291	-120.59931	-2436.07824	-1214.35098	1

220	C	68.10928	75.33851	75.11096	404.07514	-299.37480	608.84009	1
221	H	68.61887	75.66117	74.17670	-1071.07882	-841.69025	2359.66467	1
222	C	67.03680	76.39259	75.59455	-683.12807	68.71770	-390.13096	1
223	H	66.17273	76.41130	74.88740	2068.88918	1596.58590	770.89603	1
224	H	66.61192	76.09014	76.57853	1379.86429	2342.49779	-179.85638	1
225	C	67.68649	77.80817	75.68981	-176.39967	537.49466	550.97268	1
226	H	68.51967	77.82983	76.42968	-396.28051	1942.22168	1869.33314	1
227	H	68.13291	78.11679	74.71829	-94.44700	586.00678	-2659.20016	1
228	C	66.48654	78.77830	76.11212	-291.69381	-718.18079	-150.72929	1
229	H	65.59825	78.78256	75.43108	-2303.38776	1089.76242	964.62032	1
230	H	66.12725	78.62057	77.16125	884.16729	2568.80533	-207.74283	1
231	N	67.07901	80.04523	76.05677	-594.49522	-252.81478	342.29276	1
232	H	68.08364	80.07249	76.14314	-1735.17426	2084.05705	-263.71605	1
233	C	66.44605	81.14193	75.93951	595.23177	-271.52487	442.22352	1
234	N	65.05106	81.09701	75.84818	585.53813	-424.79750	-105.81303	1
235	H	64.42282	80.29521	75.88077	959.88797	1327.56823	-2177.11905	1
236	H	64.44472	81.91385	75.76620	1578.48647	16.27378	-2220.76233	1
237	N	67.32768	82.23133	75.92939	-452.17763	-390.33541	-421.51853	1
238	H	68.34216	82.26543	76.01832	470.26107	1974.25629	-1817.92087	1
239	H	67.01839	83.20185	75.86293	1856.67307	-1573.97321	-1224.35416	1
240	C	69.11551	74.97135	76.33036	-531.47271	-581.45780	-55.06206	1
241	O	70.22151	75.50797	76.37889	-243.00837	192.73507	609.52485	1
242	N	68.53146	74.16043	77.18766	343.49288	-644.25607	38.09164	1
243	H	67.58053	73.89800	76.92859	-1691.16043	-1535.97525	-1484.73099	1
244	C	69.20269	73.47251	78.22897	542.66492	350.14337	454.42563	1
245	H	68.44369	72.73492	78.57109	1209.57979	-2396.95920	463.86744	1
246	C	70.48962	72.77804	77.59537	-737.14309	145.93010	242.71942	1
247	H	70.84846	73.34337	76.70726	-1050.18303	159.36419	-2509.06125	1
248	C	71.63986	72.62855	78.64632	-706.77696	-252.88343	-245.16230	1
249	H	72.48119	72.01230	78.24987	-1624.64039	-1665.49085	1417.86935	1
250	H	72.06421	73.63121	78.92378	2566.10521	598.51109	693.22305	1
251	H	71.27889	72.14161	79.58334	-1972.69758	107.10018	-1876.34312	1
252	C	70.04665	71.32898	77.19986	412.85148	672.58832	-27.69222	1
253	H	70.90744	70.72332	76.82964	1447.02277	1762.76533	-1490.78944	1
254	H	69.60582	70.78065	78.06554	1320.77379	-145.20455	2378.68491	1
255	H	69.26786	71.35766	76.37391	-1512.10848	1470.52031	1724.75147	1
256	C	69.61289	74.47247	79.46097	-607.11113	499.56689	73.73769	1
257	O	69.31567	74.13435	80.58334	357.97126	460.81534	356.68785	1
258	N	70.30302	75.53648	79.07419	536.55407	-368.62270	332.76306	1
259	H	70.52752	75.71127	78.06059	524.38866	2297.69985	1367.20941	1
260	C	70.66424	76.44066	80.10609	46.50277	-774.29190	-147.97904	1
261	H	70.01620	76.16140	80.97017	1676.51875	1883.29066	1032.55549	1
262	C	72.23636	76.26196	80.44762	-559.41456	-34.19198	-556.30433	1
263	H	72.82889	76.37001	79.50875	-64.66664	395.18769	2695.05373	1
264	H	72.57668	77.08341	81.12155	-2703.44278	-60.40056	333.79418	1
265	C	72.49784	74.92469	81.08096	-519.76435	377.31045	459.42366	1
266	H	72.10105	74.12417	80.40606	-1746.74323	1667.50644	-1261.73691	1
267	C	73.99638	74.70943	81.25817	570.95554	16.46261	-545.27700	1
268	H	74.22059	73.70476	81.70044	2391.58273	28.05277	-1305.07271	1
269	H	74.54180	74.77125	80.28153	175.75588	917.63458	2559.43867	1
270	H	74.44569	75.47795	81.93813	-1063.97851	-2155.34650	1283.00462	1
271	C	71.79998	74.78397	82.42672	193.76014	2.62946	-765.53141	1
272	H	72.09604	73.83643	82.94685	507.39394	-846.55087	2539.60089	1
273	H	72.04684	75.63272	83.11528	1337.57841	1818.19054	1526.01994	1
274	H	70.68358	74.75589	82.30628	1100.88635	-1172.91350	-2199.08909	1
275	C	70.46377	77.95330	79.57915	-549.21115	475.64486	-309.38218	1
276	O	70.38766	78.26167	78.41947	556.06106	-390.37755	-78.24250	1
277	O	70.48265	78.94852	80.58751	-572.27940	-310.19032	-209.75862	1
278	H	70.55141	78.35478	81.38547	-1380.08193	2212.14486	790.85944	1

Listing 77: C00077.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.9895	3958
		0.2500	300.00	0.00	0.00	0.00	-1293.5337	0.0000	300.0000
3	H	60.27662	77.58934	65.25431	-2043.14101	-1757.64893	399.89339		1
4	N	60.57299	78.39843	65.79713	426.75047	490.45733	-334.42467		1
5	H	60.91634	77.97449	66.66003	442.25559	-1110.30854	-2448.52907		1
6	C	61.55314	79.20249	65.17606	415.32972	-666.39213	83.73172		1
7	H	61.42972	79.10115	64.07536	879.32219	2491.00447	667.35213		1
8	C	61.35094	80.71706	65.70533	31.35357	477.41777	628.23362		1
9	H	61.48197	80.72715	66.81420	1168.38489	2240.25337	-1019.71136		1
10	H	62.14094	81.38798	65.29256	-360.43770	2534.90498	931.67112		1
11	C	59.98500	81.22970	65.33484	463.18208	512.70242	-382.34388		1
12	H	59.24155	80.42906	65.54941	1725.29117	1863.52247	-987.07854		1
13	C	59.63926	82.45167	66.17737	710.42801	-144.27427	-313.15367		1
14	H	58.62469	82.85545	65.92669	364.20195	-1033.13725	2494.72524		1
15	H	59.64143	82.21244	67.27235	2567.61904	335.80679	847.48802		1
16	H	60.37486	83.28207	66.01970	-2587.99029	680.92867	-512.16411		1
17	C	59.91114	81.59135	63.85763	268.17616	741.64379	-40.42634		1
18	H	58.89999	81.98648	63.57931	1283.54314	-1945.37420	-1411.27812		1
19	H	60.65926	82.38116	63.58881	-1258.57796	1317.15249	-2026.02085		1
20	H	60.11382	80.70559	63.20228	-2502.84526	909.80597	575.92391		1
21	C	62.97488	78.67632	65.75271	619.36578	-458.64843	-172.09273		1
22	O	63.11212	78.21689	66.88982	-81.40433	433.87611	522.34594		1
23	N	63.90201	78.97195	64.87047	175.23996	-622.20190	341.55523		1
24	H	63.58864	79.33259	63.97134	-876.57256	-303.22879	-2561.90213		1
25	C	65.24128	78.48452	65.05159	-571.88214	-534.10783	-106.15033		1
26	H	65.07726	77.43237	65.37798	-2713.20841	-16.25800	-248.80809		1
27	C	65.98755	78.62543	63.64232	166.60354	288.16399	-716.09568		1
28	H	66.18886	79.71349	63.44383	-2097.85574	1636.78449	-586.18044		1
29	O	65.26987	78.12807	62.50112	-317.80580	-363.38227	484.43082		1
30	H	65.24655	78.92311	61.93032	1863.74748	-1451.84923	1357.29467		1
31	C	67.35083	77.91074	63.96752	503.80731	517.99032	318.51606		1
32	H	68.08028	78.01984	63.13178	640.61020	-2157.10410	-1536.29104		1
33	H	67.82734	78.32648	64.88910	1687.88455	465.60692	2087.56452		1
34	H	67.20446	76.81859	64.13657	-1293.07895	-1899.88581	-1463.57452		1
35	C	66.04322	79.31877	66.18504	-153.07550	-733.68902	248.70981		1
36	O	66.78128	78.64817	66.89489	186.15459	-480.78787	-449.34387		1
37	N	65.91245	80.64465	66.14932	-487.53139	543.18517	42.03850		1
38	C	66.77979	81.50571	66.90199	-699.35871	69.34393	360.10701		1
39	H	67.79750	81.06215	66.81306	2.81126	-221.99807	-2715.58072		1
40	C	66.55704	82.90518	66.19087	-507.46439	-592.59194	122.07761		1
41	H	66.86583	83.76575	66.82630	-1975.08116	525.87560	-1801.71556		1
42	H	67.13072	82.98105	65.24007	1588.27743	-1913.22100	1113.83566		1
43	C	65.01926	82.85728	65.92665	-613.62442	-457.55993	-194.14490		1
44	H	64.45341	83.07087	66.86171	1707.54637	-721.27992	1996.92523		1
45	H	64.67041	83.59322	65.16755	758.23357	2100.81767	1560.55011		1
46	C	64.82914	81.34712	65.47181	-352.41524	704.96076	49.21465		1
47	H	63.88579	80.86507	65.81452	1714.76886	-2070.42778	443.35792		1
48	H	64.96370	81.16637	64.37971	1224.15040	1801.50881	1636.97633		1
49	C	66.24475	81.53292	68.45095	566.85117	537.05831	117.62814		1
50	O	65.82379	82.55189	68.93902	-550.26779	-406.08867	4.21666		1
51	N	66.42222	80.33371	69.00031	566.34832	-425.77725	180.18749		1
52	H	66.76796	79.53863	68.41241	644.44502	2646.80550	-52.73430		1
53	C	65.77969	80.11887	70.25623	612.34801	-281.48662	411.56221		1
54	H	65.29387	81.10034	70.47371	1667.23498	-1490.75142	1556.16753		1
55	C	64.71246	78.94982	70.01115	-714.45746	-175.43074	286.98927		1
56	H	65.20001	78.11451	69.43704	-787.09484	1763.03619	-1922.46060		1
57	O	63.57628	79.35684	69.25648	-429.46514	516.51932	-128.40526		1
58	H	63.61933	78.76316	68.43316	1981.82785	436.16847	-1818.18182		1
59	C	64.40676	78.47276	71.47479	630.79189	-468.94448	76.03230		1
60	H	63.67485	77.63193	71.48314	-1775.71861	2062.30353	131.89849		1

61	H	65.32253	78.11555	72.00041	-1855.14608	88.94118	1993.53760	1
62	H	63.97170	79.29640	72.08717	-1504.82350	-780.94249	-2132.90992	1
63	C	66.98015	79.81903	71.33243	288.57638	618.62814	-397.00270	1
64	O	67.36229	80.75769	71.98786	321.70495	-185.26452	574.37218	1
65	N	67.38314	78.56398	71.37801	-447.05792	-446.53431	367.76425	1
66	H	67.06298	77.79454	70.76337	350.31316	1975.63644	-1843.31522	1
67	C	68.48348	78.22452	72.25100	-511.23061	374.03917	-471.51480	1
68	H	69.33780	78.82860	71.86892	2234.79579	-898.70890	-1273.45190	1
69	C	68.14667	78.61796	73.77115	529.53781	-159.34528	563.72604	1
70	H	69.09764	78.49378	74.35911	654.59388	2347.94251	1217.51488	1
71	H	67.90463	79.71841	73.77921	-1526.55661	2103.42026	817.87394	1
72	O	67.12511	77.83265	74.43309	-554.84278	14.12789	399.58769	1
73	H	66.33304	78.32746	74.14787	1297.06236	2061.84854	1220.68812	1
74	C	68.60086	76.65644	71.96341	-662.15484	-412.13544	123.62687	1
75	O	67.97602	76.18756	71.02659	-540.01537	-317.05804	274.91456	1
76	N	69.50693	76.04477	72.74795	-202.76299	-690.00100	-131.49145	1
77	H	69.85685	76.62084	73.51678	-702.62132	-2617.37191	281.70413	1
78	C	69.45512	74.57861	72.88726	-491.73914	576.34187	222.73509	1
79	H	68.40310	74.33257	72.61157	1977.17978	-1823.58850	-434.68928	1
80	C	70.46656	73.99220	71.92528	-649.50797	-328.66843	306.11224	1
81	H	71.45677	74.45156	72.14089	2075.07803	1452.16490	-1004.45904	1
82	C	70.59491	72.48911	72.09585	-615.18735	-489.99689	-70.96352	1
83	H	71.30707	72.04667	71.34672	-1226.32661	-1724.38906	-1716.47170	1
84	H	70.97155	72.21933	73.12155	2381.64273	-969.84735	900.46860	1
85	H	69.60552	71.97234	71.95841	2122.74991	1702.23946	-141.36228	1
86	C	70.11835	74.32009	70.48385	-501.86074	-479.61276	-376.42482	1
87	H	70.89753	73.94561	69.76480	993.79261	-2246.95401	-1177.81305	1
88	H	69.13469	73.86394	70.18492	42.71279	-626.15391	-2651.37258	1
89	H	70.01781	75.43204	70.33114	-2026.39012	-1590.33709	-887.82922	1
90	C	69.82058	74.19694	74.45731	-672.89153	382.57394	-156.34072	1
91	O	69.00924	73.57608	75.10154	410.04627	221.86223	500.35950	1
92	N	71.02478	74.59072	74.83497	-378.11782	-443.79414	-441.10984	1
93	H	71.61348	75.08926	74.17196	2404.15973	-568.14894	1149.30085	1
94	C	71.40152	74.30364	76.19522	-544.54484	466.16019	331.29119	1
95	H	70.47260	74.52913	76.76883	-1409.80988	-170.17955	2325.32679	1
96	C	71.75531	72.75614	76.26937	-184.48284	116.78282	-758.89137	1
97	H	70.88406	72.16029	75.91352	1893.78641	1861.14652	611.04528	1
98	H	72.60160	72.49996	75.59361	-2170.79665	-974.19311	1327.50117	1
99	C	72.09318	72.42877	77.75794	389.51668	672.81878	-138.49152	1
100	H	73.06593	72.90257	78.06188	510.64577	1933.03327	1851.02484	1
101	H	71.34440	72.90412	78.43075	-2302.30869	-1105.72939	-948.89774	1
102	C	72.13650	70.89009	78.05918	-559.93427	-126.34590	542.30857	1
103	O	72.28031	70.51381	79.20059	-670.36003	-111.83166	76.36448	1
104	N	72.00483	70.11269	76.96803	-216.06729	-537.07037	446.51379	1
105	H	71.80916	70.38251	75.99715	-1251.96487	1074.12894	-2168.52500	1
106	H	71.96769	69.08735	76.99209	-2451.83023	-720.73851	944.84612	1
107	C	72.69893	75.18859	76.57533	546.24052	-563.88337	-85.11809	1
108	O	73.78177	74.95302	76.05056	71.70702	-307.40463	606.69673	1
109	N	72.38301	76.11127	77.47479	479.90863	-504.50129	222.86849	1
110	C	73.38238	76.89974	78.13592	75.51268	-600.91904	506.73700	1
111	H	74.21693	77.04351	77.40774	-2033.61562	1795.30103	254.89480	1
112	C	72.56081	78.20039	78.51382	523.79067	517.99274	284.45581	1
113	H	73.02926	78.78468	79.33717	1599.61665	-1127.00911	1895.98173	1
114	H	72.46747	78.88941	77.64517	-1881.83093	1275.82488	-1501.55016	1
115	C	71.17816	77.58751	78.90397	-600.05639	-404.05026	316.64485	1
116	H	71.22397	77.12341	79.91682	-2597.05260	496.36221	657.73249	1
117	H	70.34713	78.32801	78.92567	-1666.24518	1294.38985	-1723.90591	1
118	C	71.00217	76.48194	77.78232	493.57570	-129.95376	-602.56394	1
119	H	70.45738	75.56474	78.11091	-1469.08415	-637.84797	2204.22581	1
120	H	70.56597	76.84745	76.82242	-1038.97840	1068.88701	-2280.71789	1
121	C	73.85068	76.12316	79.50272	188.88100	241.05089	-727.87821	1
122	O	73.05640	75.84599	80.37189	531.88613	-49.19943	427.07960	1

123	N	75.17723	76.02799	79.51199	708.14833	26.93417	-179.73509	1
124	H	75.61676	76.35504	78.65056	-2232.69501	-1179.09831	1023.94816	1
125	C	75.92698	75.18003	80.43122	-738.32412	259.92548	104.42456	1
126	H	76.99022	75.46582	80.24597	2028.89123	1260.02983	1311.33324	1
127	C	75.46092	75.50000	81.83926	-258.65678	-345.52513	661.28459	1
128	H	74.35470	75.31473	81.87475	-1826.06090	-1801.46097	-918.64554	1
129	C	76.11883	74.64897	82.90899	-541.23400	531.92970	-218.41428	1
130	H	75.76535	74.93551	83.93768	1311.73218	-2219.18200	882.19023	1
131	H	75.89168	73.55597	82.77645	-1048.71298	1223.58118	-2196.97971	1
132	H	77.23791	74.76322	82.90204	419.06414	1903.92898	1903.44670	1
133	C	75.68566	76.96607	82.17009	-423.86431	152.66566	-648.55262	1
134	H	75.28675	77.22956	83.18768	105.68386	-2342.50080	1387.51238	1
135	H	76.77864	77.22985	82.16115	-1695.63603	-1484.73621	-1531.02793	1
136	H	75.17445	77.63477	81.42450	-1853.57121	-487.39031	1936.59343	1
137	C	75.65485	73.59622	80.00344	539.71428	-510.58232	267.58633	1
138	O	74.79921	73.26471	79.18233	-15.93758	-278.34085	-624.49402	1
139	N	76.52384	72.81183	80.61634	-676.81886	12.05292	276.17960	1
140	H	77.13262	73.43031	81.15178	-1694.44250	-373.84189	-2100.66098	1
141	C	76.25039	71.47891	81.03232	412.33078	-664.70360	108.35451	1
142	H	76.92163	71.31785	81.90524	1765.77476	1294.44366	1621.76594	1
143	C	74.71089	71.37245	81.37547	-179.66635	-721.95667	-264.73915	1
144	H	74.37831	72.19848	82.04313	-607.34922	2587.87032	-598.10018	1
145	H	74.10764	71.48612	80.43986	-359.69332	-1479.13954	-2259.74260	1
146	C	74.47879	69.97288	82.03809	-240.01076	616.02425	431.85322	1
147	H	75.00198	69.17581	81.45936	-1359.17131	782.54425	2227.99181	1
148	H	74.89768	69.93196	83.06866	-820.36667	85.81767	-2596.78715	1
149	C	72.92038	69.71756	82.03346	-513.07015	236.18570	-551.87280	1
150	H	72.39665	70.41729	82.72567	1816.11944	-1183.11722	-1650.94321	1
151	H	72.50483	69.93190	80.99518	-1800.04429	-1361.53473	1526.34643	1
152	C	72.67045	68.24501	82.43395	726.08972	-253.19732	-179.64713	1
153	H	73.11873	67.49797	81.74858	1224.27271	-456.51798	-2390.90304	1
154	H	72.92699	67.99878	83.48345	1206.40339	-1150.93514	-2154.90344	1
155	N	71.12892	68.00527	82.32060	329.70796	-633.68968	-155.67358	1
156	H	70.78714	67.03188	82.56791	1348.31305	1938.76845	1359.00643	1
157	H	70.49518	68.61169	82.91849	2096.92035	1446.54551	-966.48890	1
158	H	70.70968	68.13668	81.35509	-1197.07217	-2303.53719	827.28733	1
159	C	76.51031	70.39288	79.83157	-378.01186	-556.17301	-413.96481	1
160	O	76.81891	69.25540	80.08904	-409.44433	-307.55053	-453.30833	1
161	N	76.15687	70.92562	78.66920	-429.02477	524.70884	274.08502	1
162	H	75.81512	71.90923	78.65403	1706.34263	-1425.96036	1574.38926	1
163	C	76.61650	70.29372	77.46684	-45.25864	-626.22952	478.93267	1
164	H	76.59295	69.22251	77.77917	1988.63164	570.90773	1772.87287	1
165	C	75.53155	70.71418	76.39390	551.77128	-20.49526	-564.54996	1
166	H	74.53250	70.76209	76.88431	1434.61535	-1753.10253	1513.99471	1
167	H	75.73006	71.75024	76.03843	-714.67738	1819.09770	1898.36494	1
168	C	75.46380	69.72759	75.18258	446.99263	-555.77305	338.97221	1
169	H	76.43892	69.64374	74.64684	1953.68466	1892.25957	-161.67766	1
170	H	75.20336	68.69588	75.50957	-403.03785	2688.07032	-188.43591	1
171	C	74.33972	70.33945	74.25093	567.86262	335.74681	434.04421	1
172	H	73.36200	70.35420	74.78217	-1080.02275	1568.26081	-1948.78900	1
173	H	74.56383	71.40448	74.00983	-919.54108	2111.34692	1456.13463	1
174	C	74.23665	69.50140	72.95689	195.81897	173.33862	-745.11536	1
175	H	75.11875	69.57127	72.28965	1405.67949	-2301.21089	-390.08113	1
176	H	73.95965	68.43941	73.11070	-940.37328	-1118.32446	2299.72133	1
177	N	73.05333	70.10649	72.12644	319.26422	656.36007	-42.02424	1
178	H	72.87745	69.67989	71.17054	1961.03633	619.91968	1787.09422	1
179	H	72.08503	70.05522	72.55867	854.14343	-2156.80752	1429.08711	1
180	H	73.13216	71.13596	71.88571	1237.02905	-1378.50857	-1998.28500	1
181	C	78.13363	70.80246	77.19675	532.53319	-268.57236	517.55729	1
182	O	78.94332	70.91087	78.11458	266.16714	-290.73804	-558.88002	1
183	N	78.33588	71.04936	75.91352	-226.25352	640.49678	-270.32839	1
184	H	77.54775	70.86872	75.29499	2007.69063	-1035.27229	1523.50231	1

185	C	79.65604	70.77361	75.39786	-540.76542	-573.33303	49.50000	1
186	H	79.99699	69.92590	76.03326	-2374.20950	-1036.76023	843.75774	1
187	C	79.47576	70.42733	73.85836	-77.09082	666.87422	-415.84136	1
188	H	79.23216	71.36888	73.29349	-985.81834	617.19825	2463.91927	1
189	O	78.41039	69.50239	73.54504	293.29899	-391.65602	-477.80926	1
190	H	77.89975	70.01905	72.89102	2528.72714	-681.76262	-751.27122	1
191	C	80.93805	69.97203	73.49669	252.47363	-605.14473	440.05134	1
192	H	81.04323	69.76108	72.40745	-2052.65063	1456.49051	-1043.51830	1
193	H	81.68803	70.75844	73.75692	-2152.98800	-1661.97574	-161.70652	1
194	H	81.22405	69.04338	74.04313	-473.12726	-1584.27339	2165.61725	1
195	C	80.58330	72.10074	75.59128	360.36307	488.46713	505.10056	1
196	O	80.96045	72.73805	74.63884	-200.08817	-528.03552	-385.82850	1
197	N	80.88325	72.26139	76.88321	-597.54095	-226.44775	355.20479	1
198	H	80.41117	71.65746	77.60456	2179.23655	-1300.70981	-991.33835	1
199	C	81.36584	73.55519	77.23297	-687.68921	297.39807	-249.45179	1
200	H	81.27730	74.16829	76.30554	-349.16256	-2467.37713	-1101.72831	1
201	C	80.47255	74.05582	78.46388	672.47345	361.54328	-201.62880	1
202	H	80.20881	73.21086	79.14070	1541.41502	582.18425	2169.97026	1
203	H	81.03973	74.80294	79.06497	-2534.67717	60.25153	997.72295	1
204	C	79.21174	74.69468	77.86592	574.26774	-389.43119	-377.02542	1
205	C	79.31342	76.02280	77.36152	688.82679	-287.33580	-257.96133	1
206	H	80.27050	76.57429	77.40390	331.14182	1470.38163	2269.80013	1
207	C	77.98002	73.98242	77.78122	-383.52382	-675.04808	144.24917	1
208	H	77.90385	72.94507	78.16338	4.09847	1517.59662	2262.86397	1
209	C	78.17895	76.60248	76.80878	-134.76730	428.45285	-649.50303	1
210	H	78.25863	77.63360	76.42268	-903.23433	1600.49020	2011.53387	1
211	C	76.87590	74.62150	77.21226	-335.53281	-615.00040	-364.39058	1
212	H	75.91695	74.07133	77.17360	1596.45398	-1369.33862	1732.02659	1
213	C	76.92785	75.94736	76.70864	585.48547	-340.24194	-406.23938	1
214	O	75.83668	76.61608	76.14883	-419.15649	-173.04408	-511.94141	1
215	H	75.13683	75.83112	76.07475	-1071.84350	1559.71507	-1960.13012	1
216	C	82.91645	73.45577	77.74080	291.41878	-183.13091	710.72246	1
217	O	83.75186	74.17838	77.19541	379.87695	523.47396	-222.23622	1
218	N	83.05905	72.64011	78.75870	564.30591	373.09380	277.24371	1
219	H	82.18965	72.17623	79.02035	-120.59931	-2436.07824	-1214.35098	1
220	C	84.31294	72.17921	79.24208	404.07514	-299.37480	608.84009	1
221	H	84.03314	71.32140	79.89377	-1071.07882	-841.69025	2359.66467	1
222	C	85.19364	71.76625	77.98725	-683.12807	68.71770	-390.13096	1
223	H	84.62400	71.10079	77.29999	2068.88918	1596.58590	770.89603	1
224	H	85.45458	72.66682	77.38288	1379.86429	2342.49779	-179.85638	1
225	C	86.47221	71.06452	78.53345	-176.39967	537.49466	550.97268	1
226	H	86.95066	71.68652	79.32344	-396.28051	1942.22168	1869.33314	1
227	H	86.22208	70.09849	79.02520	-94.44700	586.00678	-2659.20016	1
228	C	87.47756	70.84438	77.30309	-291.69381	-718.18079	-150.72929	1
229	H	87.08195	70.26369	76.43253	-2303.38776	1089.76242	964.62032	1
230	H	87.94472	71.80207	76.95483	884.16729	2568.80533	-207.74283	1
231	N	88.44350	70.08992	77.97996	-594.49522	-252.81478	342.29276	1
232	H	88.67617	70.40956	78.90993	-1735.17426	2084.05705	-263.71605	1
233	C	89.06800	69.07475	77.52688	595.23177	-271.52487	442.22352	1
234	N	88.79572	68.62839	76.23257	585.53813	-424.79750	-105.81303	1
235	H	88.16382	69.00765	75.52856	959.88797	1327.56823	-2177.11905	1
236	H	89.26077	67.83955	75.78114	1578.48647	16.27378	-2220.76233	1
237	N	89.96545	68.58907	78.48606	-452.17763	-390.33541	-421.51853	1
238	H	90.16205	68.90419	79.43501	470.26107	1974.25629	-1817.92087	1
239	H	90.56711	67.77962	78.32990	1856.67307	-1573.97321	-1224.35416	1
240	C	85.14174	73.32775	80.06896	-531.47271	-581.45780	-55.06206	1
241	O	85.50908	73.04282	81.17839	-243.00837	192.73507	609.52485	1
242	N	85.32989	74.43236	79.36434	343.49288	-644.25607	38.09164	1
243	H	84.92349	74.47978	78.38972	-1691.16043	-1535.97525	-1484.73099	1
244	C	86.06908	75.59882	79.83484	542.66492	350.14337	454.42563	1
245	H	85.50722	76.45118	79.38296	1209.57979	-2396.95920	463.86744	1
246	C	86.12640	75.65995	81.34686	-737.14309	145.93010	242.71942	1

247	H	86.61841	74.72343	81.71589	-1050.18303	159.36419	-2509.06125	1
248	C	86.94550	76.84159	81.83532	-706.77696	-252.88343	-245.16230	1
249	H	87.00274	76.87294	82.95748	-1624.64039	-1665.49085	1417.86935	1
250	H	88.00127	76.80190	81.44940	2566.10521	598.51109	693.22305	1
251	H	86.50508	77.81935	81.49786	-1972.69758	107.10018	-1876.34312	1
252	C	84.73842	75.71989	81.96101	412.85148	672.58832	-27.69222	1
253	H	84.78118	75.78221	83.08259	1447.02277	1762.76533	-1490.78944	1
254	H	84.15939	76.61167	81.59630	1320.77379	-145.20455	2378.68491	1
255	H	84.14301	74.80026	81.69867	-1512.10848	1470.52031	1724.75147	1
256	C	87.60164	75.49985	79.18690	-607.11113	499.56689	73.73769	1
257	O	88.17996	74.45314	79.01098	357.97126	460.81534	356.68785	1
258	N	88.12316	76.74620	79.09128	536.55407	-368.62270	332.76306	1
259	H	87.34228	77.36267	79.32768	524.38866	2297.69985	1367.20941	1
260	C	88.88525	77.06947	77.91098	46.50277	-774.29190	-147.97904	1
261	H	89.27367	78.08085	78.15436	1676.51875	1883.29066	1032.55549	1
262	C	90.05973	76.00155	77.67179	-559.41456	-34.19198	-556.30433	1
263	H	89.61070	75.03641	77.32746	-64.66664	395.18769	2695.05373	1
264	H	90.74604	76.33590	76.85599	-2703.44278	-60.40056	333.79418	1
265	C	90.81976	75.78552	78.95773	-519.76435	377.31045	459.42366	1
266	H	90.07572	75.50217	79.73972	-1746.74323	1667.50644	-1261.73691	1
267	C	91.81542	74.64395	78.79941	570.95554	16.46261	-545.27700	1
268	H	92.37210	74.44451	79.75145	2391.58273	28.05277	-1305.07271	1
269	H	91.30403	73.69026	78.50677	175.75588	917.63458	2559.43867	1
270	H	92.57881	74.86846	78.01008	-1063.97851	-2155.34650	1283.00462	1
271	C	91.55022	77.04599	79.39761	193.76014	2.62946	-765.53141	1
272	H	92.12713	76.88112	80.34412	507.39394	-846.55087	2539.60089	1
273	H	92.28040	77.39164	78.62086	1337.57841	1818.19054	1526.01994	1
274	H	90.84013	77.89182	79.58647	1100.88635	-1172.91350	-2199.08909	1
275	C	87.85971	77.14378	76.69621	-549.21115	475.64486	-309.38218	1
276	O	86.68691	77.37238	76.85118	556.06106	-390.37755	-78.24250	1
277	O	88.40460	77.07246	75.38559	-572.27940	-310.19032	-209.75862	1
278	H	89.36217	76.97121	75.61661	-1380.08193	2212.14486	790.85944	1

Listing 78: C00078.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.5304	0.0000	300.0000
3	H	80.62860	79.47171	76.41020	-2043.14101	-1757.64893	399.89339		1
4	N	81.21464	78.78709	75.93443	426.75047	490.45733	-334.42467		1
5	H	80.55577	78.36630	75.27195	442.25559	-1110.30854	-2448.52907		1
6	C	82.33167	79.34976	75.26651	415.32972	-666.39213	83.73172		1
7	H	82.18571	80.44353	75.40299	879.32219	2491.00447	667.35213		1
8	C	83.70431	78.83508	75.93764	31.35357	477.41777	628.23362		1
9	H	83.84318	77.75017	75.71411	1168.38489	2240.25337	-1019.71136		1
10	H	84.58151	79.35720	75.48563	-360.43770	2534.90498	931.67112		1
11	C	83.66163	79.06328	77.42506	463.18208	512.70242	-382.34388		1
12	H	82.74218	78.57767	77.82282	1725.29117	1863.52247	-987.07854		1
13	C	84.88235	78.43246	78.08424	710.42801	-144.27427	-313.15367		1
14	H	84.88283	78.58304	79.19415	364.20195	-1033.13725	2494.72524		1
15	H	84.93039	77.32883	77.89733	2567.61904	335.80679	847.48802		1
16	H	85.83387	78.87526	77.69207	-2587.99029	680.92867	-512.16411		1
17	C	83.61093	80.54829	77.75856	268.17616	741.64379	-40.42634		1
18	H	83.63157	80.72471	78.86442	1283.54314	-1945.37420	-1411.27812		1
19	H	84.48108	81.09971	77.31812	-1258.57796	1317.15249	-2026.02085		1
20	H	82.67873	81.02918	77.36569	-2502.84526	909.80597	575.92391		1
21	C	82.14841	78.86276	73.73987	619.36578	-458.64843	-172.09273		1
22	O	81.02567	78.63393	73.29226	-81.40433	433.87611	522.34594		1
23	N	83.31171	78.73462	73.12298	175.23996	-622.20190	341.55523		1
24	H	84.17253	78.94439	73.62501	-876.57256	-303.22879	-2561.90213		1
25	C	83.34730	78.21419	71.80282	-571.88214	-534.10783	-106.15033		1
26	H	82.30508	78.34600	71.43262	-2713.20841	-16.25800	-248.80809		1

27	C	84.50019	78.99899	71.01073	166.60354	288.16399	-716.09568	1
28	H	85.49412	78.67263	71.42972	-2097.85574	1636.78449	-586.18044	1
29	O	84.47005	80.43259	71.11690	-317.80580	-363.38227	484.43082	1
30	H	85.32956	80.61048	71.55078	1863.74748	-1451.84923	1357.29467	1
31	C	84.35002	78.42724	69.55318	503.80731	517.99032	318.51606	1
32	H	85.15685	78.80828	68.88456	640.61020	-2157.10410	-1536.29104	1
33	H	84.40638	77.31168	69.53952	1687.88455	465.60692	2087.56452	1
34	H	83.37679	78.72227	69.09705	-1293.07895	-1899.88581	-1463.57452	1
35	C	83.85187	76.65648	71.84261	-153.07550	-733.68902	248.70981	1
36	O	85.00590	76.44746	71.56877	186.15459	-480.78787	-449.34387	1
37	N	82.89847	75.77961	72.21340	-487.53139	543.18517	42.03850	1
38	C	83.08330	74.38307	72.02373	-699.35871	69.34393	360.10701	1
39	H	84.14785	74.22641	71.73100	2.81126	-221.99807	-2715.58072	1
40	C	82.65620	73.81175	73.44641	-507.46439	-592.59194	122.07761	1
41	H	82.42576	72.72337	73.42314	-1975.08116	525.87560	-1801.71556	1
42	H	83.45740	73.95722	74.20473	1588.27743	-1913.22100	1113.83566	1
43	C	81.41019	74.69689	73.75750	-613.62442	-457.55993	-194.14490	1
44	H	80.49401	74.32202	73.21220	1707.54637	-721.27992	1996.92523	1
45	H	81.14612	74.72925	74.83961	758.23357	2100.81767	1560.55011	1
46	C	81.85237	76.10785	73.18026	-352.41524	704.96076	49.21465	1
47	H	81.04572	76.65027	72.62147	1714.76886	-2070.42778	443.35792	1
48	H	82.32628	76.78658	73.92743	1224.15040	1801.50881	1636.97633	1
49	C	81.98592	73.77088	70.94912	566.85117	537.05831	117.62814	1
50	O	81.86819	72.56645	70.90291	-550.26779	-406.08867	4.21666	1
51	N	81.42108	74.71134	70.20880	566.34832	-425.77725	180.18749	1
52	H	81.75197	75.64447	70.45161	644.44502	2646.80550	-52.73430	1
53	C	80.18576	74.55436	69.51484	612.34801	-281.48662	411.56221	1
54	H	80.15201	75.41718	68.81399	1667.23498	-1490.75142	1556.16753	1
55	C	80.23955	73.16296	68.73016	-714.45746	-175.43074	286.98927	1
56	H	80.45083	72.33930	69.48012	-787.09484	1763.03619	-1922.46060	1
57	O	81.28710	73.11128	67.73623	-429.46514	516.51932	-128.40526	1
58	H	81.92680	72.52554	68.18819	1981.82785	436.16847	-1818.18182	1
59	C	78.79106	72.93359	68.16819	630.79189	-468.94448	76.03230	1
60	H	78.71445	71.95692	67.63601	-1775.71861	2062.30353	131.89849	1
61	H	78.02539	72.92506	68.97943	-1855.14608	88.94118	1993.53760	1
62	H	78.50294	73.72611	67.43893	-1504.82350	-780.94249	-2132.90992	1
63	C	78.99534	74.67742	70.61054	288.57638	618.62814	-397.00270	1
64	O	79.16688	74.54791	71.80917	321.70495	-185.26452	574.37218	1
65	N	77.85714	74.98628	69.99581	-447.05792	-446.53431	367.76425	1
66	H	77.84101	75.05348	68.97988	350.31316	1975.63644	-1843.31522	1
67	C	76.65364	74.73265	70.72834	-511.23061	374.03917	-471.51480	1
68	H	76.93512	74.96440	71.78253	2234.79579	-898.70890	-1273.45190	1
69	C	75.50898	75.63937	70.08241	529.53781	-159.34528	563.72604	1
70	H	74.60718	75.52849	70.74411	654.59388	2347.94251	1217.51488	1
71	H	75.80247	76.71958	70.14362	-1526.55661	2103.42026	817.87394	1
72	O	75.15962	75.30212	68.72944	-554.84278	14.12789	399.58769	1
73	H	75.01877	74.29923	68.85072	1297.06236	2061.84854	1220.68812	1
74	C	76.21624	73.17939	70.52017	-662.15484	-412.13544	123.62687	1
75	O	75.34387	72.89169	69.70602	-540.01537	-317.05804	274.91456	1
76	N	76.96246	72.40206	71.25595	-202.76299	-690.00100	-131.49145	1
77	H	77.73007	72.78169	71.85138	-702.62132	-2617.37191	281.70413	1
78	C	76.47556	71.11310	71.66145	-491.73914	576.34187	222.73509	1
79	H	75.38116	71.20880	71.84040	1977.17978	-1823.58850	-434.68928	1
80	C	76.78591	70.08252	70.48551	-649.50797	-328.66843	306.11224	1
81	H	77.64946	70.44695	69.88901	2075.07803	1452.16490	-1004.45904	1
82	C	77.04485	68.63087	71.01330	-615.18735	-489.99689	-70.96352	1
83	H	77.26412	67.92366	70.17921	-1226.32661	-1724.38906	-1716.47170	1
84	H	77.91248	68.59787	71.71296	2381.64273	-969.84735	900.46860	1
85	H	76.16125	68.22812	71.56169	2122.74991	1702.23946	-141.36228	1
86	C	75.49890	69.95078	69.60294	-501.86074	-479.61276	-376.42482	1
87	H	75.67716	69.32001	68.69995	993.79261	-2246.95401	-1177.81305	1
88	H	74.65826	69.48522	70.17042	42.71279	-626.15391	-2651.37258	1

89	H	75.14469	70.96380	69.25207	-2026.39012	-1590.33709	-887.82922	1
90	C	77.37350	70.87263	72.98665	-672.89153	382.57394	-156.34072	1
91	O	78.28434	71.67656	73.21258	410.04627	221.86223	500.35950	1
92	N	76.97385	69.83774	73.69469	-378.11782	-443.79414	-441.10984	1
93	H	76.14543	69.36984	73.32423	2404.15973	-568.14894	1149.30085	1
94	C	77.84218	69.07534	74.53502	-544.54484	466.16019	331.29119	1
95	H	77.54693	68.03195	74.28714	-1409.80988	-170.17955	2325.32679	1
96	C	79.35454	69.37633	74.18409	-184.48284	116.78282	-758.89137	1
97	H	79.59150	69.07275	73.13847	1893.78641	1861.14652	611.04528	1
98	H	79.56724	70.47617	74.21951	-2170.79665	-974.19311	1327.50117	1
99	C	80.25370	68.61646	75.21128	389.51668	672.81878	-138.49152	1
100	H	79.80493	68.65839	76.22869	510.64577	1933.03327	1851.02484	1
101	H	80.28221	67.52918	74.97928	-2302.30869	-1105.72939	-948.89774	1
102	C	81.71188	69.20871	75.26574	-559.93427	-126.34590	542.30857	1
103	O	82.48098	68.81859	76.10587	-670.36003	-111.83166	76.36448	1
104	N	81.97058	70.14145	74.32087	-216.06729	-537.07037	446.51379	1
105	H	81.39577	70.46090	73.53230	-1251.96487	1074.12894	-2168.52500	1
106	H	82.89668	70.55840	74.17881	-2451.83023	-720.73851	944.84612	1
107	C	77.41086	69.30046	76.10106	546.24052	-563.88337	-85.11809	1
108	O	76.96742	68.31343	76.63145	71.70702	-307.40463	606.69673	1
109	N	77.68156	70.49239	76.65120	479.90863	-504.50129	222.86849	1
110	C	77.10189	70.87434	77.90307	75.51268	-600.91904	506.73700	1
111	H	76.86369	69.91359	78.41802	-2033.61562	1795.30103	254.89480	1
112	C	78.29247	71.73223	78.51923	523.79067	517.99274	284.45581	1
113	H	77.99190	72.35460	79.39241	1599.61665	-1127.00911	1895.98173	1
114	H	79.12879	71.08326	78.86261	-1881.83093	1275.82488	-1501.55016	1
115	C	78.69968	72.56366	77.26543	-600.05639	-404.05026	316.64485	1
116	H	77.93656	73.35040	77.03317	-2597.05260	496.36221	657.73249	1
117	H	79.67882	73.08389	77.36778	-1666.24518	1294.38985	-1723.90591	1
118	C	78.71637	71.40328	76.17943	493.57570	-129.95376	-602.56394	1
119	H	78.43279	71.70757	75.12539	-1469.08415	-637.84797	2204.22581	1
120	H	79.66221	70.81193	76.15585	-1038.97840	1068.88701	-2280.71789	1
121	C	75.76967	71.77604	77.59208	188.88100	241.05089	-727.87821	1
122	O	74.99836	71.46453	76.71704	531.88613	-49.19943	427.07960	1
123	N	75.63797	72.73954	78.50332	708.14833	26.93417	-179.73509	1
124	H	76.37909	72.85740	79.19341	-2232.69501	-1179.09831	1023.94816	1
125	C	74.82316	73.86280	78.14388	-738.32412	259.92548	104.42456	1
126	H	74.37890	73.53531	77.17449	2028.89123	1260.02983	1311.33324	1
127	C	73.73139	74.01634	79.28683	-258.65678	-345.52513	661.28459	1
128	H	74.20773	74.17392	80.27815	-1826.06090	-1801.46097	-918.64554	1
129	C	72.73754	75.17540	78.92748	-541.23400	531.92970	-218.41428	1
130	H	71.93218	75.28059	79.69219	1311.73218	-2219.18200	882.19023	1
131	H	73.25037	76.16766	78.85248	-1048.71298	1223.58118	-2196.97971	1
132	H	72.24301	74.99599	77.94375	419.06414	1903.92898	1903.44670	1
133	C	72.87332	72.70413	79.28571	-423.86431	152.66566	-648.55262	1
134	H	72.07598	72.72908	80.06457	105.68386	-2342.50080	1387.51238	1
135	H	72.37626	72.54668	78.30011	-1695.63603	-1484.73621	-1531.02793	1
136	H	73.50720	71.80682	79.47842	-1853.57121	-487.39031	1936.59343	1
137	C	75.84036	75.12419	77.95917	539.71428	-510.58232	267.58633	1
138	O	76.67898	75.06804	77.05708	-15.93758	-278.34085	-624.49402	1
139	N	75.61052	76.07861	78.82541	-676.81886	12.05292	276.17960	1
140	H	74.88107	75.89188	79.51233	-1694.44250	-373.84189	-2100.66098	1
141	C	76.28765	77.32250	78.88708	412.33078	-664.70360	108.35451	1
142	H	75.91633	77.76463	79.83870	1765.77476	1294.44366	1621.76594	1
143	C	77.84569	77.03713	78.88572	-179.66635	-721.95667	-264.73915	1
144	H	78.10793	76.29542	79.67286	-607.34922	2587.87032	-598.10018	1
145	H	78.16305	76.57403	77.92190	-359.69332	-1479.13954	-2259.74260	1
146	C	78.56198	78.40571	79.13441	-240.01076	616.02425	431.85322	1
147	H	78.42338	79.08854	78.26610	-1359.17131	782.54425	2227.99181	1
148	H	78.10239	78.92635	80.00429	-820.36667	85.81767	-2596.78715	1
149	C	80.09619	78.13991	79.41082	-513.07015	236.18570	-551.87280	1
150	H	80.22514	77.38711	80.22189	1816.11944	-1183.11722	-1650.94321	1

151	H	80.59587	77.71017	78.51199	-1800.04429	-1361.53473	1526.34643	1
152	C	80.74029	79.48665	79.81660	726.08972	-253.19732	-179.64713	1
153	H	80.96037	80.16877	78.97139	1224.27271	-456.51798	-2390.90304	1
154	H	80.19967	80.03422	80.61433	1206.40339	-1150.93514	-2154.90344	1
155	N	82.12947	79.17098	80.46743	329.70796	-633.68968	-155.67358	1
156	H	82.69008	80.01385	80.78474	1348.31305	1938.76845	1359.00643	1
157	H	82.12329	78.58404	81.35175	2096.92035	1446.54551	-966.48890	1
158	H	82.84111	78.65742	79.87273	-1197.07217	-2303.53719	827.28733	1
159	C	75.95214	78.29954	77.60393	-378.01186	-556.17301	-413.96481	1
160	O	75.68413	79.45811	77.80071	-409.44433	-307.55053	-453.30833	1
161	N	76.11816	77.66415	76.45609	-429.02477	524.70884	274.08502	1
162	H	76.42253	76.66127	76.44537	1706.34263	-1425.96036	1574.38926	1
163	C	75.93861	78.39666	75.24966	-45.25864	-626.22952	478.93267	1
164	H	76.06001	79.46547	75.54575	1988.63164	570.90773	1772.87287	1
165	C	77.05743	77.83593	74.27905	551.77128	-20.49526	-564.54996	1
166	H	78.05245	77.89105	74.77547	1434.61535	-1753.10253	1513.99471	1
167	H	76.88786	76.75277	74.08509	-714.67738	1819.09770	1898.36494	1
168	C	77.07747	78.62981	72.93218	446.99263	-555.77305	338.97221	1
169	H	76.11177	78.50946	72.38728	1953.68466	1892.25957	-161.67766	1
170	H	77.20102	79.72256	73.10618	-403.03785	2688.07032	-188.43591	1
171	C	78.28857	78.04275	72.10238	567.86262	335.74681	434.04421	1
172	H	79.28404	78.28028	72.60523	-1080.02275	1568.26081	-1948.78900	1
173	H	78.23213	76.92938	72.05559	-919.54108	2111.34692	1456.13463	1
174	C	78.25903	78.63370	70.67455	195.81897	173.33862	-745.11536	1
175	H	77.42947	78.27108	70.03471	1405.67949	-2301.21089	-390.08113	1
176	H	78.32742	79.73928	70.62287	-940.37328	-1118.32446	2299.72133	1
177	N	79.56719	78.11715	69.98910	319.26422	656.36007	-42.02424	1
178	H	79.71503	78.36422	68.96752	1961.03633	619.91968	1787.09422	1
179	H	80.47460	78.44938	70.42425	854.14343	-2156.80752	1429.08711	1
180	H	79.69728	77.06526	69.98246	1237.02905	-1378.50857	-1998.28500	1
181	C	74.45118	78.10896	74.61744	532.53319	-268.57236	517.55729	1
182	O	74.15347	78.61255	73.55882	266.16714	-290.73804	-558.88002	1
183	N	73.72147	77.30309	75.37851	-226.25352	640.49678	-270.32839	1
184	H	74.12566	77.00207	76.26590	2007.69063	-1035.27229	1523.50231	1
185	C	72.36713	77.06312	75.03915	-540.76542	-573.33303	49.50000	1
186	H	72.15025	77.66921	74.12873	-2374.20950	-1036.76023	843.75774	1
187	C	72.24730	75.47872	74.80661	-77.09082	666.87422	-415.84136	1
188	H	72.55157	74.95833	75.75574	-985.81834	617.19825	2463.91927	1
189	O	73.09322	74.93374	73.77871	293.29899	-391.65602	-477.80926	1
190	H	73.66423	74.33596	74.30234	2528.72714	-681.76262	-751.27122	1
191	C	70.70294	75.29280	74.58088	252.47363	-605.14473	440.05134	1
192	H	70.43441	74.21753	74.46439	-2052.65063	1456.49051	-1043.51830	1
193	H	70.10383	75.69202	75.43222	-2152.98800	-1661.97574	-161.70652	1
194	H	70.36080	75.81877	73.65967	-473.12726	-1584.27339	2165.61725	1
195	C	71.48652	77.43742	76.36584	360.36307	488.46713	505.10056	1
196	O	71.92329	77.20859	77.47433	-200.08817	-528.03552	-385.82850	1
197	N	70.27502	77.87103	76.03485	-597.54095	-226.44775	355.20479	1
198	H	70.03428	77.99677	75.05268	2179.23655	-1300.70981	-991.33835	1
199	C	69.41004	78.21098	77.10979	-687.68921	297.39807	-249.45179	1
200	H	70.09826	78.40935	77.96406	-349.16256	-2467.37713	-1101.72831	1
201	C	68.49575	79.45160	76.67469	672.47345	361.54328	-201.62880	1
202	H	67.98611	79.25256	75.70460	1541.41502	582.18425	2169.97026	1
203	H	67.70019	79.61514	77.43776	-2534.67717	60.25153	997.72295	1
204	C	69.41110	80.67957	76.57765	574.26774	-389.43119	-377.02542	1
205	C	69.84343	81.32014	77.77789	688.82679	-287.33580	-257.96133	1
206	H	69.51704	80.94748	78.76593	331.14182	1470.38163	2269.80013	1
207	C	69.85502	81.15026	75.30539	-383.52382	-675.04808	144.24917	1
208	H	69.53612	80.64551	74.37567	4.09847	1517.59662	2262.86397	1
209	C	70.69311	82.42087	77.67759	-134.76730	428.45285	-649.50303	1
210	H	71.03180	82.91390	78.60567	-903.23433	1600.49020	2011.53387	1
211	C	70.70476	82.25799	75.25795	-335.53281	-615.00040	-364.39058	1
212	H	71.04175	82.61435	74.26887	1596.45398	-1369.33862	1732.02659	1

213	C	71.15121	82.93546	76.42991	585.48547	-340.24194	-406.23938	1
214	O	72.00475	84.06834	76.39071	-419.15649	-173.04408	-511.94141	1
215	H	72.16626	84.12241	75.41943	-1071.84350	1559.71507	-1960.13012	1
216	C	68.39279	76.97852	77.45311	291.41878	-183.13091	710.72246	1
217	O	68.22070	76.66253	78.60955	379.87695	523.47396	-222.23622	1
218	N	67.80327	76.44098	76.36999	564.30591	373.09380	277.24371	1
219	H	68.02051	76.92135	75.49634	-120.59931	-2436.07824	-1214.35098	1
220	C	66.50019	75.89096	76.66329	404.07514	-299.37480	608.84009	1
221	H	66.18661	76.41996	77.59320	-1071.07882	-841.69025	2359.66467	1
222	C	65.57974	76.15815	75.41129	-683.12807	68.71770	-390.13096	1
223	H	65.50971	77.24912	75.19888	2068.88918	1596.58590	770.89603	1
224	H	66.01901	75.70283	74.49505	1379.86429	2342.49779	-179.85638	1
225	C	64.16813	75.55471	75.70218	-176.39967	537.49466	550.97268	1
226	H	64.23932	74.46029	75.89342	-396.28051	1942.22168	1869.33314	1
227	H	63.72649	75.98979	76.62606	-94.44700	586.00678	-2659.20016	1
228	C	63.25643	75.86416	74.42742	-291.69381	-718.18079	-150.72929	1
229	H	63.01603	76.94244	74.24556	-2303.38776	1089.76242	964.62032	1
230	H	63.62834	75.42826	73.46671	884.16729	2568.80533	-207.74283	1
231	N	62.06344	75.19311	74.72884	-594.49522	-252.81478	342.29276	1
232	H	62.08216	74.56950	75.52092	-1735.17426	2084.05705	-263.71605	1
233	C	60.98296	75.30026	74.06805	595.23177	-271.52487	442.22352	1
234	N	60.97143	76.15867	72.96319	585.53813	-424.79750	-105.81303	1
235	H	61.72171	76.73108	72.57845	959.88797	1327.56823	-2177.11905	1
236	H	60.16587	76.31934	72.35757	1578.48647	16.27378	-2220.76233	1
237	N	59.97511	74.49011	74.61044	-452.17763	-390.33541	-421.51853	1
238	H	59.98437	73.85443	75.40665	470.26107	1974.25629	-1817.92087	1
239	H	59.03587	74.42872	74.21548	1856.67307	-1573.97321	-1224.35416	1
240	C	66.64467	74.28664	76.94019	-531.47271	-581.45780	-55.06206	1
241	O	65.94099	73.78404	77.81751	-243.00837	192.73507	609.52485	1
242	N	67.43669	73.69165	76.06047	343.49288	-644.25607	38.09164	1
243	H	67.81237	74.42517	75.45506	-1691.16043	-1535.97525	-1484.73099	1
244	C	68.25191	72.55765	76.35956	542.66492	350.14337	454.42563	1
245	H	68.99050	72.55449	75.52724	1209.57979	-2396.95920	463.86744	1
246	C	68.92843	72.82066	77.77849	-737.14309	145.93010	242.71942	1
247	H	68.14734	72.97361	78.55427	-1050.18303	159.36419	-2509.06125	1
248	C	69.83440	71.58824	78.11442	-706.77696	-252.88343	-245.16230	1
249	H	70.32007	71.69223	79.11246	-1624.64039	-1665.49085	1417.86935	1
250	H	69.24617	70.64056	78.12772	2566.10521	598.51109	693.22305	1
251	H	70.64448	71.45916	77.35826	-1972.69758	107.10018	-1876.34312	1
252	C	69.85331	74.08066	77.69058	412.85148	672.58832	-27.69222	1
253	H	70.36642	74.27511	78.66049	1447.02277	1762.76533	-1490.78944	1
254	H	70.64017	73.96072	76.90932	1320.77379	-145.20455	2378.68491	1
255	H	69.26625	74.99961	77.44095	-1512.10848	1470.52031	1724.75147	1
256	C	67.46605	71.14819	76.47156	-607.11113	499.56689	73.73769	1
257	O	67.96620	70.15559	75.93713	357.97126	460.81534	356.68785	1
258	N	66.38652	71.19857	77.21365	536.55407	-368.62270	332.76306	1
259	H	66.05675	72.11971	77.61181	524.38866	2297.69985	1367.20941	1
260	C	66.06178	69.99212	77.92739	46.50277	-774.29190	-147.97904	1
261	H	67.05023	69.51108	78.10195	1676.51875	1883.29066	1032.55549	1
262	C	65.26333	70.38865	79.27166	-559.41456	-34.19198	-556.30433	1
263	H	64.39803	71.04228	79.00613	-64.66664	395.18769	2695.05373	1
264	H	64.82456	69.47463	79.73961	-2703.44278	-60.40056	333.79418	1
265	C	66.18115	71.09070	80.23649	-519.76435	377.31045	459.42366	1
266	H	66.70736	71.90891	79.69584	-1746.74323	1667.50644	-1261.73691	1
267	C	65.38088	71.71115	81.37539	570.95554	16.46261	-545.27700	1
268	H	66.04581	72.23147	82.11226	2391.58273	28.05277	-1305.07271	1
269	H	64.64697	72.46976	80.99877	175.75588	917.63458	2559.43867	1
270	H	64.79982	70.93801	81.94144	-1063.97851	-2155.34650	1283.00462	1
271	C	67.21786	70.13277	80.80845	193.76014	2.62946	-765.53141	1
272	H	67.88484	70.64149	81.55127	507.39394	-846.55087	2539.60089	1
273	H	66.73356	69.27018	81.33507	1337.57841	1818.19054	1526.01994	1
274	H	67.87728	69.70558	80.01033	1100.88635	-1172.91350	-2199.08909	1

275	C	65.14165	69.09743	76.97395	-549.21115	475.64486	-309.38218	1
276	O	64.05253	68.73092	77.32493	556.06106	-390.37755	-78.24250	1
277	O	65.71674	68.72433	75.77121	-572.27940	-310.19032	-209.75862	1
278	H	66.62853	69.27183	75.81667	-1380.08193	2212.14486	790.85944	1

Listing 79: C00079.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.6012	2405
		0.2500	300.00	0.00	0.00	0.00	-1293.5268	0.0000	300.0000
3	H	75.57644	83.27698	68.29153	-2043.14101	-1757.64893	399.89339		1
4	N	75.74152	83.95922	69.03344	426.75047	490.45733	-334.42467		1
5	H	75.87190	83.38944	69.88857	442.25559	-1110.30854	-2448.52907		1
6	C	76.83404	84.81634	68.77747	415.32972	-666.39213	83.73172		1
7	H	77.14503	84.64159	67.72401	879.32219	2491.00447	667.35213		1
8	C	76.40396	86.34689	69.04126	31.35357	477.41777	628.23362		1
9	H	76.18776	86.48428	70.12771	1168.38489	2240.25337	-1019.71136		1
10	H	77.25091	87.03565	68.80758	-360.43770	2534.90498	931.67112		1
11	C	75.18852	86.69121	68.22131	463.18208	512.70242	-382.34388		1
12	H	74.38974	85.95382	68.46328	1725.29117	1863.52247	-987.07854		1
13	C	74.69096	88.08680	68.57778	710.42801	-144.27427	-313.15367		1
14	H	73.76286	88.35336	68.00951	364.20195	-1033.13725	2494.72524		1
15	H	74.45033	88.17505	69.66854	2567.61904	335.80679	847.48802		1
16	H	75.45805	88.86926	68.34369	-2587.99029	680.92867	-512.16411		1
17	C	75.47425	86.62155	66.72749	268.17616	741.64379	-40.42634		1
18	H	74.57847	86.91659	66.12215	1283.54314	-1945.37420	-1411.27812		1
19	H	76.31222	87.30517	66.43449	-1258.57796	1317.15249	-2026.02085		1
20	H	75.76145	85.58669	66.40866	-2502.84526	909.80597	575.92391		1
21	C	77.89338	84.29995	69.89291	619.36578	-458.64843	-172.09273		1
22	O	77.54047	83.39157	70.64918	-81.40433	433.87611	522.34594		1
23	N	79.00642	84.99163	69.82843	175.23996	-622.20190	341.55523		1
24	H	79.01382	85.72077	69.11420	-876.57256	-303.22879	-2561.90213		1
25	C	80.17415	84.81022	70.61741	-571.88214	-534.10783	-106.15033		1
26	H	80.56874	85.84392	70.71247	-2713.20841	-16.25800	-248.80809		1
27	C	79.79376	84.15378	72.02412	166.60354	288.16399	-716.09568		1
28	H	79.27701	83.17053	71.82272	-2097.85574	1636.78449	-586.18044		1
29	O	78.86909	84.94054	72.80602	-317.80580	-363.38227	484.43082		1
30	H	78.03248	84.46795	72.59717	1863.74748	-1451.84923	1357.29467		1
31	C	81.18459	83.85494	72.69363	503.80731	517.99032	318.51606		1
32	H	81.07595	83.26238	73.63533	640.61020	-2157.10410	-1536.29104		1
33	H	81.85946	83.27655	72.01716	1687.88455	465.60692	2087.56452		1
34	H	81.71524	84.79568	72.96659	-1293.07895	-1899.88581	-1463.57452		1
35	C	81.19342	83.85517	69.77161	-153.07550	-733.68902	248.70981		1
36	O	80.79299	82.83661	69.27087	186.15459	-480.78787	-449.34387		1
37	N	82.44222	84.34061	69.81716	-487.53139	543.18517	42.03850		1
38	C	83.52915	83.62350	69.21995	-699.35871	69.34393	360.10701		1
39	H	83.14448	83.17947	68.27407	2.81126	-221.99807	-2715.58072		1
40	C	84.62650	84.76032	69.05552	-507.46439	-592.59194	122.07761		1
41	H	85.66147	84.35545	68.99570	-1975.08116	525.87560	-1801.71556		1
42	H	84.46524	85.35662	68.12979	1588.27743	-1913.22100	1113.83566		1
43	C	84.37597	85.61963	70.33209	-613.62442	-457.55993	-194.14490		1
44	H	84.77622	85.10909	71.23825	1707.54637	-721.27992	1996.92523		1
45	H	84.83779	86.63231	70.29406	758.23357	2100.81767	1560.55011		1
46	C	82.78658	85.65207	70.34766	-352.41524	704.96076	49.21465		1
47	H	82.33125	85.77172	71.35732	1714.76886	-2070.42778	443.35792		1
48	H	82.33134	86.39316	69.64794	1224.15040	1801.50881	1636.97633		1
49	C	84.07191	82.49440	70.27505	566.85117	537.05831	117.62814		1
50	O	84.32402	82.79073	71.43937	-550.26779	-406.08867	4.21666		1
51	N	84.20321	81.35285	69.63784	566.34832	-425.77725	180.18749		1
52	H	83.87905	81.38642	68.67113	644.44502	2646.80550	-52.73430		1
53	C	85.06094	80.28637	70.00954	612.34801	-281.48662	411.56221		1
54	H	85.10479	79.66542	69.08701	1667.23498	-1490.75142	1556.16753		1

55	C	86.47995	80.92334	70.38804	-714.45746	-175.43074	286.98927	1
56	H	86.32705	81.62782	71.25327	-787.09484	1763.03619	-1922.46060	1
57	O	87.11583	81.69481	69.35231	-429.46514	516.51932	-128.40526	1
58	H	87.16288	82.57425	69.77774	1981.82785	436.16847	-1818.18182	1
59	C	87.26932	79.65098	70.86818	630.79189	-468.94448	76.03230	1
60	H	88.27729	79.91832	71.26208	-1775.71861	2062.30353	131.89849	1
61	H	86.72809	79.10464	71.67768	-1855.14608	88.94118	1993.53760	1
62	H	87.42283	78.92996	70.03160	-1504.82350	-780.94249	-2132.90992	1
63	C	84.48867	79.42322	71.27802	288.57638	618.62814	-397.00270	1
64	O	84.65272	78.22817	71.28218	321.70495	-185.26452	574.37218	1
65	N	84.06264	80.20619	72.26556	-447.05792	-446.53431	367.76425	1
66	H	84.05139	81.24901	72.12221	350.31316	1975.63644	-1843.31522	1
67	C	83.11960	79.60992	73.16140	-511.23061	374.03917	-471.51480	1
68	H	83.48389	78.55821	73.21891	2234.79579	-898.70890	-1273.45190	1
69	C	83.27282	80.45119	74.51106	529.53781	-159.34528	563.72604	1
70	H	82.83773	79.84377	75.34903	654.59388	2347.94251	1217.51488	1
71	H	84.37339	80.53028	74.71317	-1526.55661	2103.42026	817.87394	1
72	O	82.64422	81.76200	74.50558	-554.84278	14.12789	399.58769	1
73	H	83.31931	82.25795	74.00359	1297.06236	2061.84854	1220.68812	1
74	C	81.65122	79.69790	72.47480	-662.15484	-412.13544	123.62687	1
75	O	81.51203	79.56833	71.27430	-540.01537	-317.05804	274.91456	1
76	N	80.64165	79.68466	73.40277	-202.76299	-690.00100	-131.49145	1
77	H	81.16359	79.88666	74.26581	-702.62132	-2617.37191	281.70413	1
78	C	79.53883	80.59182	73.12658	-491.73914	576.34187	222.73509	1
79	H	80.00636	81.57931	72.93756	1977.17978	-1823.58850	-434.68928	1
80	C	78.66898	80.07286	71.91969	-649.50797	-328.66843	306.11224	1
81	H	78.61982	78.96290	71.95162	2075.07803	1452.16490	-1004.45904	1
82	C	77.24396	80.71841	72.04948	-615.18735	-489.99689	-70.96352	1
83	H	76.50809	80.22485	71.37230	-1226.32661	-1724.38906	-1716.47170	1
84	H	76.84564	80.63892	73.09083	2381.64273	-969.84735	900.46860	1
85	H	77.26840	81.81739	71.77261	2122.74991	1702.23946	-141.36228	1
86	C	79.10629	80.57408	70.49665	-501.86074	-479.61276	-376.42482	1
87	H	78.29828	80.41626	69.74357	993.79261	-2246.95401	-1177.81305	1
88	H	79.33891	81.66812	70.49449	42.71279	-626.15391	-2651.37258	1
89	H	80.02514	80.03688	70.11248	-2026.39012	-1590.33709	-887.82922	1
90	C	78.61309	80.56490	74.45865	-672.89153	382.57394	-156.34072	1
91	O	78.01649	81.55497	74.82702	410.04627	221.86223	500.35950	1
92	N	78.45410	79.29801	74.87981	-378.11782	-443.79414	-441.10984	1
93	H	79.11455	78.65852	74.43496	2404.15973	-568.14894	1149.30085	1
94	C	78.06542	79.07061	76.25493	-544.54484	466.16019	331.29119	1
95	H	78.84035	79.61518	76.83605	-1409.80988	-170.17955	2325.32679	1
96	C	76.65006	79.73583	76.44288	-184.48284	116.78282	-758.89137	1
97	H	76.70768	80.84213	76.26101	1893.78641	1861.14652	611.04528	1
98	H	75.94761	79.35578	75.66548	-2170.79665	-974.19311	1327.50117	1
99	C	76.11212	79.44328	77.88324	389.51668	672.81878	-138.49152	1
100	H	76.37550	78.40987	78.20198	510.64577	1933.03327	1851.02484	1
101	H	76.62578	80.08910	78.62869	-2302.30869	-1105.72939	-948.89774	1
102	C	74.55003	79.63498	77.97473	-559.93427	-126.34590	542.30857	1
103	O	73.95356	79.26332	78.95228	-670.36003	-111.83166	76.36448	1
104	N	74.00804	80.23039	76.88832	-216.06729	-537.07037	446.51379	1
105	H	74.47691	80.64679	76.07582	-1251.96487	1074.12894	-2168.52500	1
106	H	73.02059	80.49737	76.81691	-2451.83023	-720.73851	944.84612	1
107	C	78.21178	77.46168	76.43021	546.24052	-563.88337	-85.11809	1
108	O	79.32852	77.09321	76.69650	71.70702	-307.40463	606.69673	1
109	N	77.12084	76.70512	76.21944	479.90863	-504.50129	222.86849	1
110	C	77.23992	75.28058	76.20564	75.51268	-600.91904	506.73700	1
111	H	78.07419	74.99413	76.88701	-2033.61562	1795.30103	254.89480	1
112	C	75.76456	74.86687	76.64134	523.79067	517.99274	284.45581	1
113	H	75.52205	73.80414	76.41392	1599.61665	-1127.00911	1895.98173	1
114	H	75.60567	75.00273	77.73656	-1881.83093	1275.82488	-1501.55016	1
115	C	74.90454	75.87828	75.82377	-600.05639	-404.05026	316.64485	1
116	H	74.71907	75.50515	74.78782	-2597.05260	496.36221	657.73249	1

117	H	73.90166	76.05248	76.27446	-1666.24518	1294.38985	-1723.90591	1
118	C	75.81067	77.18487	75.80761	493.57570	-129.95376	-602.56394	1
119	H	75.94987	77.64096	74.79831	-1469.08415	-637.84797	2204.22581	1
120	H	75.50259	77.97358	76.53669	-1038.97840	1068.88701	-2280.71789	1
121	C	77.46562	74.84910	74.64315	188.88100	241.05089	-727.87821	1
122	O	76.62973	75.11192	73.78821	531.88613	-49.19943	427.07960	1
123	N	78.60099	74.20322	74.48523	708.14833	26.93417	-179.73509	1
124	H	79.15535	74.06555	75.32678	-2232.69501	-1179.09831	1023.94816	1
125	C	79.00465	73.72338	73.16520	-738.32412	259.92548	104.42456	1
126	H	78.54666	74.49746	72.50291	2028.89123	1260.02983	1311.33324	1
127	C	80.52333	73.65779	73.11156	-258.65678	-345.52513	661.28459	1
128	H	80.86198	72.94239	73.89379	-1826.06090	-1801.46097	-918.64554	1
129	C	81.01284	73.15040	71.76820	-541.23400	531.92970	-218.41428	1
130	H	82.13559	73.08702	71.73040	1311.73218	-2219.18200	882.19023	1
131	H	80.60961	72.12089	71.54700	-1048.71298	1223.58118	-2196.97971	1
132	H	80.68902	73.82455	70.92758	419.06414	1903.92898	1903.44670	1
133	C	81.14930	75.00623	73.41647	-423.86431	152.66566	-648.55262	1
134	H	82.27240	74.95030	73.44392	105.68386	-2342.50080	1387.51238	1
135	H	80.87441	75.77398	72.64127	-1695.63603	-1484.73621	-1531.02793	1
136	H	80.80696	75.40759	74.41067	-1853.57121	-487.39031	1936.59343	1
137	C	78.24914	72.25122	72.97338	539.71428	-510.58232	267.58633	1
138	O	78.90009	71.25715	72.77154	-15.93758	-278.34085	-624.49402	1
139	N	76.95117	72.40914	73.09051	-676.81886	12.05292	276.17960	1
140	H	76.57825	73.36976	73.21540	-1694.44250	-373.84189	-2100.66098	1
141	C	76.04686	71.33103	72.78991	412.33078	-664.70360	108.35451	1
142	H	76.11231	71.27737	71.68162	1765.77476	1294.44366	1621.76594	1
143	C	76.55470	70.00373	73.46469	-179.66635	-721.95667	-264.73915	1
144	H	77.59782	69.75427	73.12829	-607.34922	2587.87032	-598.10018	1
145	H	76.62455	70.12385	74.56998	-359.69332	-1479.13954	-2259.74260	1
146	C	75.56711	68.84863	73.07596	-240.01076	616.02425	431.85322	1
147	H	74.52326	69.09530	73.37257	-1359.17131	782.54425	2227.99181	1
148	H	75.54427	68.69924	71.97362	-820.36667	85.81767	-2596.78715	1
149	C	76.06994	67.54477	73.81356	-513.07015	236.18570	-551.87280	1
150	H	77.11097	67.29329	73.50537	1816.11944	-1183.11722	-1650.94321	1
151	H	76.11143	67.70524	74.91562	-1800.04429	-1361.53473	1526.34643	1
152	C	75.10126	66.39036	73.46541	726.08972	-253.19732	-179.64713	1
153	H	74.07720	66.50823	73.87244	1224.27271	-456.51798	-2390.90304	1
154	H	75.05382	66.13609	72.38781	1206.40339	-1150.93514	-2154.90344	1
155	N	75.65754	65.09600	74.14978	329.70796	-633.68968	-155.67358	1
156	H	75.08564	64.21451	74.00410	1348.31305	1938.76845	1359.00643	1
157	H	76.62169	64.77001	73.84818	2096.92035	1446.54551	-966.48890	1
158	H	75.75313	65.11153	75.20679	-1197.07217	-2303.53719	827.28733	1
159	C	74.57872	71.84772	73.29033	-378.01186	-556.17301	-413.96481	1
160	O	74.00063	72.69579	72.65086	-409.44433	-307.55053	-453.30833	1
161	N	74.17781	71.24843	74.40541	-429.02477	524.70884	274.08502	1
162	H	74.75652	70.55744	74.88026	1706.34263	-1425.96036	1574.38926	1
163	C	72.92414	71.60772	74.96892	-45.25864	-626.22952	478.93267	1
164	H	72.65441	72.59946	74.53600	1988.63164	570.90773	1772.87287	1
165	C	71.91732	70.45267	74.55091	551.77128	-20.49526	-564.54996	1
166	H	71.90951	70.33061	73.44496	1434.61535	-1753.10253	1513.99471	1
167	H	72.25861	69.47427	74.95645	-714.67738	1819.09770	1898.36494	1
168	C	70.48914	70.80519	75.07908	446.99263	-555.77305	338.97221	1
169	H	70.49736	70.87187	76.19345	1953.68466	1892.25957	-161.67766	1
170	H	70.16991	71.80713	74.71407	-403.03785	2688.07032	-188.43591	1
171	C	69.47128	69.69373	74.60032	567.86262	335.74681	434.04421	1
172	H	69.38798	69.67750	73.48968	-1080.02275	1568.26081	-1948.78900	1
173	H	69.82279	68.67864	74.89347	-919.54108	2111.34692	1456.13463	1
174	C	68.10064	69.99995	75.25858	195.81897	173.33862	-745.11536	1
175	H	68.09895	69.91634	76.37894	1405.67949	-2301.21089	-390.08113	1
176	H	67.64361	70.96359	74.94850	-940.37328	-1118.32446	2299.72133	1
177	N	67.07814	68.93367	74.80435	319.26422	656.36007	-42.02424	1
178	H	66.05613	69.22288	75.05206	1961.03633	619.91968	1787.09422	1

179	H	67.02800	68.76674	73.75262	854.14343	-2156.80752	1429.08711	1
180	H	67.20976	67.93279	75.24021	1237.02905	-1378.50857	-1998.28500	1
181	C	73.15094	71.55048	76.59427	532.53319	-268.57236	517.55729	1
182	O	73.81414	70.67588	77.10350	266.16714	-290.73804	-558.88002	1
183	N	72.47957	72.53338	77.18462	-226.25352	640.49678	-270.32839	1
184	H	71.92107	73.17388	76.62299	2007.69063	-1035.27229	1523.50231	1
185	C	72.54751	72.60443	78.60197	-540.76542	-573.33303	49.50000	1
186	H	73.48941	72.06418	78.85180	-2374.20950	-1036.76023	843.75774	1
187	C	72.48848	74.12552	79.07038	-77.09082	666.87422	-415.84136	1
188	H	71.47493	74.54453	78.82462	-985.81834	617.19825	2463.91927	1
189	O	73.45074	75.01891	78.47543	293.29899	-391.65602	-477.80926	1
190	H	72.87107	75.74575	78.17317	2528.72714	-681.76262	-751.27122	1
191	C	72.61101	73.94404	80.62925	252.47363	-605.14473	440.05134	1
192	H	72.46818	74.91095	81.16480	-2052.65063	1456.49051	-1043.51830	1
193	H	71.85317	73.22885	81.02375	-2152.98800	-1661.97574	-161.70652	1
194	H	73.61410	73.55304	80.91692	-473.12726	-1584.27339	2165.61725	1
195	C	71.18924	71.84098	79.17558	360.36307	488.46713	505.10056	1
196	O	70.12579	72.40920	79.22451	-200.08817	-528.03552	-385.82850	1
197	N	71.56362	70.64867	79.60333	-597.54095	-226.44775	355.20479	1
198	H	72.54854	70.42007	79.46303	2179.23655	-1300.70981	-991.33835	1
199	C	70.68104	69.60656	79.97484	-687.68921	297.39807	-249.45179	1
200	H	71.31756	68.87829	80.52362	-349.16256	-2467.37713	-1101.72831	1
201	C	69.46048	70.18970	80.83018	672.47345	361.54328	-201.62880	1
202	H	68.89308	70.94288	80.22829	1541.41502	582.18425	2169.97026	1
203	H	68.74450	69.37359	81.08518	-2534.67717	60.25153	997.72295	1
204	C	70.05895	70.82527	82.09364	574.26774	-389.43119	-377.02542	1
205	C	70.64897	70.00850	83.10453	688.82679	-287.33580	-257.96133	1
206	H	70.63920	68.90671	83.01911	331.14182	1470.38163	2269.80013	1
207	C	70.08166	72.24755	82.20626	-383.52382	-675.04808	144.24917	1
208	H	69.64181	72.87763	81.40952	4.09847	1517.59662	2262.86397	1
209	C	71.25625	70.63476	84.19264	-134.76730	428.45285	-649.50303	1
210	H	71.72035	70.00612	84.97250	-903.23433	1600.49020	2011.53387	1
211	C	70.70034	72.82772	83.31603	-335.53281	-615.00040	-364.39058	1
212	H	70.72033	73.92924	83.38733	1596.45398	-1369.33862	1732.02659	1
213	C	71.31024	72.05093	84.34356	585.48547	-340.24194	-406.23938	1
214	O	71.95091	72.62996	85.46998	-419.15649	-173.04408	-511.94141	1
215	H	71.79779	73.58473	85.27570	-1071.84350	1559.71507	-1960.13012	1
216	C	70.02945	68.96454	78.61864	291.41878	-183.13091	710.72246	1
217	O	69.49705	69.63136	77.75411	379.87695	523.47396	-222.23622	1
218	N	70.09302	67.64474	78.71573	564.30591	373.09380	277.24371	1
219	H	70.56935	67.22725	79.51373	-120.59931	-2436.07824	-1214.35098	1
220	C	69.73448	66.88959	77.54083	404.07514	-299.37480	608.84009	1
221	H	70.21256	67.43223	76.69371	-1071.07882	-841.69025	2359.66467	1
222	C	70.26268	65.40902	77.73935	-683.12807	68.71770	-390.13096	1
223	H	71.35035	65.39566	77.97604	2068.88918	1596.58590	770.89603	1
224	H	69.75850	64.92562	78.60624	1379.86429	2342.49779	-179.85638	1
225	C	69.96053	64.63897	76.41666	-176.39967	537.49466	550.97268	1
226	H	68.88501	64.74542	76.14053	-396.28051	1942.22168	1869.33314	1
227	H	70.53204	65.06775	75.56358	-94.44700	586.00678	-2659.20016	1
228	C	70.35103	63.10979	76.66397	-291.69381	-718.18079	-150.72929	1
229	H	71.43568	62.91180	76.86017	-2303.38776	1089.76242	964.62032	1
230	H	69.76062	62.58411	77.45710	884.16729	2568.80533	-207.74283	1
231	N	70.02330	62.52305	75.43266	-594.49522	-252.81478	342.29276	1
232	H	69.62558	63.12974	74.73259	-1735.17426	2084.05705	-263.71605	1
233	C	70.18660	61.29464	75.14972	595.23177	-271.52487	442.22352	1
234	N	70.73705	60.46495	76.13286	585.53813	-424.79750	-105.81303	1
235	H	71.03298	60.69462	77.08064	959.88797	1327.56823	-2177.11905	1
236	H	70.90843	59.46480	76.02490	1578.48647	16.27378	-2220.76233	1
237	N	69.75921	61.01734	73.84328	-452.17763	-390.33541	-421.51853	1
238	H	69.34884	61.62097	73.13254	470.26107	1974.25629	-1817.92087	1
239	H	69.79802	60.08531	73.42917	1856.67307	-1573.97321	-1224.35416	1
240	C	68.12279	66.88707	77.39414	-531.47271	-581.45780	-55.06206	1

241	O	67.60643	66.68840	76.28761	-243.00837	192.73507	609.52485	1
242	N	67.52320	66.97413	78.56491	343.49288	-644.25607	38.09164	1
243	H	68.17877	67.13755	79.33146	-1691.16043	-1535.97525	-1484.73099	1
244	C	66.14259	67.41727	78.67332	542.66492	350.14337	454.42563	1
245	H	65.67331	67.09995	77.71067	1209.57979	-2396.95920	463.86744	1
246	C	65.51232	66.85493	79.93874	-737.14309	145.93010	242.71942	1
247	H	66.09916	67.24470	80.80160	-1050.18303	159.36419	-2509.06125	1
248	C	64.08087	67.33629	80.08908	-706.77696	-252.88343	-245.16230	1
249	H	63.61956	66.98164	81.05137	-1624.64039	-1665.49085	1417.86935	1
250	H	64.02336	68.46031	80.08521	2566.10521	598.51109	693.22305	1
251	H	63.42940	66.96709	79.24987	-1972.69758	107.10018	-1876.34312	1
252	C	65.56756	65.34038	79.99303	412.85148	672.58832	-27.69222	1
253	H	65.18164	64.94488	80.97338	1447.02277	1762.76533	-1490.78944	1
254	H	64.94697	64.87542	79.17813	1320.77379	-145.20455	2378.68491	1
255	H	66.61947	64.96187	79.86594	-1512.10848	1470.52031	1724.75147	1
256	C	66.19185	69.07504	78.90192	-607.11113	499.56689	73.73769	1
257	O	66.44759	69.54419	79.98570	357.97126	460.81534	356.68785	1
258	N	65.93392	69.68708	77.75387	536.55407	-368.62270	332.76306	1
259	H	65.76741	69.04840	76.97472	524.38866	2297.69985	1367.20941	1
260	C	65.12731	70.88497	77.81090	46.50277	-774.29190	-147.97904	1
261	H	64.33600	70.65921	78.56012	1676.51875	1883.29066	1032.55549	1
262	C	66.06775	72.10306	78.29307	-559.41456	-34.19198	-556.30433	1
263	H	67.13869	71.81397	78.15881	-64.66664	395.18769	2695.05373	1
264	H	65.90064	73.00829	77.66091	-2703.44278	-60.40056	333.79418	1
265	C	65.77253	72.40818	79.73778	-519.76435	377.31045	459.42366	1
266	H	65.81037	71.44253	80.31282	-1746.74323	1667.50644	-1261.73691	1
267	C	66.83967	73.33692	80.30318	570.95554	16.46261	-545.27700	1
268	H	66.69589	73.51305	81.40076	2391.58273	28.05277	-1305.07271	1
269	H	67.86863	72.91369	80.16256	175.75588	917.63458	2559.43867	1
270	H	66.82271	74.33788	79.80013	-1063.97851	-2155.34650	1283.00462	1
271	C	64.39951	73.04446	79.89932	193.76014	2.62946	-765.53141	1
272	H	64.18591	73.30367	80.96837	507.39394	-846.55087	2539.60089	1
273	H	64.31402	73.99215	79.30695	1337.57841	1818.19054	1526.01994	1
274	H	63.57761	72.36579	79.55416	1100.88635	-1172.91350	-2199.08909	1
275	C	64.56320	71.12702	76.35038	-549.21115	475.64486	-309.38218	1
276	O	64.92153	70.45966	75.38859	556.06106	-390.37755	-78.24250	1
277	O	63.63119	72.16416	76.18959	-572.27940	-310.19032	-209.75862	1
278	H	63.58045	72.47397	77.14328	-1380.08193	2212.14486	790.85944	1

Listing 80: C00080.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.5263	0.0000	300.0000
3	H	79.02095	77.29813	83.72580	-2043.14101	-1757.64893	399.89339		1
4	N	79.97342	77.03808	83.47662	426.75047	490.45733	-334.42467		1
5	H	79.83678	76.53445	82.60082	442.25559	-1110.30854	-2448.52907		1
6	C	80.86905	78.12254	83.34954	415.32972	-666.39213	83.73172		1
7	H	80.53529	78.92242	84.04633	879.32219	2491.00447	667.35213		1
8	C	82.35210	77.56385	83.66986	31.35357	477.41777	628.23362		1
9	H	82.52957	76.63876	83.07163	1168.38489	2240.25337	-1019.71136		1
10	H	83.13159	78.30125	83.35513	-360.43770	2534.90498	931.67112		1
11	C	82.43414	77.27966	85.14531	463.18208	512.70242	-382.34388		1
12	H	81.49781	76.75553	85.44473	1725.29117	1863.52247	-987.07854		1
13	C	83.61015	76.36667	85.46815	710.42801	-144.27427	-313.15367		1
14	H	83.61630	76.07052	86.54875	364.20195	-1033.13725	2494.72524		1
15	H	83.58049	75.42249	84.86526	2567.61904	335.80679	847.48802		1
16	H	84.59191	76.86300	85.26138	-2587.99029	680.92867	-512.16411		1
17	C	82.55670	78.57079	85.94400	268.17616	741.64379	-40.42634		1
18	H	82.64891	78.36928	87.04235	1283.54314	-1945.37420	-1411.27812		1
19	H	83.45943	79.16011	85.63820	-1258.57796	1317.15249	-2026.02085		1
20	H	81.66516	79.23412	85.80319	-2502.84526	909.80597	575.92391		1

21	C	80.85277	78.54700	81.78483	619.36578	-458.64843	-172.09273	1
22	O	80.78575	77.72534	80.86771	-81.40433	433.87611	522.34594	1
23	N	81.00521	79.84985	81.72878	175.23996	-622.20190	341.55523	1
24	H	81.01675	80.37759	82.60007	-876.57256	-303.22879	-2561.90213	1
25	C	81.06251	80.48489	80.45296	-571.88214	-534.10783	-106.15033	1
26	H	80.40883	79.81556	79.84879	-2713.20841	-16.25800	-248.80809	1
27	C	80.48240	81.96823	80.63144	166.60354	288.16399	-716.09568	1
28	H	81.21341	82.57499	81.23105	-2097.85574	1636.78449	-586.18044	1
29	O	79.22000	82.05018	81.31557	-317.80580	-363.38227	484.43082	1
30	H	79.45284	82.62570	82.07108	1863.74748	-1451.84923	1357.29467	1
31	C	80.47248	82.50298	79.15317	503.80731	517.99032	318.51606	1
32	H	80.10472	83.55417	79.10443	640.61020	-2157.10410	-1536.29104	1
33	H	81.48935	82.48637	78.69350	1687.88455	465.60692	2087.56452	1
34	H	79.80433	81.89041	78.50418	-1293.07895	-1899.88581	-1463.57452	1
35	C	82.58136	80.48249	79.85394	-153.07550	-733.68902	248.70981	1
36	O	82.64083	80.52345	78.64810	186.15459	-480.78787	-449.34387	1
37	N	83.60448	80.51901	80.72177	-487.53139	543.18517	42.03850	1
38	C	84.94189	80.55371	80.21470	-699.35871	69.34393	360.10701	1
39	H	84.89953	81.08552	79.23573	2.81126	-221.99807	-2715.58072	1
40	C	85.71644	81.30616	81.38177	-507.46439	-592.59194	122.07761	1
41	H	86.81437	81.12352	81.35854	-1975.08116	525.87560	-1801.71556	1
42	H	85.57154	82.40823	81.33059	1588.27743	-1913.22100	1113.83566	1
43	C	85.01761	80.69841	82.63657	-613.62442	-457.55993	-194.14490	1
44	H	85.40730	79.66652	82.83408	1707.54637	-721.27992	1996.92523	1
45	H	85.17556	81.28559	83.56956	758.23357	2100.81767	1560.55011	1
46	C	83.50030	80.66078	82.16796	-352.41524	704.96076	49.21465	1
47	H	82.92028	79.79206	82.56003	1714.76886	-2070.42778	443.35792	1
48	H	82.92602	81.59958	82.34708	1224.15040	1801.50881	1636.97633	1
49	C	85.54549	79.03505	80.06185	566.85117	537.05831	117.62814	1
50	O	86.61251	78.88714	79.51312	-550.26779	-406.08867	4.21666	1
51	N	84.75252	78.10707	80.58995	566.34832	-425.77725	180.18749	1
52	H	83.88747	78.43254	81.01887	644.44502	2646.80550	-52.73430	1
53	C	85.29596	76.80804	80.81076	612.34801	-281.48662	411.56221	1
54	H	86.24556	76.83858	80.22260	1667.23498	-1490.75142	1556.16753	1
55	C	85.55672	76.60282	82.37525	-714.45746	-175.43074	286.98927	1
56	H	84.58162	76.35744	82.87338	-787.09484	1763.03619	-1922.46060	1
57	O	86.10098	77.73074	83.10067	-429.46514	516.51932	-128.40526	1
58	H	85.42457	77.83644	83.79736	1981.82785	436.16847	-1818.18182	1
59	C	86.46706	75.32357	82.37170	630.79189	-468.94448	76.03230	1
60	H	86.68928	74.97854	83.40856	-1775.71861	2062.30353	131.89849	1
61	H	85.97866	74.46833	81.82995	-1855.14608	88.94118	1993.53760	1
62	H	87.44602	75.52153	81.87488	-1504.82350	-780.94249	-2132.90992	1
63	C	84.21825	75.69757	80.29642	288.57638	618.62814	-397.00270	1
64	O	84.25121	74.56212	80.72802	321.70495	-185.26452	574.37218	1
65	N	83.38784	76.17849	79.37827	-447.05792	-446.53431	367.76425	1
66	H	83.51705	77.14564	79.08494	350.31316	1975.63644	-1843.31522	1
67	C	82.62169	75.20577	78.63780	-511.23061	374.03917	-471.51480	1
68	H	83.40666	74.42307	78.52019	2234.79579	-898.70890	-1273.45190	1
69	C	81.48862	74.68069	79.62204	529.53781	-159.34528	563.72604	1
70	H	81.23638	73.63143	79.30910	654.59388	2347.94251	1217.51488	1
71	H	81.97004	74.61097	80.63502	-1526.55661	2103.42026	817.87394	1
72	O	80.24406	75.40826	79.68971	-554.84278	14.12789	399.58769	1
73	H	80.57249	76.25943	80.16355	1297.06236	2061.84854	1220.68812	1
74	C	82.19266	75.88713	77.23729	-662.15484	-412.13544	123.62687	1
75	O	83.07810	76.34210	76.51443	-540.01537	-317.05804	274.91456	1
76	N	80.90397	75.74723	76.99471	-202.76299	-690.00100	-131.49145	1
77	H	80.34172	75.29631	77.72777	-702.62132	-2617.37191	281.70413	1
78	C	80.20375	76.58771	76.08590	-491.73914	576.34187	222.73509	1
79	H	79.14462	76.48765	76.41054	1977.17978	-1823.58850	-434.68928	1
80	C	80.75549	78.07172	76.21815	-649.50797	-328.66843	306.11224	1
81	H	81.84780	78.10458	75.99920	2075.07803	1452.16490	-1004.45904	1
82	C	79.96124	78.99614	75.23326	-615.18735	-489.99689	-70.96352	1

83	H	80.31590	80.05253	75.28718	-1226.32661	-1724.38906	-1716.47170	1
84	H	80.07625	78.65971	74.17572	2381.64273	-969.84735	900.46860	1
85	H	78.87006	78.99958	75.46326	2122.74991	1702.23946	-141.36228	1
86	C	80.48022	78.60014	77.66742	-501.86074	-479.61276	-376.42482	1
87	H	80.83930	79.65328	77.78477	993.79261	-2246.95401	-1177.81305	1
88	H	79.39251	78.58582	77.91390	42.71279	-626.15391	-2651.37258	1
89	H	81.00316	77.98217	78.43845	-2026.39012	-1590.33709	-887.82922	1
90	C	80.40021	76.07089	74.54046	-672.89153	382.57394	-156.34072	1
91	O	79.42836	75.96677	73.83595	410.04627	221.86223	500.35950	1
92	N	81.68139	75.92587	74.22737	-378.11782	-443.79414	-441.10984	1
93	H	82.42389	76.13114	74.94273	2404.15973	-568.14894	1149.30085	1
94	C	81.98351	75.21802	73.01542	-544.54484	466.16019	331.29119	1
95	H	81.32248	75.71133	72.26780	-1409.80988	-170.17955	2325.32679	1
96	C	83.53504	75.40493	72.76317	-184.48284	116.78282	-758.89137	1
97	H	83.82338	76.47997	72.80546	1893.78641	1861.14652	611.04528	1
98	H	84.12358	74.90237	73.56952	-2170.79665	-974.19311	1327.50117	1
99	C	83.86781	74.78076	71.37175	389.51668	672.81878	-138.49152	1
100	H	83.45692	73.74558	71.31147	510.64577	1933.03327	1851.02484	1
101	H	83.32972	75.32628	70.56555	-2302.30869	-1105.72939	-948.89774	1
102	C	85.41066	74.75444	71.05633	-559.93427	-126.34590	542.30857	1
103	O	85.79257	74.29459	70.01107	-670.36003	-111.83166	76.36448	1
104	N	86.18865	75.27056	72.03244	-216.06729	-537.07037	446.51379	1
105	H	85.92635	75.68761	72.93313	-1251.96487	1074.12894	-2168.52500	1
106	H	87.21131	75.33113	71.97625	-2451.83023	-720.73851	944.84612	1
107	C	81.65276	73.62310	73.08558	546.24052	-563.88337	-85.11809	1
108	O	81.38154	73.11037	72.02868	71.70702	-307.40463	606.69673	1
109	N	81.85915	73.01454	74.26677	479.90863	-504.50129	222.86849	1
110	C	81.48433	71.64982	74.44965	75.51268	-600.91904	506.73700	1
111	H	81.33783	71.22247	73.42892	-2033.61562	1795.30103	254.89480	1
112	C	82.71289	71.08666	75.28867	523.79067	517.99274	284.45581	1
113	H	82.46449	70.14327	75.82524	1599.61665	-1127.00911	1895.98173	1
114	H	83.58806	70.86859	74.63699	-1881.83093	1275.82488	-1501.55016	1
115	C	83.00177	72.28240	76.24901	-600.05639	-404.05026	316.64485	1
116	H	82.30506	72.27609	77.11624	-2597.05260	496.36221	657.73249	1
117	H	84.02910	72.26656	76.67680	-1666.24518	1294.38985	-1723.90591	1
118	C	82.73862	73.53366	75.30773	493.57570	-129.95376	-602.56394	1
119	H	82.18149	74.36786	75.79727	-1469.08415	-637.84797	2204.22581	1
120	H	83.64238	73.93981	74.78930	-1038.97840	1068.88701	-2280.71789	1
121	C	80.16339	71.53605	75.41676	188.88100	241.05089	-727.87821	1
122	O	80.05876	70.58927	76.16684	531.88613	-49.19943	427.07960	1
123	N	79.32228	72.54586	75.25715	708.14833	26.93417	-179.73509	1
124	H	79.55672	73.26220	74.57034	-2232.69501	-1179.09831	1023.94816	1
125	C	78.03464	72.43127	75.88342	-738.32412	259.92548	104.42456	1
126	H	77.91359	71.32318	75.87393	2028.89123	1260.02983	1311.33324	1
127	C	78.12643	72.94631	77.38390	-258.65678	-345.52513	661.28459	1
128	H	78.27213	74.04746	77.41748	-1826.06090	-1801.46097	-918.64554	1
129	C	76.83747	72.50070	78.15654	-541.23400	531.92970	-218.41428	1
130	H	76.85099	72.85758	79.21291	1311.73218	-2219.18200	882.19023	1
131	H	75.90528	72.89229	77.68618	-1048.71298	1223.58118	-2196.97971	1
132	H	76.74479	71.38969	78.18384	419.06414	1903.92898	1903.44670	1
133	C	79.31440	72.21223	78.09857	-423.86431	152.66566	-648.55262	1
134	H	79.44053	72.56220	79.15056	105.68386	-2342.50080	1387.51238	1
135	H	79.15320	71.10592	78.12805	-1695.63603	-1484.73621	-1531.02793	1
136	H	80.27702	72.38752	77.56108	-1853.57121	-487.39031	1936.59343	1
137	C	76.98346	73.20155	74.91675	539.71428	-510.58232	267.58633	1
138	O	76.93274	72.86709	73.73116	-15.93758	-278.34085	-624.49402	1
139	N	76.25733	74.08635	75.55810	-676.81886	12.05292	276.17960	1
140	H	76.47522	74.23259	76.54056	-1694.44250	-373.84189	-2100.66098	1
141	C	75.18528	74.80301	74.96368	412.33078	-664.70360	108.35451	1
142	H	74.93267	75.57195	75.72741	1765.77476	1294.44366	1621.76594	1
143	C	75.74458	75.41387	73.61412	-179.66635	-721.95667	-264.73915	1
144	H	76.76333	75.83393	73.78148	-607.34922	2587.87032	-598.10018	1

145	H	75.87912	74.62554	72.83520	-359.69332	-1479.13954	-2259.74260	1
146	C	74.74930	76.51810	73.12829	-240.01076	616.02425	431.85322	1
147	H	73.82812	76.06347	72.69746	-1359.17131	782.54425	2227.99181	1
148	H	74.40941	77.15239	73.97785	-820.36667	85.81767	-2596.78715	1
149	C	75.51698	77.39518	72.05832	-513.07015	236.18570	-551.87280	1
150	H	76.45387	77.81529	72.49199	1816.11944	-1183.11722	-1650.94321	1
151	H	75.83950	76.77163	71.19276	-1800.04429	-1361.53473	1526.34643	1
152	C	74.57411	78.53175	71.60087	726.08972	-253.19732	-179.64713	1
153	H	73.70276	78.19643	71.00388	1224.27271	-456.51798	-2390.90304	1
154	H	74.24011	79.20882	72.41216	1206.40339	-1150.93514	-2154.90344	1
155	N	75.39135	79.45908	70.63794	329.70796	-633.68968	-155.67358	1
156	H	74.85767	80.27497	70.21981	1348.31305	1938.76845	1359.00643	1
157	H	76.23504	79.95441	71.04989	2096.92035	1446.54551	-966.48890	1
158	H	75.80490	79.01144	69.76899	-1197.07217	-2303.53719	827.28733	1
159	C	73.91255	73.79218	74.69683	-378.01186	-556.17301	-413.96481	1
160	O	72.85858	74.04511	75.22187	-409.44433	-307.55053	-453.30833	1
161	N	74.25550	72.76644	73.93616	-429.02477	524.70884	274.08502	1
162	H	75.23179	72.70886	73.55044	1706.34263	-1425.96036	1574.38926	1
163	C	73.24567	71.92485	73.37981	-45.25864	-626.22952	478.93267	1
164	H	73.86759	71.08550	72.99402	1988.63164	570.90773	1772.87287	1
165	C	72.22560	71.48234	74.50757	551.77128	-20.49526	-564.54996	1
166	H	72.75251	71.29988	75.47085	1434.61535	-1753.10253	1513.99471	1
167	H	71.49865	72.30129	74.72221	-714.67738	1819.09770	1898.36494	1
168	C	71.50276	70.18591	74.00939	446.99263	-555.77305	338.97221	1
169	H	71.13395	70.31450	72.96750	1953.68466	1892.25957	-161.67766	1
170	H	72.21326	69.33061	73.96925	-403.03785	2688.07032	-188.43591	1
171	C	70.29491	69.86525	74.97852	567.86262	335.74681	434.04421	1
172	H	70.65756	69.62968	76.00553	-1080.02275	1568.26081	-1948.78900	1
173	H	69.62581	70.75018	75.08717	-919.54108	2111.34692	1456.13463	1
174	C	69.52276	68.67036	74.37189	195.81897	173.33862	-745.11536	1
175	H	68.99102	68.89974	73.42686	1405.67949	-2301.21089	-390.08113	1
176	H	70.12204	67.74564	74.25363	-940.37328	-1118.32446	2299.72133	1
177	N	68.38638	68.26923	75.37277	319.26422	656.36007	-42.02424	1
178	H	67.76492	67.46742	75.06211	1961.03633	619.91968	1787.09422	1
179	H	68.68690	67.93595	76.33473	854.14343	-2156.80752	1429.08711	1
180	H	67.66588	69.01135	75.61111	1237.02905	-1378.50857	-1998.28500	1
181	C	72.58084	72.77146	72.15224	532.53319	-268.57236	517.55729	1
182	O	73.26681	73.39758	71.38196	266.16714	-290.73804	-558.88002	1
183	N	71.26491	72.59278	72.11966	-226.25352	640.49678	-270.32839	1
184	H	70.69429	72.14601	72.84825	2007.69063	-1035.27229	1523.50231	1
185	C	70.55860	72.98769	70.95279	-540.76542	-573.33303	49.50000	1
186	H	71.16078	73.76762	70.43186	-2374.20950	-1036.76023	843.75774	1
187	C	70.31636	71.66035	70.08191	-77.09082	666.87422	-415.84136	1
188	H	69.63780	70.97716	70.66395	-985.81834	617.19825	2463.91927	1
189	O	71.47931	70.87301	69.77410	293.29899	-391.65602	-477.80926	1
190	H	71.26556	70.03276	70.22806	2528.72714	-681.76262	-751.27122	1
191	C	69.55120	72.22484	68.83227	252.47363	-605.14473	440.05134	1
192	H	69.28151	71.40677	68.12392	-2052.65063	1456.49051	-1043.51830	1
193	H	68.58449	72.75213	69.11563	-2152.98800	-1661.97574	-161.70652	1
194	H	70.17911	72.95210	68.26623	-473.12726	-1584.27339	2165.61725	1
195	C	69.15982	73.43650	71.68257	360.36307	488.46713	505.10056	1
196	O	68.82023	72.84298	72.68938	-200.08817	-528.03552	-385.82850	1
197	N	68.55636	74.42233	71.03400	-597.54095	-226.44775	355.20479	1
198	H	68.98128	74.78079	70.17793	2179.23655	-1300.70981	-991.33835	1
199	C	67.21032	74.72464	71.36284	-687.68921	297.39807	-249.45179	1
200	H	67.04970	74.25169	72.36196	-349.16256	-2467.37713	-1101.72831	1
201	C	67.01303	76.31752	71.33432	672.47345	361.54328	-201.62880	1
202	H	66.89909	76.66063	70.28113	1541.41502	582.18425	2169.97026	1
203	H	66.06611	76.57877	71.86412	-2534.67717	60.25153	997.72295	1
204	C	68.20868	77.02210	71.98591	574.26774	-389.43119	-377.02542	1
205	C	68.28013	77.16107	73.40511	688.82679	-287.33580	-257.96133	1
206	H	67.48033	76.75503	74.05287	331.14182	1470.38163	2269.80013	1

207	C	69.25547	77.52793	71.15577	-383.52382	-675.04808	144.24917	1
208	H	69.21105	77.40527	70.05872	4.09847	1517.59662	2262.86397	1
209	C	69.38066	77.82063	73.95335	-134.76730	428.45285	-649.50303	1
210	H	69.43440	77.93394	75.05037	-903.23433	1600.49020	2011.53387	1
211	C	70.33582	78.18027	71.75261	-335.53281	-615.00040	-364.39058	1
212	H	71.13592	78.57168	71.10003	1596.45398	-1369.33862	1732.02659	1
213	C	70.43982	78.35693	73.16375	585.48547	-340.24194	-406.23938	1
214	O	71.53455	79.02527	73.77186	-419.15649	-173.04408	-511.94141	1
215	H	72.03262	79.29478	72.96329	-1071.84350	1559.71507	-1960.13012	1
216	C	66.30237	74.09672	70.16492	291.41878	-183.13091	710.72246	1
217	O	66.80670	73.45432	69.26232	379.87695	523.47396	-222.23622	1
218	N	65.04434	74.41069	70.38938	564.30591	373.09380	277.24371	1
219	H	64.81266	74.94919	71.24237	-120.59931	-2436.07824	-1214.35098	1
220	C	64.00155	74.14627	69.44810	404.07514	-299.37480	608.84009	1
221	H	63.46499	75.11671	69.36638	-1071.07882	-841.69025	2359.66467	1
222	C	64.57180	73.58946	68.08844	-683.12807	68.71770	-390.13096	1
223	H	65.36395	74.26402	67.68595	2068.88918	1596.58590	770.89603	1
224	H	65.07394	72.60674	68.27294	1379.86429	2342.49779	-179.85638	1
225	C	63.41080	73.41390	67.05772	-176.39967	537.49466	550.97268	1
226	H	62.57990	72.81100	67.48663	-396.28051	1942.22168	1869.33314	1
227	H	62.96380	74.39102	66.76953	-94.44700	586.00678	-2659.20016	1
228	C	64.08146	72.67598	65.80978	-291.69381	-718.18079	-150.72929	1
229	H	64.85763	73.26431	65.25704	-2303.38776	1089.76242	964.62032	1
230	H	64.51512	71.66715	66.03140	884.16729	2568.80533	-207.74283	1
231	N	62.99342	72.48004	64.94888	-594.49522	-252.81478	342.29276	1
232	H	62.08823	72.76105	65.29245	-1735.17426	2084.05705	-263.71605	1
233	C	63.07623	71.96931	63.78745	595.23177	-271.52487	442.22352	1
234	N	64.34257	71.58266	63.33543	585.53813	-424.79750	-105.81303	1
235	H	65.24384	71.64365	63.80761	959.88797	1327.56823	-2177.11905	1
236	H	64.53627	71.16196	62.42616	1578.48647	16.27378	-2220.76233	1
237	N	61.81420	71.89964	63.18151	-452.17763	-390.33541	-421.51853	1
238	H	60.89473	72.18200	63.51775	470.26107	1974.25629	-1817.92087	1
239	H	61.66416	71.51998	62.24602	1856.67307	-1573.97321	-1224.35416	1
240	C	63.06089	72.97848	70.12055	-531.47271	-581.45780	-55.06206	1
241	O	63.39825	71.81677	70.18200	-243.00837	192.73507	609.52485	1
242	N	61.92782	73.54736	70.52973	343.49288	-644.25607	38.09164	1
243	H	61.88095	74.55616	70.38115	-1691.16043	-1535.97525	-1484.73099	1
244	C	60.97283	72.90342	71.42562	542.66492	350.14337	454.42563	1
245	H	60.06177	73.54413	71.34962	1209.57979	-2396.95920	463.86744	1
246	C	60.72671	71.47999	70.95491	-737.14309	145.93010	242.71942	1
247	H	61.72110	70.95803	70.90942	-1050.18303	159.36419	-2509.06125	1
248	C	59.82789	70.71360	71.90591	-706.77696	-252.88343	-245.16230	1
249	H	59.68662	69.64663	71.57768	-1624.64039	-1665.49085	1417.86935	1
250	H	60.25156	70.69264	72.95006	2566.10521	598.51109	693.22305	1
251	H	58.80633	71.17984	71.97450	-1972.69758	107.10018	-1876.34312	1
252	C	60.14082	71.45274	69.55453	412.85148	672.58832	-27.69222	1
253	H	60.01792	70.40219	69.17283	1447.02277	1762.76533	-1490.78944	1
254	H	59.12927	71.94265	69.51795	1320.77379	-145.20455	2378.68491	1
255	H	60.80208	71.99853	68.82669	-1512.10848	1470.52031	1724.75147	1
256	C	61.57407	72.94525	72.97399	-607.11113	499.56689	73.73769	1
257	O	60.82569	72.69547	73.89069	357.97126	460.81534	356.68785	1
258	N	62.85956	73.23637	73.02863	536.55407	-368.62270	332.76306	1
259	H	63.36754	73.40373	72.16160	524.38866	2297.69985	1367.20941	1
260	C	63.47712	73.40111	74.29739	46.50277	-774.29190	-147.97904	1
261	H	62.62940	73.55291	75.00483	1676.51875	1883.29066	1032.55549	1
262	C	64.33417	72.07022	74.63937	-559.41456	-34.19198	-556.30433	1
263	H	65.11720	71.92996	73.85683	-64.66664	395.18769	2695.05373	1
264	H	64.88257	72.20142	75.60194	-2703.44278	-60.40056	333.79418	1
265	C	63.43617	70.86687	74.69726	-519.76435	377.31045	459.42366	1
266	H	62.88184	70.79972	73.73296	-1746.74323	1667.50644	-1261.73691	1
267	C	64.26099	69.59703	74.87386	570.95554	16.46261	-545.27700	1
268	H	63.61276	68.68355	74.89723	2391.58273	28.05277	-1305.07271	1

269	H	64.99582	69.46200	74.03899	175.75588	917.63458	2559.43867	1
270	H	64.84436	69.61374	75.83004	-1063.97851	-2155.34650	1283.00462	1
271	C	62.42158	70.97227	75.82755	193.76014	2.62946	-765.53141	1
272	H	61.84911	70.01810	75.95947	507.39394	-846.55087	2539.60089	1
273	H	62.91230	71.20348	76.80804	1337.57841	1818.19054	1526.01994	1
274	H	61.66571	71.78256	75.62407	1100.88635	-1172.91350	-2199.08909	1
275	C	64.50838	74.62364	74.17064	-549.21115	475.64486	-309.38218	1
276	O	64.88288	75.06694	73.10387	556.06106	-390.37755	-78.24250	1
277	O	65.04237	75.11804	75.37502	-572.27940	-310.19032	-209.75862	1
278	H	64.53322	74.53693	76.01521	-1380.08193	2212.14486	790.85944	1

Listing 81: C00081.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.2750	1100
		0.2500	300.00	0.00	0.00	0.00	-1293.5211	0.0000	300.0000
3	H	74.17324	77.32821	70.79415	-2043.14101	-1757.64893	399.89339		1
4	N	74.49287	77.73899	69.90037	426.75047	490.45733	-334.42467		1
5	H	73.63175	78.04654	69.43224	442.25559	-1110.30854	-2448.52907		1
6	C	75.47937	78.75883	69.96965	415.32972	-666.39213	83.73172		1
7	H	75.60893	79.00154	71.05019	879.32219	2491.00447	667.35213		1
8	C	76.84202	78.12605	69.34476	31.35357	477.41777	628.23362		1
9	H	76.66678	77.83199	68.28329	1168.38489	2240.25337	-1019.71136		1
10	H	77.66430	78.87748	69.32788	-360.43770	2534.90498	931.67112		1
11	C	77.20127	76.92789	70.16848	463.18208	512.70242	-382.34388		1
12	H	76.27862	76.32468	70.32906	1725.29117	1863.52247	-987.07854		1
13	C	78.21257	76.04510	69.44504	710.42801	-144.27427	-313.15367		1
14	H	78.50395	75.16027	70.06842	364.20195	-1033.13725	2494.72524		1
15	H	77.80216	75.65105	68.47988	2567.61904	335.80679	847.48802		1
16	H	79.15247	76.60424	69.20470	-2587.99029	680.92867	-512.16411		1
17	C	77.75814	77.31986	71.53218	268.17616	741.64379	-40.42634		1
18	H	78.17611	76.43340	72.07554	1283.54314	-1945.37420	-1411.27812		1
19	H	78.58667	78.06703	71.44174	-1258.57796	1317.15249	-2026.02085		1
20	H	76.97261	77.77134	72.19086	-2502.84526	909.80597	575.92391		1
21	C	74.86742	79.93108	69.11174	619.36578	-458.64843	-172.09273		1
22	O	73.64699	79.91459	68.64311	-81.40433	433.87611	522.34594		1
23	N	75.68246	80.90619	68.86402	175.23996	-622.20190	341.55523		1
24	H	76.61718	80.91017	69.26534	-876.57256	-303.22879	-2561.90213		1
25	C	75.04456	81.98278	68.16751	-571.88214	-534.10783	-106.15033		1
26	H	74.51772	82.50064	68.99331	-2713.20841	-16.25800	-248.80809		1
27	C	76.12225	82.94138	67.54742	166.60354	288.16399	-716.09568		1
28	H	76.90816	82.35411	66.99656	-2097.85574	1636.78449	-586.18044		1
29	O	76.88913	83.71109	68.51892	-317.80580	-363.38227	484.43082		1
30	H	77.79863	83.49284	68.25948	1863.74748	-1451.84923	1357.29467		1
31	C	75.27029	83.78576	66.52861	503.80731	517.99032	318.51606		1
32	H	75.90442	84.51734	65.97501	640.61020	-2157.10410	-1536.29104		1
33	H	74.76736	83.13989	65.77023	1687.88455	465.60692	2087.56452		1
34	H	74.47356	84.36591	67.05019	-1293.07895	-1899.88581	-1463.57452		1
35	C	73.82357	81.26402	67.20996	-153.07550	-733.68902	248.70981		1
36	O	72.80099	81.94669	67.08633	186.15459	-480.78787	-449.34387		1
37	N	74.35213	80.51860	66.17862	-487.53139	543.18517	42.03850		1
38	C	73.57971	80.04334	65.09536	-699.35871	69.34393	360.10701		1
39	H	72.92234	80.89404	64.80268	2.81126	-221.99807	-2715.58072		1
40	C	74.67551	79.59085	64.02998	-507.46439	-592.59194	122.07761		1
41	H	74.28648	78.82628	63.32006	-1975.08116	525.87560	-1801.71556		1
42	H	75.04037	80.44363	63.41623	1588.27743	-1913.22100	1113.83566		1
43	C	75.78991	79.04216	64.96715	-613.62442	-457.55993	-194.14490		1
44	H	75.52698	78.03571	65.36157	1707.54637	-721.27992	1996.92523		1
45	H	76.78529	78.94713	64.47986	758.23357	2100.81767	1560.55011		1
46	C	75.74969	80.15221	66.11848	-352.41524	704.96076	49.21465		1
47	H	76.07191	79.80491	67.12758	1714.76886	-2070.42778	443.35792		1
48	H	76.30173	81.08923	65.86349	1224.15040	1801.50881	1636.97633		1

49	C	72.69819	78.66054	65.32483	566.85117	537.05831	117.62814	1
50	O	72.08722	78.22384	64.38110	-550.26779	-406.08867	4.21666	1
51	N	72.84164	78.15753	66.53694	566.34832	-425.77725	180.18749	1
52	H	73.37707	78.70558	67.22300	644.44502	2646.80550	-52.73430	1
53	C	72.12839	76.97629	66.89561	612.34801	-281.48662	411.56221	1
54	H	71.60777	76.69982	65.94894	1667.23498	-1490.75142	1556.16753	1
55	C	73.29808	75.93069	67.20212	-714.45746	-175.43074	286.98927	1
56	H	74.04857	76.43903	67.86618	-787.09484	1763.03619	-1922.46060	1
57	O	74.04625	75.57110	66.01382	-429.46514	516.51932	-128.40526	1
58	H	74.90821	75.97957	66.20977	1981.82785	436.16847	-1818.18182	1
59	C	72.75325	74.66266	67.95244	630.79189	-468.94448	76.03230	1
60	H	73.45823	73.80872	67.82133	-1775.71861	2062.30353	131.89849	1
61	H	72.66979	74.82170	69.05697	-1855.14608	88.94118	1993.53760	1
62	H	71.76195	74.32560	67.56169	-1504.82350	-780.94249	-2132.90992	1
63	C	71.04719	77.46226	68.00551	288.57638	618.62814	-397.00270	1
64	O	70.52423	78.54912	67.91162	321.70495	-185.26452	574.37218	1
65	N	70.69046	76.49251	68.85558	-447.05792	-446.53431	367.76425	1
66	H	71.18598	75.60073	68.87280	350.31316	1975.63644	-1843.31522	1
67	C	70.14941	76.94643	70.11503	-511.23061	374.03917	-471.51480	1
68	H	69.28286	77.60888	69.88324	2234.79579	-898.70890	-1273.45190	1
69	C	69.82086	75.58191	70.86233	529.53781	-159.34528	563.72604	1
70	H	69.41201	75.85366	71.86838	654.59388	2347.94251	1217.51488	1
71	H	68.99327	75.02980	70.34302	-1526.55661	2103.42026	817.87394	1
72	O	70.94569	74.66333	70.98012	-554.84278	14.12789	399.58769	1
73	H	71.66108	75.30816	71.18995	1297.06236	2061.84854	1220.68812	1
74	C	71.33968	77.68937	70.92138	-662.15484	-412.13544	123.62687	1
75	O	72.42410	77.09816	71.11505	-540.01537	-317.05804	274.91456	1
76	N	70.95262	78.83305	71.42004	-202.76299	-690.00100	-131.49145	1
77	H	69.99609	79.08188	71.16699	-702.62132	-2617.37191	281.70413	1
78	C	71.91754	79.85374	71.72306	-491.73914	576.34187	222.73509	1
79	H	72.71421	79.67587	70.96556	1977.17978	-1823.58850	-434.68928	1
80	C	71.15966	81.23299	71.55244	-649.50797	-328.66843	306.11224	1
81	H	70.15524	81.17875	72.02604	2075.07803	1452.16490	-1004.45904	1
82	C	71.98264	82.42779	72.14885	-615.18735	-489.99689	-70.96352	1
83	H	71.53522	83.41325	71.87862	-1226.32661	-1724.38906	-1716.47170	1
84	H	72.02517	82.38707	73.27235	2381.64273	-969.84735	900.46860	1
85	H	73.03386	82.42539	71.77590	2122.74991	1702.23946	-141.36228	1
86	C	71.03706	81.51904	70.01458	-501.86074	-479.61276	-376.42482	1
87	H	70.46460	82.45563	69.81524	993.79261	-2246.95401	-1177.81305	1
88	H	72.03828	81.63371	69.53330	42.71279	-626.15391	-2651.37258	1
89	H	70.51846	80.68936	69.47750	-2026.39012	-1590.33709	-887.82922	1
90	C	72.51437	79.66531	73.22627	-672.89153	382.57394	-156.34072	1
91	O	72.40745	80.54636	74.05183	410.04627	221.86223	500.35950	1
92	N	73.16870	78.52109	73.32163	-378.11782	-443.79414	-441.10984	1
93	H	73.12996	77.81364	72.55506	2404.15973	-568.14894	1149.30085	1
94	C	73.79564	78.18502	74.57749	-544.54484	466.16019	331.29119	1
95	H	74.52756	78.99154	74.80297	-1409.80988	-170.17955	2325.32679	1
96	C	72.59949	78.17614	75.62305	-184.48284	116.78282	-758.89137	1
97	H	72.12370	79.18915	75.65090	1893.78641	1861.14652	611.04528	1
98	H	71.80386	77.47601	75.28148	-2170.79665	-974.19311	1327.50117	1
99	C	73.09017	77.79979	77.05425	389.51668	672.81878	-138.49152	1
100	H	73.45673	76.75027	77.06523	510.64577	1933.03327	1851.02484	1
101	H	73.97069	78.41027	77.34640	-2302.30869	-1105.72939	-948.89774	1
102	C	71.95170	78.00757	78.12311	-559.93427	-126.34590	542.30857	1
103	O	72.23217	78.02789	79.29778	-670.36003	-111.83166	76.36448	1
104	N	70.71585	78.10660	77.59644	-216.06729	-537.07037	446.51379	1
105	H	70.42264	78.13168	76.61213	-1251.96487	1074.12894	-2168.52500	1
106	H	69.86920	78.28172	78.14844	-2451.83023	-720.73851	944.84612	1
107	C	74.43573	76.72634	74.36020	546.24052	-563.88337	-85.11809	1
108	O	73.75764	75.88657	73.77672	71.70702	-307.40463	606.69673	1
109	N	75.64503	76.58626	74.89872	479.90863	-504.50129	222.86849	1
110	C	76.37732	75.35763	74.75144	75.51268	-600.91904	506.73700	1

111	H	76.20706	75.05322	73.69475	-2033.61562	1795.30103	254.89480	1
112	C	77.85840	75.78385	75.10834	523.79067	517.99274	284.45581	1
113	H	78.46782	74.93288	75.48938	1599.61665	-1127.00911	1895.98173	1
114	H	78.39726	76.18211	74.21671	-1881.83093	1275.82488	-1501.55016	1
115	C	77.62782	76.89933	76.17752	-600.05639	-404.05026	316.64485	1
116	H	77.37981	76.45302	77.16703	-2597.05260	496.36221	657.73249	1
117	H	78.51146	77.55779	76.33314	-1666.24518	1294.38985	-1723.90591	1
118	C	76.37829	77.65948	75.55731	493.57570	-129.95376	-602.56394	1
119	H	75.70403	78.14507	76.29993	-1469.08415	-637.84797	2204.22581	1
120	H	76.63674	78.39236	74.75598	-1038.97840	1068.88701	-2280.71789	1
121	C	75.77834	74.24867	75.80141	188.88100	241.05089	-727.87821	1
122	O	76.45599	73.88069	76.73437	531.88613	-49.19943	427.07960	1
123	N	74.55518	73.94517	75.43653	708.14833	26.93417	-179.73509	1
124	H	74.14553	74.43814	74.60230	-2232.69501	-1179.09831	1023.94816	1
125	C	73.73578	72.94707	76.03268	-738.32412	259.92548	104.42456	1
126	H	72.73578	73.30657	75.70006	2028.89123	1260.02983	1311.33324	1
127	C	74.04376	71.53254	75.36390	-258.65678	-345.52513	661.28459	1
128	H	75.13013	71.30506	75.38376	-1826.06090	-1801.46097	-918.64554	1
129	C	73.19439	70.46089	76.13225	-541.23400	531.92970	-218.41428	1
130	H	72.92601	69.58711	75.49385	1311.73218	-2219.18200	882.19023	1
131	H	73.74946	70.06715	77.02221	-1048.71298	1223.58118	-2196.97971	1
132	H	72.23896	70.89844	76.50451	419.06414	1903.92898	1903.44670	1
133	C	73.51248	71.56059	73.89265	-423.86431	152.66566	-648.55262	1
134	H	73.70487	70.59783	73.36531	105.68386	-2342.50080	1387.51238	1
135	H	72.41341	71.74469	73.85871	-1695.63603	-1484.73621	-1531.02793	1
136	H	74.00046	72.36811	73.29994	-1853.57121	-487.39031	1936.59343	1
137	C	73.87311	72.88092	77.64932	539.71428	-510.58232	267.58633	1
138	O	74.09029	71.79625	78.21287	-15.93758	-278.34085	-624.49402	1
139	N	73.51557	74.02924	78.19669	-676.81886	12.05292	276.17960	1
140	H	73.48571	74.74498	77.46752	-1694.44250	-373.84189	-2100.66098	1
141	C	73.97842	74.30417	79.53502	412.33078	-664.70360	108.35451	1
142	H	75.08036	74.15956	79.48915	1765.77476	1294.44366	1621.76594	1
143	C	73.53670	75.78145	79.85538	-179.66635	-721.95667	-264.73915	1
144	H	73.90388	76.48953	79.07899	-607.34922	2587.87032	-598.10018	1
145	H	72.42369	75.84505	79.81917	-359.69332	-1479.13954	-2259.74260	1
146	C	74.06551	76.20081	81.26984	-240.01076	616.02425	431.85322	1
147	H	73.78071	75.44605	82.03942	-1359.17131	782.54425	2227.99181	1
148	H	75.17663	76.25292	81.28569	-820.36667	85.81767	-2596.78715	1
149	C	73.43106	77.61180	81.59324	-513.07015	236.18570	-551.87280	1
150	H	73.79329	78.38373	80.87306	1816.11944	-1183.11722	-1650.94321	1
151	H	72.32105	77.57981	81.47009	-1800.04429	-1361.53473	1526.34643	1
152	C	73.80826	77.99695	83.04506	726.08972	-253.19732	-179.64713	1
153	H	73.20784	77.49495	83.82936	1224.27271	-456.51798	-2390.90304	1
154	H	74.88595	77.91342	83.28246	1206.40339	-1150.93514	-2154.90344	1
155	N	73.51864	79.52367	83.20921	329.70796	-633.68968	-155.67358	1
156	H	73.64961	79.91026	84.18775	1348.31305	1938.76845	1359.00643	1
157	H	74.13206	80.17839	82.64287	2096.92035	1446.54551	-966.48890	1
158	H	72.54502	79.87104	82.96815	-1197.07217	-2303.53719	827.28733	1
159	C	73.25004	73.30939	80.59742	-378.01186	-556.17301	-413.96481	1
160	O	73.68814	73.21686	81.72435	-409.44433	-307.55053	-453.30833	1
161	N	72.12868	72.78096	80.11009	-429.02477	524.70884	274.08502	1
162	H	71.91346	72.96074	79.13095	1706.34263	-1425.96036	1574.38926	1
163	C	71.29880	72.03377	80.99752	-45.25864	-626.22952	478.93267	1
164	H	71.54466	72.46261	81.99806	1988.63164	570.90773	1772.87287	1
165	C	69.80152	72.26062	80.52459	551.77128	-20.49526	-564.54996	1
166	H	69.57903	73.34770	80.43421	1434.61535	-1753.10253	1513.99471	1
167	H	69.64745	71.84161	79.50474	-714.67738	1819.09770	1898.36494	1
168	C	68.82451	71.58433	81.53956	446.99263	-555.77305	338.97221	1
169	H	69.03781	70.49068	81.60401	1953.68466	1892.25957	-161.67766	1
170	H	68.97497	71.98673	82.56624	-403.03785	2688.07032	-188.43591	1
171	C	67.34368	71.84682	81.04393	567.86262	335.74681	434.04421	1
172	H	67.10231	72.93385	81.07982	-1080.02275	1568.26081	-1948.78900	1

173	H	67.22177	71.54700	79.97825	-919.54108	2111.34692	1456.13463	1
174	C	66.38027	71.03477	81.93882	195.81897	173.33862	-745.11536	1
175	H	66.50931	69.93618	81.87238	1405.67949	-2301.21089	-390.08113	1
176	H	66.35864	71.35066	83.00003	-940.37328	-1118.32446	2299.72133	1
177	N	64.92022	71.28554	81.42762	319.26422	656.36007	-42.02424	1
178	H	64.15956	70.75850	81.94571	1961.03633	619.91968	1787.09422	1
179	H	64.54935	72.27896	81.47168	854.14343	-2156.80752	1429.08711	1
180	H	64.70964	71.01660	80.42308	1237.02905	-1378.50857	-1998.28500	1
181	C	71.69657	70.45209	80.93790	532.53319	-268.57236	517.55729	1
182	O	71.18038	69.70813	81.74077	266.16714	-290.73804	-558.88002	1
183	N	72.57709	70.15491	79.98566	-226.25352	640.49678	-270.32839	1
184	H	72.92686	70.90372	79.36456	2007.69063	-1035.27229	1523.50231	1
185	C	72.80019	68.76370	79.76362	-540.76542	-573.33303	49.50000	1
186	H	72.36382	68.26585	80.66527	-2374.20950	-1036.76023	843.75774	1
187	C	72.00458	68.37078	78.42458	-77.09082	666.87422	-415.84136	1
188	H	72.22672	69.13975	77.63833	-985.81834	617.19825	2463.91927	1
189	O	70.57127	68.37423	78.54640	293.29899	-391.65602	-477.80926	1
190	H	70.33494	69.12002	77.95836	2528.72714	-681.76262	-751.27122	1
191	C	72.64656	67.00357	77.99120	252.47363	-605.14473	440.05134	1
192	H	72.07587	66.53256	77.15759	-2052.65063	1456.49051	-1043.51830	1
193	H	73.69592	67.12833	77.62839	-2152.98800	-1661.97574	-161.70652	1
194	H	72.66568	66.27602	78.83726	-473.12726	-1584.27339	2165.61725	1
195	C	74.38708	68.45105	79.55891	360.36307	488.46713	505.10056	1
196	O	74.75824	67.30409	79.63906	-200.08817	-528.03552	-385.82850	1
197	N	75.08966	69.53783	79.27484	-597.54095	-226.44775	355.20479	1
198	H	74.65486	70.48588	79.21044	2179.23655	-1300.70981	-991.33835	1
199	C	76.46594	69.38622	78.95767	-687.68921	297.39807	-249.45179	1
200	H	76.71117	68.38442	79.37521	-349.16256	-2467.37713	-1101.72831	1
201	C	76.62910	69.45163	77.36698	672.47345	361.54328	-201.62880	1
202	H	76.08121	70.33408	76.96656	1541.41502	582.18425	2169.97026	1
203	H	77.70497	69.59671	77.11739	-2534.67717	60.25153	997.72295	1
204	C	76.16225	68.17291	76.64985	574.26774	-389.43119	-377.02542	1
205	C	76.71391	66.90102	76.99109	688.82679	-287.33580	-257.96133	1
206	H	77.40764	66.79750	77.84580	331.14182	1470.38163	2269.80013	1
207	C	75.26095	68.27808	75.54806	-383.52382	-675.04808	144.24917	1
208	H	74.84275	69.25616	75.25696	4.09847	1517.59662	2262.86397	1
209	C	76.37468	65.79189	76.21460	-134.76730	428.45285	-649.50303	1
210	H	76.80719	64.81064	76.47577	-903.23433	1600.49020	2011.53387	1
211	C	74.94261	67.13931	74.80343	-335.53281	-615.00040	-364.39058	1
212	H	74.24387	67.24579	73.95584	1596.45398	-1369.33862	1732.02659	1
213	C	75.49729	65.85766	75.09216	585.48547	-340.24194	-406.23938	1
214	O	75.20289	64.69672	74.33169	-419.15649	-173.04408	-511.94141	1
215	H	74.63324	65.09418	73.63180	-1071.84350	1559.71507	-1960.13012	1
216	C	77.22828	70.62736	79.69498	291.41878	-183.13091	710.72246	1
217	O	77.25395	70.65646	80.90186	379.87695	523.47396	-222.23622	1
218	N	77.86451	71.42804	78.82764	564.30591	373.09380	277.24371	1
219	H	77.67151	71.21772	77.84341	-120.59931	-2436.07824	-1214.35098	1
220	C	77.97375	72.83709	79.11144	404.07514	-299.37480	608.84009	1
221	H	77.44045	73.29473	78.21539	-1071.07882	-841.69025	2359.66467	1
222	C	77.39897	73.23905	80.52066	-683.12807	68.71770	-390.13096	1
223	H	76.37024	72.82777	80.67316	2068.88918	1596.58590	770.89603	1
224	H	78.03448	72.75962	81.30622	1379.86429	2342.49779	-179.85638	1
225	C	77.42806	74.79544	80.68450	-176.39967	537.49466	550.97268	1
226	H	78.41993	75.21320	80.39938	-396.28051	1942.22168	1869.33314	1
227	H	76.68688	75.30260	80.02661	-94.44700	586.00678	-2659.20016	1
228	C	77.12798	75.03788	82.23267	-291.69381	-718.18079	-150.72929	1
229	H	76.10230	74.75548	82.58337	-2303.38776	1089.76242	964.62032	1
230	H	77.86395	74.55415	82.92306	884.16729	2568.80533	-207.74283	1
231	N	77.29873	76.42017	82.38172	-594.49522	-252.81478	342.29276	1
232	H	77.75010	76.91700	81.62983	-1735.17426	2084.05705	-263.71605	1
233	C	76.95474	77.08618	83.40735	595.23177	-271.52487	442.22352	1
234	N	76.33650	76.38396	84.44921	585.53813	-424.79750	-105.81303	1

235	H	76.13039	75.38862	84.52947	959.88797	1327.56823	-2177.11905	1
236	H	76.02371	76.79691	85.32787	1578.48647	16.27378	-2220.76233	1
237	N	77.26501	78.44766	83.26286	-452.17763	-390.33541	-421.51853	1
238	H	77.74288	78.94750	82.51393	470.26107	1974.25629	-1817.92087	1
239	H	77.05743	79.15070	83.97385	1856.67307	-1573.97321	-1224.35416	1
240	C	79.55329	73.20777	79.20409	-531.47271	-581.45780	-55.06206	1
241	O	80.00920	73.57864	80.26650	-243.00837	192.73507	609.52485	1
242	N	80.19986	73.09666	78.03146	343.49288	-644.25607	38.09164	1
243	H	79.66697	72.64613	77.28613	-1691.16043	-1535.97525	-1484.73099	1
244	C	81.63075	73.00371	78.15565	542.66492	350.14337	454.42563	1
245	H	81.86585	73.71221	78.98334	1209.57979	-2396.95920	463.86744	1
246	C	82.00390	71.51139	78.56965	-737.14309	145.93010	242.71942	1
247	H	81.51311	70.77046	77.90369	-1050.18303	159.36419	-2509.06125	1
248	C	83.56337	71.37906	78.48335	-706.77696	-252.88343	-245.16230	1
249	H	83.93943	70.49495	79.05066	-1624.64039	-1665.49085	1417.86935	1
250	H	83.90493	71.25788	77.42647	2566.10521	598.51109	693.22305	1
251	H	84.07562	72.28506	78.88850	-1972.69758	107.10018	-1876.34312	1
252	C	81.51839	71.31556	80.04591	412.85148	672.58832	-27.69222	1
253	H	81.86659	70.34748	80.48164	1447.02277	1762.76533	-1490.78944	1
254	H	81.88218	72.13966	80.70439	1320.77379	-145.20455	2378.68491	1
255	H	80.40236	71.33048	80.10834	-1512.10848	1470.52031	1724.75147	1
256	C	82.42020	73.35121	76.78326	-607.11113	499.56689	73.73769	1
257	O	83.63300	73.44284	76.84059	357.97126	460.81534	356.68785	1
258	N	81.63829	73.39825	75.70844	536.55407	-368.62270	332.76306	1
259	H	80.63746	73.26893	75.86576	524.38866	2297.69985	1367.20941	1
260	C	82.01312	74.31522	74.66802	46.50277	-774.29190	-147.97904	1
261	H	82.49731	75.17112	75.18533	1676.51875	1883.29066	1032.55549	1
262	C	83.02404	73.59076	73.64492	-559.41456	-34.19198	-556.30433	1
263	H	82.76890	72.50424	73.60209	-64.66664	395.18769	2695.05373	1
264	H	82.87460	73.98860	72.61183	-2703.44278	-60.40056	333.79418	1
265	C	84.46095	73.78933	74.05360	-519.76435	377.31045	459.42366	1
266	H	84.56498	73.52575	75.14943	-1746.74323	1667.50644	-1261.73691	1
267	C	85.35503	72.87491	73.22643	570.95554	16.46261	-545.27700	1
268	H	86.43232	72.96302	73.52267	2391.58273	28.05277	-1305.07271	1
269	H	85.06514	71.79828	73.34078	175.75588	917.63458	2559.43867	1
270	H	85.29122	73.11944	72.13425	-1063.97851	-2155.34650	1283.00462	1
271	C	84.89749	75.23442	73.86626	193.76014	2.62946	-765.53141	1
272	H	85.99237	75.36664	74.06848	507.39394	-846.55087	2539.60089	1
273	H	84.70862	75.58944	72.82025	1337.57841	1818.19054	1526.01994	1
274	H	84.35146	75.92864	74.55608	1100.88635	-1172.91350	-2199.08909	1
275	C	80.66561	74.68519	73.88763	-549.21115	475.64486	-309.38218	1
276	O	79.71166	73.95140	73.83519	556.06106	-390.37755	-78.24250	1
277	O	80.67303	75.90369	73.16361	-572.27940	-310.19032	-209.75862	1
278	H	81.59889	76.20287	73.37560	-1380.08193	2212.14486	790.85944	1

Listing 82: C00082.xmolout

1		276								
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100	
		0.2500	300.00	0.00	0.00	0.00	-1293.5150	0.0000	300.0000	
3	H	68.47668	71.60640	66.00199	-2043.14101	-1757.64893	399.89339		1	
4	N	68.39853	72.62203	66.01249	426.75047	490.45733	-334.42467		1	
5	H	68.04860	72.81031	66.95495	442.25559	-1110.30854	-2448.52907		1	
6	C	69.61628	73.30066	65.78637	415.32972	-666.39213	83.73172		1	
7	H	70.19153	72.72999	65.02594	879.32219	2491.00447	667.35213		1	
8	C	69.24416	74.80102	65.33003	31.35357	477.41777	628.23362		1	
9	H	68.83606	75.35502	66.20934	1168.38489	2240.25337	-1019.71136		1	
10	H	70.15844	75.35871	65.01428	-360.43770	2534.90498	931.67112		1	
11	C	68.21772	74.75343	64.22681	463.18208	512.70242	-382.34388		1	
12	H	67.42317	74.03379	64.52977	1725.29117	1863.52247	-987.07854		1	
13	C	67.57280	76.11893	64.02856	710.42801	-144.27427	-313.15367		1	
14	H	66.78631	76.09256	63.23051	364.20195	-1033.13725	2494.72524		1	

15	H	67.08071	76.48491	64.96662	2567.61904	335.80679	847.48802	1
16	H	68.32599	76.89124	63.72581	-2587.99029	680.92867	-512.16411	1
17	C	68.82684	74.27636	62.91594	268.17616	741.64379	-40.42634	1
18	H	68.06173	74.23103	62.09802	1283.54314	-1945.37420	-1411.27812	1
19	H	69.64452	74.95894	62.56784	-1258.57796	1317.15249	-2026.02085	1
20	H	69.26743	73.25086	63.01518	-2502.84526	909.80597	575.92391	1
21	C	70.28916	73.32770	67.26943	619.36578	-458.64843	-172.09273	1
22	O	69.58245	73.53122	68.24685	-81.40433	433.87611	522.34594	1
23	N	71.60212	73.18811	67.19968	175.23996	-622.20190	341.55523	1
24	H	72.00188	73.02229	66.27683	-876.57256	-303.22879	-2561.90213	1
25	C	72.32301	72.80463	68.37912	-571.88214	-534.10783	-106.15033	1
26	H	71.63020	72.13691	68.93387	-2713.20841	-16.25800	-248.80809	1
27	C	73.67838	72.11058	67.90638	166.60354	288.16399	-716.09568	1
28	H	74.22235	72.80894	67.21286	-2097.85574	1636.78449	-586.18044	1
29	O	73.52537	70.87274	67.18805	-317.80580	-363.38227	484.43082	1
30	H	73.98342	71.07682	66.34876	1863.74748	-1451.84923	1357.29467	1
31	C	74.45544	72.04424	69.27356	503.80731	517.99032	318.51606	1
32	H	75.49209	71.65771	69.13847	640.61020	-2157.10410	-1536.29104	1
33	H	74.53185	73.05667	69.74425	1687.88455	465.60692	2087.56452	1
34	H	73.94377	71.37474	70.00312	-1293.07895	-1899.88581	-1463.57452	1
35	C	72.71650	74.15089	69.21387	-153.07550	-733.68902	248.70981	1
36	O	73.56328	74.88641	68.77493	186.15459	-480.78787	-449.34387	1
37	N	72.06903	74.22047	70.38855	-487.53139	543.18517	42.03850	1
38	C	72.11549	75.42304	71.16184	-699.35871	69.34393	360.10701	1
39	H	72.37103	76.23482	70.44144	2.81126	-221.99807	-2715.58072	1
40	C	70.64675	75.44796	71.76731	-507.46439	-592.59194	122.07761	1
41	H	70.57067	76.14351	72.65659	-1975.08116	525.87560	-1801.71556	1
42	H	69.89643	75.79090	71.01864	1588.27743	-1913.22100	1113.83566	1
43	C	70.44142	73.94435	72.12262	-613.62442	-457.55993	-194.14490	1
44	H	71.01846	73.66464	73.03589	1707.54637	-721.27992	1996.92523	1
45	H	69.38066	73.66441	72.30964	758.23357	2100.81767	1560.55011	1
46	C	71.04348	73.27715	70.81234	-352.41524	704.96076	49.21465	1
47	H	71.50525	72.27113	70.95366	1714.76886	-2070.42778	443.35792	1
48	H	70.32577	73.26201	69.92664	1224.15040	1801.50881	1636.97633	1
49	C	73.22931	75.24678	72.35432	566.85117	537.05831	117.62814	1
50	O	72.94865	74.70932	73.42596	-550.26779	-406.08867	4.21666	1
51	N	74.38637	75.66280	71.91337	566.34832	-425.77725	180.18749	1
52	H	74.35544	76.01817	70.95595	644.44502	2646.80550	-52.73430	1
53	C	75.38603	76.22181	72.78794	612.34801	-281.48662	411.56221	1
54	H	75.04893	77.25831	73.00663	1667.23498	-1490.75142	1556.16753	1
55	C	75.44500	75.34983	74.12089	-714.45746	-175.43074	286.98927	1
56	H	75.15244	74.29674	73.84050	-787.09484	1763.03619	-1922.46060	1
57	O	74.50007	75.74677	75.11833	-429.46514	516.51932	-128.40526	1
58	H	73.68702	75.20219	74.80076	1981.82785	436.16847	-1818.18182	1
59	C	76.95302	75.38070	74.55578	630.79189	-468.94448	76.03230	1
60	H	77.10644	74.85277	75.52609	-1775.71861	2062.30353	131.89849	1
61	H	77.60673	74.88092	73.80352	-1855.14608	88.94118	1993.53760	1
62	H	77.32173	76.42511	74.67942	-1504.82350	-780.94249	-2132.90992	1
63	C	76.69993	76.24784	71.84112	288.57638	618.62814	-397.00270	1
64	O	77.33959	77.31089	71.76761	321.70495	-185.26452	574.37218	1
65	N	76.93461	75.07700	71.29494	-447.05792	-446.53431	367.76425	1
66	H	76.20815	74.39341	71.52015	350.31316	1975.63644	-1843.31522	1
67	C	77.82851	74.82847	70.22519	-511.23061	374.03917	-471.51480	1
68	H	77.57941	73.77862	69.95030	2234.79579	-898.70890	-1273.45190	1
69	C	77.46333	75.84440	69.04893	529.53781	-159.34528	563.72604	1
70	H	77.87454	75.46007	68.07453	654.59388	2347.94251	1217.51488	1
71	H	76.34450	75.80670	68.94594	-1526.55661	2103.42026	817.87394	1
72	O	77.90152	77.20754	69.17416	-554.84278	14.12789	399.58769	1
73	H	77.72836	77.34543	70.17519	1297.06236	2061.84854	1220.68812	1
74	C	79.39258	74.97623	70.66721	-662.15484	-412.13544	123.62687	1
75	O	80.26522	74.94120	69.83166	-540.01537	-317.05804	274.91456	1
76	N	79.52591	74.96339	71.99610	-202.76299	-690.00100	-131.49145	1

77	H	78.65244	74.99746	72.52027	-702.62132	-2617.37191	281.70413	1
78	C	80.76388	75.40344	72.55461	-491.73914	576.34187	222.73509	1
79	H	81.22858	76.05727	71.78318	1977.17978	-1823.58850	-434.68928	1
80	C	80.41063	76.12396	73.92292	-649.50797	-328.66843	306.11224	1
81	H	79.67003	75.53011	74.49935	2075.07803	1452.16490	-1004.45904	1
82	C	81.71864	76.33504	74.76000	-615.18735	-489.99689	-70.96352	1
83	H	81.50406	76.81181	75.74526	-1226.32661	-1724.38906	-1716.47170	1
84	H	82.23409	75.36241	74.95836	2381.64273	-969.84735	900.46860	1
85	H	82.44642	76.98742	74.22331	2122.74991	1702.23946	-141.36228	1
86	C	79.82181	77.54104	73.60696	-501.86074	-479.61276	-376.42482	1
87	H	79.50921	78.06549	74.53923	993.79261	-2246.95401	-1177.81305	1
88	H	80.56752	78.19119	73.09200	42.71279	-626.15391	-2651.37258	1
89	H	78.91660	77.46833	72.93214	-2026.39012	-1590.33709	-887.82922	1
90	C	81.71381	74.10754	72.87422	-672.89153	382.57394	-156.34072	1
91	O	82.89829	74.27076	73.06123	410.04627	221.86223	500.35950	1
92	N	81.00130	72.99218	72.98559	-378.11782	-443.79414	-441.10984	1
93	H	80.01574	73.07550	72.74011	2404.15973	-568.14894	1149.30085	1
94	C	81.56726	71.78059	73.46322	-544.54484	466.16019	331.29119	1
95	H	80.71291	71.06652	73.43736	-1409.80988	-170.17955	2325.32679	1
96	C	82.73493	71.42208	72.44553	-184.48284	116.78282	-758.89137	1
97	H	82.39803	71.60460	71.39992	1893.78641	1861.14652	611.04528	1
98	H	83.60199	72.10707	72.60825	-2170.79665	-974.19311	1327.50117	1
99	C	83.13291	69.92840	72.64840	389.51668	672.81878	-138.49152	1
100	H	83.58932	69.78877	73.65796	510.64577	1933.03327	1851.02484	1
101	H	82.22181	69.29033	72.67303	-2302.30869	-1105.72939	-948.89774	1
102	C	84.11186	69.37753	71.54378	-559.93427	-126.34590	542.30857	1
103	O	84.43466	68.21779	71.56471	-670.36003	-111.83166	76.36448	1
104	N	84.50249	70.29948	70.63768	-216.06729	-537.07037	446.51379	1
105	H	84.28773	71.30206	70.58491	-1251.96487	1074.12894	-2168.52500	1
106	H	85.14868	70.10419	69.86511	-2451.83023	-720.73851	944.84612	1
107	C	82.23543	71.93869	74.94471	546.24052	-563.88337	-85.11809	1
108	O	83.29243	71.38944	75.12606	71.70702	-307.40463	606.69673	1
109	N	81.47126	72.59104	75.83348	479.90863	-504.50129	222.86849	1
110	C	81.90691	72.81523	77.17635	75.51268	-600.91904	506.73700	1
111	H	83.01519	72.93299	77.16630	-2033.61562	1795.30103	254.89480	1
112	C	81.06635	74.10991	77.56612	523.79067	517.99274	284.45581	1
113	H	80.97884	74.25500	78.66608	1599.61665	-1127.00911	1895.98173	1
114	H	81.53459	75.03338	77.16102	-1881.83093	1275.82488	-1501.55016	1
115	C	79.69659	73.81969	76.87899	-600.05639	-404.05026	316.64485	1
116	H	79.06357	73.15697	77.51308	-2597.05260	496.36221	657.73249	1
117	H	79.09710	74.74415	76.68859	-1666.24518	1294.38985	-1723.90591	1
118	C	80.13160	73.08366	75.54094	493.57570	-129.95376	-602.56394	1
119	H	79.50398	72.20738	75.25460	-1469.08415	-637.84797	2204.22581	1
120	H	80.25007	73.75208	74.65976	-1038.97840	1068.88701	-2280.71789	1
121	C	81.39643	71.57388	78.10861	188.88100	241.05089	-727.87821	1
122	O	80.49290	70.84272	77.79243	531.88613	-49.19943	427.07960	1
123	N	82.01069	71.67140	79.29676	708.14833	26.93417	-179.73509	1
124	H	82.76361	72.35739	79.31837	-2232.69501	-1179.09831	1023.94816	1
125	C	81.86154	70.61648	80.31301	-738.32412	259.92548	104.42456	1
126	H	82.13336	69.67454	79.78156	2028.89123	1260.02983	1311.33324	1
127	C	82.77846	70.94029	81.47121	-258.65678	-345.52513	661.28459	1
128	H	82.57950	71.99212	81.77743	-1826.06090	-1801.46097	-918.64554	1
129	C	82.51313	70.04419	82.66875	-541.23400	531.92970	-218.41428	1
130	H	83.17085	70.30711	83.54198	1311.73218	-2219.18200	882.19023	1
131	H	81.44462	70.12344	83.01675	-1048.71298	1223.58118	-2196.97971	1
132	H	82.69857	68.96256	82.42405	419.06414	1903.92898	1903.44670	1
133	C	84.24499	70.84009	81.08705	-423.86431	152.66566	-648.55262	1
134	H	84.91814	71.13848	81.93671	105.68386	-2342.50080	1387.51238	1
135	H	84.52282	69.79020	80.79646	-1695.63603	-1484.73621	-1531.02793	1
136	H	84.49486	71.50117	80.21335	-1853.57121	-487.39031	1936.59343	1
137	C	80.28467	70.58784	80.80413	539.71428	-510.58232	267.58633	1
138	O	79.86432	69.64481	81.43559	-15.93758	-278.34085	-624.49402	1

139	N	79.62976	71.76746	80.57438	-676.81886	12.05292	276.17960	1
140	H	80.31142	72.24442	79.96755	-1694.44250	-373.84189	-2100.66098	1
141	C	78.29069	71.57375	80.03619	412.33078	-664.70360	108.35451	1
142	H	78.42007	70.85142	79.20032	1765.77476	1294.44366	1621.76594	1
143	C	77.46197	70.96900	81.22330	-179.66635	-721.95667	-264.73915	1
144	H	77.79768	69.91825	81.42323	-607.34922	2587.87032	-598.10018	1
145	H	77.68711	71.53114	82.15868	-359.69332	-1479.13954	-2259.74260	1
146	C	75.91986	70.98776	80.94305	-240.01076	616.02425	431.85322	1
147	H	75.51883	72.02669	80.98664	-1359.17131	782.54425	2227.99181	1
148	H	75.67952	70.60110	79.92741	-820.36667	85.81767	-2596.78715	1
149	C	75.31028	70.06562	82.07442	-513.07015	236.18570	-551.87280	1
150	H	75.67848	69.01981	81.96061	1816.11944	-1183.11722	-1650.94321	1
151	H	75.66497	70.39893	83.07684	-1800.04429	-1361.53473	1526.34643	1
152	C	73.76614	70.09850	82.02237	726.08972	-253.19732	-179.64713	1
153	H	73.31396	71.07586	82.28468	1224.27271	-456.51798	-2390.90304	1
154	H	73.32294	69.71386	81.08232	1206.40339	-1150.93514	-2154.90344	1
155	N	73.26021	69.11514	83.13342	329.70796	-633.68968	-155.67358	1
156	H	72.20740	69.05534	83.24534	1348.31305	1938.76845	1359.00643	1
157	H	73.51868	68.09079	83.02922	2096.92035	1446.54551	-966.48890	1
158	H	73.56366	69.31675	84.13029	-1197.07217	-2303.53719	827.28733	1
159	C	77.71522	73.00216	79.51891	-378.01186	-556.17301	-413.96481	1
160	O	76.84930	73.01071	78.67359	-409.44433	-307.55053	-453.30833	1
161	N	78.32444	74.04114	80.09761	-429.02477	524.70884	274.08502	1
162	H	79.00925	73.78540	80.80978	1706.34263	-1425.96036	1574.38926	1
163	C	77.73779	75.34041	80.10016	-45.25864	-626.22952	478.93267	1
164	H	78.52419	75.92798	80.62478	1988.63164	570.90773	1772.87287	1
165	C	77.51307	75.79242	78.59990	551.77128	-20.49526	-564.54996	1
166	H	78.22585	75.26193	77.92443	1434.61535	-1753.10253	1513.99471	1
167	H	76.49896	75.49001	78.25058	-714.67738	1819.09770	1898.36494	1
168	C	77.70601	77.34189	78.48870	446.99263	-555.77305	338.97221	1
169	H	77.02710	77.88736	79.18408	1953.68466	1892.25957	-161.67766	1
170	H	78.73894	77.63597	78.78084	-403.03785	2688.07032	-188.43591	1
171	C	77.41040	77.74469	76.98853	567.86262	335.74681	434.04421	1
172	H	78.19844	77.34095	76.31259	-1080.02275	1568.26081	-1948.78900	1
173	H	76.44845	77.29875	76.64130	-919.54108	2111.34692	1456.13463	1
174	C	77.34478	79.28808	76.90715	195.81897	173.33862	-745.11536	1
175	H	76.39416	79.72493	77.27389	1405.67949	-2301.21089	-390.08113	1
176	H	78.20549	79.81779	77.36273	-940.37328	-1118.32446	2299.72133	1
177	N	77.41333	79.67593	75.39146	319.26422	656.36007	-42.02424	1
178	H	77.22759	80.69210	75.14124	1961.03633	619.91968	1787.09422	1
179	H	78.34662	79.53305	74.91264	854.14343	-2156.80752	1429.08711	1
180	H	76.75564	79.16408	74.73421	1237.02905	-1378.50857	-1998.28500	1
181	C	76.35811	75.27662	80.96925	532.53319	-268.57236	517.55729	1
182	O	76.17589	74.47789	81.85824	266.16714	-290.73804	-558.88002	1
183	N	75.54247	76.25005	80.56010	-226.25352	640.49678	-270.32839	1
184	H	75.83938	76.84652	79.78888	2007.69063	-1035.27229	1523.50231	1
185	C	74.57560	76.75159	81.47688	-540.76542	-573.33303	49.50000	1
186	H	74.49040	75.93883	82.23543	-2374.20950	-1036.76023	843.75774	1
187	C	75.14109	78.11714	82.08882	-77.09082	666.87422	-415.84136	1
188	H	75.05029	78.92181	81.30843	-985.81834	617.19825	2463.91927	1
189	O	76.52105	78.11519	82.49594	293.29899	-391.65602	-477.80926	1
190	H	76.88639	78.82498	81.93071	2528.72714	-681.76262	-751.27122	1
191	C	74.11010	78.39604	83.24353	252.47363	-605.14473	440.05134	1
192	H	74.32219	79.36476	83.75314	-2052.65063	1456.49051	-1043.51830	1
193	H	73.05556	78.44590	82.85559	-2152.98800	-1661.97574	-161.70652	1
194	H	74.14552	77.60034	84.02389	-473.12726	-1584.27339	2165.61725	1
195	C	73.20877	77.05267	80.62700	360.36307	488.46713	505.10056	1
196	O	72.44636	77.92893	80.98878	-200.08817	-528.03552	-385.82850	1
197	N	73.04850	76.15546	79.66702	-597.54095	-226.44775	355.20479	1
198	H	73.81680	75.48974	79.58714	2179.23655	-1300.70981	-991.33835	1
199	C	72.09284	76.29503	78.62719	-687.68921	297.39807	-249.45179	1
200	H	72.12668	75.32243	78.08635	-349.16256	-2467.37713	-1101.72831	1

201	C	70.66290	76.60637	79.29082	672.47345	361.54328	-201.62880	1
202	H	70.71098	77.58058	79.84159	1541.41502	582.18425	2169.97026	1
203	H	69.88414	76.71281	78.49939	-2534.67717	60.25153	997.72295	1
204	C	70.30285	75.46723	80.25255	574.26774	-389.43119	-377.02542	1
205	C	69.72871	74.25381	79.76655	688.82679	-287.33580	-257.96133	1
206	H	69.48728	74.13384	78.69348	331.14182	1470.38163	2269.80013	1
207	C	70.57830	75.62316	81.64549	-383.52382	-675.04808	144.24917	1
208	H	71.00980	76.56724	82.02860	4.09847	1517.59662	2262.86397	1
209	C	69.47916	73.22555	80.67632	-134.76730	428.45285	-649.50303	1
210	H	69.03664	72.28629	80.30145	-903.23433	1600.49020	2011.53387	1
211	C	70.31162	74.56639	82.51669	-335.53281	-615.00040	-364.39058	1
212	H	70.53920	74.70283	83.58859	1596.45398	-1369.33862	1732.02659	1
213	C	69.76280	73.32877	82.06971	585.48547	-340.24194	-406.23938	1
214	O	69.50464	72.24455	82.94819	-419.15649	-173.04408	-511.94141	1
215	H	69.75421	72.66383	83.80646	-1071.84350	1559.71507	-1960.13012	1
216	C	72.53357	77.53462	77.68386	291.41878	-183.13091	710.72246	1
217	O	73.49026	78.24285	77.90437	379.87695	523.47396	-222.23622	1
218	N	71.70885	77.56314	76.63809	564.30591	373.09380	277.24371	1
219	H	70.90799	76.90582	76.53692	-120.59931	-2436.07824	-1214.35098	1
220	C	71.68493	78.80145	75.88227	404.07514	-299.37480	608.84009	1
221	H	71.32980	79.59103	76.58066	-1071.07882	-841.69025	2359.66467	1
222	C	73.15681	79.04861	75.36877	-683.12807	68.71770	-390.13096	1
223	H	73.85442	79.27686	76.22135	2068.88918	1596.58590	770.89603	1
224	H	73.55848	78.12463	74.88965	1379.86429	2342.49779	-179.85638	1
225	C	73.11282	80.24650	74.36379	-176.39967	537.49466	550.97268	1
226	H	72.52080	79.98979	73.45836	-396.28051	1942.22168	1869.33314	1
227	H	72.61474	81.13488	74.81157	-94.44700	586.00678	-2659.20016	1
228	C	74.62830	80.55905	73.99948	-291.69381	-718.18079	-150.72929	1
229	H	75.26989	80.75105	74.89334	-2303.38776	1089.76242	964.62032	1
230	H	75.13309	79.77865	73.38004	884.16729	2568.80533	-207.74283	1
231	N	74.66412	81.78840	73.24912	-594.49522	-252.81478	342.29276	1
232	H	73.89909	82.44016	73.09858	-1735.17426	2084.05705	-263.71605	1
233	C	75.70945	82.29104	72.69995	595.23177	-271.52487	442.22352	1
234	N	76.95633	81.56431	72.78877	585.53813	-424.79750	-105.81303	1
235	H	76.93200	80.54898	72.82486	959.88797	1327.56823	-2177.11905	1
236	H	77.60993	81.76367	72.03571	1578.48647	16.27378	-2220.76233	1
237	N	75.67549	83.51837	72.03425	-452.17763	-390.33541	-421.51853	1
238	H	74.89657	84.16960	71.92229	470.26107	1974.25629	-1817.92087	1
239	H	76.50604	83.95673	71.63402	1856.67307	-1573.97321	-1224.35416	1
240	C	70.71310	78.54206	74.61635	-531.47271	-581.45780	-55.06206	1
241	O	70.89395	77.55802	73.88640	-243.00837	192.73507	609.52485	1
242	N	69.86703	79.52949	74.45043	343.49288	-644.25607	38.09164	1
243	H	69.92358	80.24715	75.17272	-1691.16043	-1535.97525	-1484.73099	1
244	C	68.79987	79.55414	73.46678	542.66492	350.14337	454.42563	1
245	H	68.39272	80.59189	73.53765	1209.57979	-2396.95920	463.86744	1
246	C	69.38483	79.22760	72.09837	-737.14309	145.93010	242.71942	1
247	H	70.04100	78.32579	72.21941	-1050.18303	159.36419	-2509.06125	1
248	C	68.30840	78.89606	71.08350	-706.77696	-252.88343	-245.16230	1
249	H	68.74854	78.59191	70.09304	-1624.64039	-1665.49085	1417.86935	1
250	H	67.65481	78.05016	71.43399	2566.10521	598.51109	693.22305	1
251	H	67.63357	79.77651	70.89398	-1972.69758	107.10018	-1876.34312	1
252	C	70.25315	80.35811	71.57899	412.85148	672.58832	-27.69222	1
253	H	70.80368	80.06524	70.64222	1447.02277	1762.76533	-1490.78944	1
254	H	69.64165	81.27037	71.33442	1320.77379	-145.20455	2378.68491	1
255	H	71.02222	80.66975	72.33745	-1512.10848	1470.52031	1724.75147	1
256	C	67.63818	78.43873	73.90010	-607.11113	499.56689	73.73769	1
257	O	66.48343	78.78648	73.91181	357.97126	460.81534	356.68785	1
258	N	68.14674	77.23800	74.09708	536.55407	-368.62270	332.76306	1
259	H	69.17310	77.09314	74.00707	524.38866	2297.69985	1367.20941	1
260	C	67.33534	76.29837	74.79283	46.50277	-774.29190	-147.97904	1
261	H	66.39118	76.84815	75.01853	1676.51875	1883.29066	1032.55549	1
262	C	67.09338	75.01218	73.83802	-559.41456	-34.19198	-556.30433	1

263	H	68.05809	74.47178	73.69910	-64.66664	395.18769	2695.05373	1
264	H	66.40680	74.28599	74.33323	-2703.44278	-60.40056	333.79418	1
265	C	66.54156	75.44756	72.51006	-519.76435	377.31045	459.42366	1
266	H	67.27169	76.14686	72.04423	-1746.74323	1667.50644	-1261.73691	1
267	C	66.36163	74.25220	71.58182	570.95554	16.46261	-545.27700	1
268	H	65.93984	74.55898	70.59026	2391.58273	28.05277	-1305.07271	1
269	H	67.33374	73.73340	71.38042	175.75588	917.63458	2559.43867	1
270	H	65.66312	73.49262	72.01773	-1063.97851	-2155.34650	1283.00462	1
271	C	65.21473	76.17645	72.67174	193.76014	2.62946	-765.53141	1
272	H	64.74062	76.40035	71.68154	507.39394	-846.55087	2539.60089	1
273	H	64.47827	75.57253	73.26225	1337.57841	1818.19054	1526.01994	1
274	H	65.35399	77.16265	73.20412	1100.88635	-1172.91350	-2199.08909	1
275	C	68.13896	75.80112	76.08782	-549.21115	475.64486	-309.38218	1
276	O	69.26229	76.17461	76.36887	556.06106	-390.37755	-78.24250	1
277	O	67.47955	74.87180	76.91116	-572.27940	-310.19032	-209.75862	1
278	H	66.60255	74.83765	76.42227	-1380.08193	2212.14486	790.85944	1

Listing 83: C00083.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.5132	0.0000	300.0000
3	H	60.66996	78.22632	70.47444	-2043.14101	-1757.64893	399.89339		1
4	N	61.44609	78.22228	71.13595	426.75047	490.45733	-334.42467		1
5	H	61.84231	77.27864	71.02556	442.25559	-1110.30854	-2448.52907		1
6	C	62.42125	79.21167	70.87528	415.32972	-666.39213	83.73172		1
7	H	61.98947	79.89384	70.11024	879.32219	2491.00447	667.35213		1
8	C	62.77628	79.98422	72.24645	31.35357	477.41777	628.23362		1
9	H	63.10441	79.24138	73.01196	1168.38489	2240.25337	-1019.71136		1
10	H	63.64116	80.67364	80.67364	-360.43770	2534.90498	931.67112		1
11	C	61.56993	80.74274	72.73125	463.18208	512.70242	-382.34388		1
12	H	60.71778	80.02971	72.80487	1725.29117	1863.52247	-987.07854		1
13	C	61.83799	81.32958	74.11224	710.42801	-144.27427	-313.15367		1
14	H	60.94564	81.87854	74.50954	364.20195	-1033.13725	2494.72524		1
15	H	62.09882	80.53446	74.85729	2567.61904	335.80679	847.48802		1
16	H	62.69079	82.05621	74.09140	-2587.99029	680.92867	-512.16411		1
17	C	61.18477	81.86566	71.77745	268.17616	741.64379	-40.42634		1
18	H	60.32460	82.46530	72.17291	1283.54314	-1945.37420	-1411.27812		1
19	H	62.03510	82.57633	71.61216	-1258.57796	1317.15249	-2026.02085		1
20	H	60.87846	81.47412	70.77377	-2502.84526	909.80597	575.92391		1
21	C	63.68875	78.34928	70.34545	619.36578	-458.64843	-172.09273		1
22	O	63.65895	77.13509	70.24279	-81.40433	433.87611	522.34594		1
23	N	64.67925	79.17933	70.03615	175.23996	-622.20190	341.55523		1
24	H	64.56886	80.17548	70.21921	-876.57256	-303.22879	-2561.90213		1
25	C	65.90185	78.61250	69.57759	-571.88214	-534.10783	-106.15033		1
26	H	65.58446	77.66559	69.08715	-2713.20841	-16.25800	-248.80809		1
27	C	66.53215	79.70913	68.59558	166.60354	288.16399	-716.09568		1
28	H	66.54892	80.69796	69.13009	-2097.85574	1636.78449	-586.18044		1
29	O	65.78300	79.92738	67.38432	-317.80580	-363.38227	484.43082		1
30	H	65.53112	80.86623	67.48413	1863.74748	-1451.84923	1357.29467		1
31	C	68.01289	79.22248	68.40147	503.80731	517.99032	318.51606		1
32	H	68.57308	79.89541	67.71110	640.61020	-2157.10410	-1536.29104		1
33	H	68.57452	79.21552	69.36785	1687.88455	465.60692	2087.56452		1
34	H	68.05789	78.19519	67.97088	-1293.07895	-1899.88581	-1463.57452		1
35	C	66.83816	78.36044	70.89563	-153.07550	-733.68902	248.70981		1
36	O	67.06332	79.27586	71.64034	186.15459	-480.78787	-449.34387		1
37	N	67.32041	77.10964	70.91110	-487.53139	543.18517	42.03850		1
38	C	68.15296	76.63275	71.97555	-699.35871	69.34393	360.10701		1
39	H	67.78295	77.10117	72.91598	2.81126	-221.99807	-2715.58072		1
40	C	67.96532	75.05786	71.87478	-507.46439	-592.59194	122.07761		1
41	H	68.80960	74.49151	72.32702	-1975.08116	525.87560	-1801.71556		1
42	H	67.03940	74.72079	72.39211	1588.27743	-1913.22100	1113.83566		1

43	C	67.85448	74.86259	70.33146	-613.62442	-457.55993	-194.14490	1
44	H	68.85347	74.94383	69.84470	1707.54637	-721.27992	1996.92523	1
45	H	67.43133	73.87746	70.03181	758.23357	2100.81767	1560.55011	1
46	C	66.92020	76.09069	69.94945	-352.41524	704.96076	49.21465	1
47	H	67.06685	76.48716	68.91745	1714.76886	-2070.42778	443.35792	1
48	H	65.83037	75.92239	70.13117	1224.15040	1801.50881	1636.97633	1
49	C	69.72573	76.97347	71.70144	566.85117	537.05831	117.62814	1
50	O	70.56749	76.76224	72.57298	-550.26779	-406.08867	4.21666	1
51	N	69.90084	77.36612	70.46015	566.34832	-425.77725	180.18749	1
52	H	69.04478	77.44805	69.91814	644.44502	2646.80550	-52.73430	1
53	C	71.17520	77.78996	69.99879	612.34801	-281.48662	411.56221	1
54	H	71.90506	77.22651	70.62287	1667.23498	-1490.75142	1556.16753	1
55	C	71.22036	77.52375	68.42448	-714.45746	-175.43074	286.98927	1
56	H	70.48776	78.21735	67.92661	-787.09484	1763.03619	-1922.46060	1
57	O	70.86660	76.19856	67.99094	-429.46514	516.51932	-128.40526	1
58	H	70.09584	76.38490	67.41626	1981.82785	436.16847	-1818.18182	1
59	C	72.68472	78.00035	68.10030	630.79189	-468.94448	76.03230	1
60	H	72.87890	78.00191	67.00282	-1775.71861	2062.30353	131.89849	1
61	H	72.87624	79.03395	68.47271	-1855.14608	88.94118	1993.53760	1
62	H	73.44354	77.33171	68.56883	-1504.82350	-780.94249	-2132.90992	1
63	C	71.24499	79.41919	70.20392	288.57638	618.62814	-397.00270	1
64	O	70.65099	80.16692	69.46215	321.70495	-185.26452	574.37218	1
65	N	71.98692	79.70751	71.27732	-447.05792	-446.53431	367.76425	1
66	H	72.40701	78.88749	71.71857	350.31316	1975.63644	-1843.31522	1
67	C	72.79760	80.92168	71.17695	-511.23061	374.03917	-471.51480	1
68	H	73.33499	80.78745	70.21111	2234.79579	-898.70890	-1273.45190	1
69	C	71.83277	82.14190	71.14373	529.53781	-159.34528	563.72604	1
70	H	72.39301	83.09650	70.98629	654.59388	2347.94251	1217.51488	1
71	H	71.08681	82.02144	70.31972	-1526.55661	2103.42026	817.87394	1
72	O	71.03628	82.64390	72.46256	-554.84278	14.12789	399.58769	1
73	H	70.38098	81.96073	72.41916	1297.06236	2061.84854	1220.68812	1
74	C	73.79824	80.85856	72.45276	-662.15484	-412.13544	123.62687	1
75	O	74.81402	80.21055	72.40056	-540.01537	-317.05804	274.91456	1
76	N	73.29759	81.57224	73.45854	-202.76299	-690.00100	-131.49145	1
77	H	72.35525	82.03329	73.34180	-702.62132	-2617.37191	281.70413	1
78	C	73.97676	81.58389	74.77070	-491.73914	576.34187	222.73509	1
79	H	75.02732	81.87890	74.54289	1977.17978	-1823.58850	-434.68928	1
80	C	73.24283	82.57469	75.65641	-649.50797	-328.66843	306.11224	1
81	H	72.21860	82.17977	75.84096	2075.07803	1452.16490	-1004.45904	1
82	C	73.94072	82.71929	76.99739	-615.18735	-489.99689	-70.96352	1
83	H	73.37639	83.40248	77.68904	-1226.32661	-1724.38906	-1716.47170	1
84	H	74.04699	81.72712	77.51634	2381.64273	-969.84735	900.46860	1
85	H	74.97489	83.14403	76.88055	2122.74991	1702.23946	-141.36228	1
86	C	73.08808	83.93249	74.99527	-501.86074	-479.61276	-376.42482	1
87	H	72.55152	84.66135	75.66170	993.79261	-2246.95401	-1177.81305	1
88	H	74.08552	84.38366	74.74086	42.71279	-626.15391	-2651.37258	1
89	H	72.50097	83.86436	74.03722	-2026.39012	-1590.33709	-887.82922	1
90	C	73.88093	80.06845	75.35989	-672.89153	382.57394	-156.34072	1
91	O	74.87119	79.45796	75.92465	410.04627	221.86223	500.35950	1
92	N	72.71148	79.49626	75.22173	-378.11782	-443.79414	-441.10984	1
93	H	72.12095	80.21217	74.79399	2404.15973	-568.14894	1149.30085	1
94	C	72.53277	78.42497	76.15792	-544.54484	466.16019	331.29119	1
95	H	72.35167	78.96988	77.10657	-1409.80988	-170.17955	2325.32679	1
96	C	71.28596	77.57942	75.75103	-184.48284	116.78282	-758.89137	1
97	H	70.34092	78.08049	76.06741	1893.78641	1861.14652	611.04528	1
98	H	71.20317	77.47530	74.63663	-2170.79665	-974.19311	1327.50117	1
99	C	71.43656	76.18712	76.45764	389.51668	672.81878	-138.49152	1
100	H	72.40556	75.72756	76.16205	510.64577	1933.03327	1851.02484	1
101	H	71.50282	76.31164	77.56046	-2302.30869	-1105.72939	-948.89774	1
102	C	70.23579	75.21811	76.09596	-559.93427	-126.34590	542.30857	1
103	O	69.78635	74.46146	76.92076	-670.36003	-111.83166	76.36448	1
104	N	69.85707	75.30844	74.80788	-216.06729	-537.07037	446.51379	1

105	H	70.24686	75.89712	74.01829	-1251.96487	1074.12894	-2168.52500	1
106	H	69.11713	74.69532	74.44114	-2451.83023	-720.73851	944.84612	1
107	C	74.06826	77.70086	76.25124	546.24052	-563.88337	-85.11809	1
108	O	74.41339	77.26341	77.35261	71.70702	-307.40463	606.69673	1
109	N	74.33836	77.00979	75.07179	479.90863	-504.50129	222.86849	1
110	C	75.20669	75.91413	75.05771	75.51268	-600.91904	506.73700	1
111	H	75.28560	75.55063	76.11271	-2033.61562	1795.30103	254.89480	1
112	C	74.45620	74.97593	73.99491	523.79067	517.99274	284.45581	1
113	H	75.11437	74.17013	73.60054	1599.61665	-1127.00911	1895.98173	1
114	H	73.56612	74.48093	74.44204	-1881.83093	1275.82488	-1501.55016	1
115	C	74.04881	76.02063	72.91749	-600.05639	-404.05026	316.64485	1
116	H	74.88210	76.21186	72.20501	-2597.05260	496.36221	657.73249	1
117	H	73.17958	75.69635	72.30234	-1666.24518	1294.38985	-1723.90591	1
118	C	73.73008	77.31608	73.79872	493.57570	-129.95376	-602.56394	1
119	H	74.19203	78.26886	73.43380	-1469.08415	-637.84797	2204.22581	1
120	H	72.64126	77.49153	73.98673	-1038.97840	1068.88701	-2280.71789	1
121	C	76.67509	76.20128	74.32998	188.88100	241.05089	-727.87821	1
122	O	77.25924	75.28390	73.81024	531.88613	-49.19943	427.07960	1
123	N	77.14239	77.47740	74.50699	708.14833	26.93417	-179.73509	1
124	H	76.34908	77.88481	75.03364	-2232.69501	-1179.09831	1023.94816	1
125	C	77.44889	78.16894	73.26393	-738.32412	259.92548	104.42456	1
126	H	76.46082	78.35356	72.78874	2028.89123	1260.02983	1311.33324	1
127	C	78.19126	79.49960	73.67207	-258.65678	-345.52513	661.28459	1
128	H	79.03994	79.28368	74.35764	-1826.06090	-1801.46097	-918.64554	1
129	C	78.69081	80.19952	72.35848	-541.23400	531.92970	-218.41428	1
130	H	79.27173	81.12585	72.57760	1311.73218	-2219.18200	882.19023	1
131	H	79.35118	79.52095	71.76391	-1048.71298	1223.58118	-2196.97971	1
132	H	77.83694	80.48553	71.70059	419.06414	1903.92898	1903.44670	1
133	C	77.16299	80.47642	74.33806	-423.86431	152.66566	-648.55262	1
134	H	77.55764	81.51785	74.40653	105.68386	-2342.50080	1387.51238	1
135	H	76.20400	80.50191	73.73118	-1695.63603	-1484.73621	-1531.02793	1
136	H	76.90386	80.15012	75.37488	-1853.57121	-487.39031	1936.59343	1
137	C	78.47464	77.38404	72.29110	539.71428	-510.58232	267.58633	1
138	O	78.41840	77.54536	71.09009	-15.93758	-278.34085	-624.49402	1
139	N	79.54875	76.84817	72.98914	-676.81886	12.05292	276.17960	1
140	H	79.08761	76.69234	73.90090	-1694.44250	-373.84189	-2100.66098	1
141	C	80.13974	75.72193	72.28170	412.33078	-664.70360	108.35451	1
142	H	79.28815	75.06981	71.99108	1765.77476	1294.44366	1621.76594	1
143	C	80.92510	76.33163	71.06869	-179.66635	-721.95667	-264.73915	1
144	H	80.23031	76.86261	70.36599	-607.34922	2587.87032	-598.10018	1
145	H	81.63542	77.10792	71.43576	-359.69332	-1479.13954	-2259.74260	1
146	C	81.69591	75.18286	70.32949	-240.01076	616.02425	431.85322	1
147	H	82.33707	74.61670	71.04217	-1359.17131	782.54425	2227.99181	1
148	H	80.99244	74.44111	69.88991	-820.36667	85.81767	-2596.78715	1
149	C	82.57323	75.87588	69.21234	-513.07015	236.18570	-551.87280	1
150	H	81.92842	76.41516	68.48067	1816.11944	-1183.11722	-1650.94321	1
151	H	83.23657	76.65182	69.65944	-1800.04429	-1361.53473	1526.34643	1
152	C	83.41495	74.78783	68.50582	726.08972	-253.19732	-179.64713	1
153	H	84.14214	74.26857	69.16148	1224.27271	-456.51798	-2390.90304	1
154	H	82.82485	74.04553	67.93235	1206.40339	-1150.93514	-2154.90344	1
155	N	84.29851	75.51139	67.43378	329.70796	-633.68968	-155.67358	1
156	H	84.93944	74.88473	66.86671	1348.31305	1938.76845	1359.00643	1
157	H	83.79102	76.03989	66.66577	2096.92035	1446.54551	-966.48890	1
158	H	84.98239	76.24235	67.78716	-1197.07217	-2303.53719	827.28733	1
159	C	81.20738	75.02252	73.28764	-378.01186	-556.17301	-413.96481	1
160	O	82.21212	75.57383	73.67798	-409.44433	-307.55053	-453.30833	1
161	N	80.83128	73.75652	73.50473	-429.02477	524.70884	274.08502	1
162	H	79.92109	73.44498	73.16369	1706.34263	-1425.96036	1574.38926	1
163	C	81.69579	73.00565	74.36724	-45.25864	-626.22952	478.93267	1
164	H	82.71393	73.31253	74.03475	1988.63164	570.90773	1772.87287	1
165	C	81.43607	73.53567	75.83731	551.77128	-20.49526	-564.54996	1
166	H	81.57371	74.64049	75.87603	1434.61535	-1753.10253	1513.99471	1

167	H	80.38531	73.34857	76.15398	-714.67738	1819.09770	1898.36494	1
168	C	82.44567	72.80096	76.77925	446.99263	-555.77305	338.97221	1
169	H	82.19265	71.71127	76.83791	1953.68466	1892.25957	-161.67766	1
170	H	83.48299	72.85362	76.37803	-403.03785	2688.07032	-188.43591	1
171	C	82.35824	73.49355	78.19591	567.86262	335.74681	434.04421	1
172	H	82.75649	74.53375	78.15950	-1080.02275	1568.26081	-1948.78900	1
173	H	81.29293	73.59042	78.52203	-919.54108	2111.34692	1456.13463	1
174	C	83.17687	72.61173	79.17547	195.81897	173.33862	-745.11536	1
175	H	82.87100	71.54467	79.20414	1405.67949	-2301.21089	-390.08113	1
176	H	84.27453	72.68250	79.03194	-940.37328	-1118.32446	2299.72133	1
177	N	82.93055	73.11511	80.61824	319.26422	656.36007	-42.02424	1
178	H	83.70725	72.85364	81.29168	1961.03633	619.91968	1787.09422	1
179	H	82.91084	74.16469	80.76414	854.14343	-2156.80752	1429.08711	1
180	H	82.01209	72.72942	81.12946	1237.02905	-1378.50857	-1998.28500	1
181	C	81.42249	71.39432	74.30823	532.53319	-268.57236	517.55729	1
182	O	82.26084	70.67594	74.80059	266.16714	-290.73804	-558.88002	1
183	N	80.26129	71.07148	73.76230	-226.25352	640.49678	-270.32839	1
184	H	79.68916	71.81936	73.37128	2007.69063	-1035.27229	1523.50231	1
185	C	79.82698	69.70749	73.66974	-540.76542	-573.33303	49.50000	1
186	H	78.94795	69.79529	72.98864	-2374.20950	-1036.76023	843.75774	1
187	C	81.00601	68.81919	73.02246	-77.09082	666.87422	-415.84136	1
188	H	81.78409	68.67219	73.82281	-985.81834	617.19825	2463.91927	1
189	O	81.66899	69.40642	71.89198	293.29899	-391.65602	-477.80926	1
190	H	82.52452	69.65611	72.30350	2528.72714	-681.76262	-751.27122	1
191	C	80.29962	67.45042	72.71094	252.47363	-605.14473	440.05134	1
192	H	81.02576	66.70241	72.31595	-2052.65063	1456.49051	-1043.51830	1
193	H	79.82321	67.00071	73.61761	-2152.98800	-1661.97574	-161.70652	1
194	H	79.50190	67.57110	71.94156	-473.12726	-1584.27339	2165.61725	1
195	C	79.41134	69.22622	75.12955	360.36307	488.46713	505.10056	1
196	O	79.55708	67.93366	75.48923	-200.08817	-528.03552	-385.82850	1
197	N	78.82682	70.13499	75.80393	-597.54095	-226.44775	355.20479	1
198	H	78.79902	70.97602	75.20547	2179.23655	-1300.70981	-991.33835	1
199	C	78.35744	70.11541	77.14296	-687.68921	297.39807	-249.45179	1
200	H	77.42902	70.72546	77.12298	-349.16256	-2467.37713	-1101.72831	1
201	C	78.13866	68.60927	77.66059	672.47345	361.54328	-201.62880	1
202	H	79.11344	68.05852	77.66091	1541.41502	582.18425	2169.97026	1
203	H	77.76261	68.61870	78.71867	-2534.67717	60.25153	997.72295	1
204	C	77.15333	67.97161	76.69912	574.26774	-389.43119	-377.02542	1
205	C	75.75241	68.14032	76.71900	688.82679	-287.33580	-257.96133	1
206	H	75.25637	68.69383	77.54084	331.14182	1470.38163	2269.80013	1
207	C	77.83729	67.20394	75.62218	-383.52382	-675.04808	144.24917	1
208	H	78.57843	66.40065	75.96454	4.09847	1517.59662	2262.86397	1
209	C	75.00743	67.63935	75.63436	-134.76730	428.45285	-649.50303	1
210	H	73.91435	67.77881	75.63564	-903.23433	1600.49020	2011.53387	1
211	C	76.97848	66.79888	74.49568	-335.53281	-615.00040	-364.39058	1
212	H	77.43617	66.28776	73.63687	1596.45398	-1369.33862	1732.02659	1
213	C	75.59869	66.98565	74.51092	585.48547	-340.24194	-406.23938	1
214	O	74.73069	66.55218	73.42101	-419.15649	-173.04408	-511.94141	1
215	H	75.39454	66.16060	72.83219	-1071.84350	1559.71507	-1960.13012	1
216	C	79.48647	70.76206	78.11715	291.41878	-183.13091	710.72246	1
217	O	80.66885	70.50876	78.04388	379.87695	523.47396	-222.23622	1
218	N	78.85716	71.48337	79.05131	564.30591	373.09380	277.24371	1
219	H	77.84248	71.58697	79.00713	-120.59931	-2436.07824	-1214.35098	1
220	C	79.68094	72.36447	79.82233	404.07514	-299.37480	608.84009	1
221	H	80.67619	72.35182	79.31101	-1071.07882	-841.69025	2359.66467	1
222	C	78.97243	73.78490	79.86297	-683.12807	68.71770	-390.13096	1
223	H	78.77558	74.16952	78.83721	2068.88918	1596.58590	770.89603	1
224	H	77.97506	73.70996	80.35208	1379.86429	2342.49779	-179.85638	1
225	C	79.91584	74.73754	80.65865	-176.39967	537.49466	550.97268	1
226	H	80.21848	74.26901	81.62478	-396.28051	1942.22168	1869.33314	1
227	H	80.86423	74.92094	80.10692	-94.44700	586.00678	-2659.20016	1
228	C	79.11927	76.10005	80.90420	-291.69381	-718.18079	-150.72929	1

229	H	78.88947	76.70608	79.99111	-2303.38776	1089.76242	964.62032	1
230	H	78.17513	76.00209	81.49866	884.16729	2568.80533	-207.74283	1
231	N	80.04242	76.81269	81.68460	-594.49522	-252.81478	342.29276	1
232	H	80.87569	76.32046	81.96787	-1735.17426	2084.05705	-263.71605	1
233	C	79.89313	78.01760	82.06243	595.23177	-271.52487	442.22352	1
234	N	78.72836	78.68406	81.66710	585.53813	-424.79750	-105.81303	1
235	H	77.94793	78.34500	81.10586	959.88797	1327.56823	-2177.11905	1
236	H	78.49424	79.64756	81.90797	1578.48647	16.27378	-2220.76233	1
237	N	80.98416	78.43915	82.83549	-452.17763	-390.33541	-421.51853	1
238	H	81.82853	77.94727	83.12400	470.26107	1974.25629	-1817.92087	1
239	H	81.05604	79.37416	83.23834	1856.67307	-1573.97321	-1224.35416	1
240	C	79.80135	71.83812	81.35803	-531.47271	-581.45780	-55.06206	1
241	O	80.81959	72.10012	82.01451	-243.00837	192.73507	609.52485	1
242	N	78.70025	71.25464	81.76552	343.49288	-644.25607	38.09164	1
243	H	77.99917	71.24932	81.02713	-1691.16043	-1535.97525	-1484.73099	1
244	C	78.69076	70.29903	82.87597	542.66492	350.14337	454.42563	1
245	H	79.71902	69.86434	82.85351	1209.57979	-2396.95920	463.86744	1
246	C	78.41285	71.04841	84.17172	-737.14309	145.93010	242.71942	1
247	H	77.38241	71.46443	84.10677	-1050.18303	159.36419	-2509.06125	1
248	C	78.47465	70.12044	85.36978	-706.77696	-252.88343	-245.16230	1
249	H	78.22365	70.65490	86.32718	-1624.64039	-1665.49085	1417.86935	1
250	H	77.74609	69.26336	85.25860	2566.10521	598.51109	693.22305	1
251	H	79.49951	69.67391	85.49628	-1972.69758	107.10018	-1876.34312	1
252	C	79.36791	72.21233	84.36200	412.85148	672.58832	-27.69222	1
253	H	79.15956	72.78224	85.30907	1447.02277	1762.76533	-1490.78944	1
254	H	80.43719	71.86343	84.40137	1320.77379	-145.20455	2378.68491	1
255	H	79.30282	72.93824	83.50265	-1512.10848	1470.52031	1724.75147	1
256	C	77.49444	69.21921	82.50921	-607.11113	499.56689	73.73769	1
257	O	76.84029	68.70410	83.39028	357.97126	460.81534	356.68785	1
258	N	77.47049	68.96534	81.20075	536.55407	-368.62270	332.76306	1
259	H	78.18853	69.47989	80.68968	524.38866	2297.69985	1367.20941	1
260	C	76.20126	68.77285	80.56697	46.50277	-774.29190	-147.97904	1
261	H	76.43326	68.62665	79.48503	1676.51875	1883.29066	1032.55549	1
262	C	75.49495	67.48264	81.21403	-559.41456	-34.19198	-556.30433	1
263	H	75.50940	67.55127	82.33722	-64.66664	395.18769	2695.05373	1
264	H	74.42379	67.40075	80.90712	-2703.44278	-60.40056	333.79418	1
265	C	76.29938	66.29623	80.74445	-519.76435	377.31045	459.42366	1
266	H	77.37084	66.60044	80.71631	-1746.74323	1667.50644	-1261.73691	1
267	C	76.16898	65.13212	81.71744	570.95554	16.46261	-545.27700	1
268	H	76.77680	64.24938	81.38952	2391.58273	28.05277	-1305.07271	1
269	H	76.51930	65.41373	82.74451	175.75588	917.63458	2559.43867	1
270	H	75.10690	64.78787	81.81104	-1063.97851	-2155.34650	1283.00462	1
271	C	75.87574	65.86027	79.34877	193.76014	2.62946	-765.53141	1
272	H	76.50058	65.00952	78.97294	507.39394	-846.55087	2539.60089	1
273	H	74.80807	65.52075	79.32937	1337.57841	1818.19054	1526.01994	1
274	H	75.97079	66.69221	78.60559	1100.88635	-1172.91350	-2199.08909	1
275	C	75.40840	70.16149	80.75768	-549.21115	475.64486	-309.38218	1
276	O	75.52452	71.04544	79.94862	556.06106	-390.37755	-78.24250	1
277	O	74.61503	70.33264	81.91568	-572.27940	-310.19032	-209.75862	1
278	H	74.96556	69.57284	82.46299	-1380.08193	2212.14486	790.85944	1

Listing 84: C00084.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.5003	0.0000	300.0000
3	H	74.99049	62.39079	74.38730	-2043.14101	-1757.64893	399.89339		1
4	N	74.91929	63.40443	74.31773	426.75047	490.45733	-334.42467		1
5	H	74.61490	63.66701	75.25539	442.25559	-1110.30854	-2448.52907		1
6	C	76.11801	64.05675	73.95908	415.32972	-666.39213	83.73172		1
7	H	76.66978	63.39464	73.25746	879.32219	2491.00447	667.35213		1
8	C	75.72620	65.49312	73.33932	31.35357	477.41777	628.23362		1

9	H	75.22750	66.09959	74.13331	1168.38489	2240.25337	-1019.71136	1
10	H	76.64416	66.05879	73.04904	-360.43770	2534.90498	931.67112	1
11	C	74.80008	65.31484	72.16317	463.18208	512.70242	-382.34388	1
12	H	74.00320	64.59446	72.45721	1725.29117	1863.52247	-987.07854	1
13	C	74.14230	66.64081	71.80288	710.42801	-144.27427	-313.15367	1
14	H	73.43243	66.53107	70.94279	364.20195	-1033.13725	2494.72524	1
15	H	73.55954	67.06072	72.66328	2567.61904	335.80679	847.48802	1
16	H	74.90170	67.41091	71.50966	-2587.99029	680.92867	-512.16411	1
17	C	75.53705	64.76057	70.95226	268.17616	741.64379	-40.42634	1
18	H	74.85373	64.64263	70.07161	1283.54314	-1945.37420	-1411.27812	1
19	H	76.37360	65.43538	70.63458	-1258.57796	1317.15249	-2026.02085	1
20	H	75.98288	63.75455	71.16376	-2502.84526	909.80597	575.92391	1
21	C	76.87865	64.34746	75.37110	619.36578	-458.64843	-172.09273	1
22	O	76.28551	64.82106	76.32532	-81.40433	433.87611	522.34594	1
23	N	78.17216	64.09436	75.23967	175.23996	-622.20190	341.55523	1
24	H	78.51533	63.73578	74.34961	-876.57256	-303.22879	-2561.90213	1
25	C	78.98174	64.07271	76.41206	-571.88214	-534.10783	-106.15033	1
26	H	78.25920	64.25095	77.24205	-2713.20841	-16.25800	-248.80809	1
27	C	79.73713	62.65729	76.47935	166.60354	288.16399	-716.09568	1
28	H	80.42293	62.58125	75.59209	-2097.85574	1636.78449	-586.18044	1
29	O	78.89442	61.49652	76.45113	-317.80580	-363.38227	484.43082	1
30	H	79.21334	61.04898	75.64070	1863.74748	-1451.84923	1357.29467	1
31	C	80.59791	62.84822	77.78140	503.80731	517.99032	318.51606	1
32	H	81.29760	61.99459	77.93829	640.61020	-2157.10410	-1536.29104	1
33	H	81.21237	63.78267	77.73726	1687.88455	465.60692	2087.56452	1
34	H	79.95534	62.91811	78.68953	-1293.07895	-1899.88581	-1463.57452	1
35	C	80.10283	65.23902	76.22547	-153.07550	-733.68902	248.70981	1
36	O	81.20216	64.95522	75.77679	186.15459	-480.78787	-449.34387	1
37	N	79.64130	66.42483	76.62343	-487.53139	543.18517	42.03850	1
38	C	80.30006	67.64777	76.26815	-699.35871	69.34393	360.10701	1
39	H	80.71850	67.48768	75.24774	2.81126	-221.99807	-2715.58072	1
40	C	79.10519	68.68394	76.38120	-507.46439	-592.59194	122.07761	1
41	H	79.44829	69.74021	76.44270	-1975.08116	525.87560	-1801.71556	1
42	H	78.42399	68.61989	75.50361	1588.27743	-1913.22100	1113.83566	1
43	C	78.40521	68.17110	77.67984	-613.62442	-457.55993	-194.14490	1
44	H	78.96774	68.49474	78.58495	1707.54637	-721.27992	1996.92523	1
45	H	77.36453	68.54650	77.80538	758.23357	2100.81767	1560.55011	1
46	C	78.48355	66.59723	77.49263	-352.41524	704.96076	49.21465	1
47	H	78.67655	66.01965	78.42771	1714.76886	-2070.42778	443.35792	1
48	H	77.61337	66.12930	76.94219	1224.15040	1801.50881	1636.97633	1
49	C	81.46923	67.89900	77.38967	566.85117	537.05831	117.62814	1
50	O	81.45243	68.86288	78.11314	-550.26779	-406.08867	4.21666	1
51	N	82.36767	66.92149	77.31303	566.34832	-425.77725	180.18749	1
52	H	82.22568	66.12321	76.65427	644.44502	2646.80550	-52.73430	1
53	C	83.47361	67.01181	78.22072	612.34801	-281.48662	411.56221	1
54	H	83.00284	67.42196	79.14359	1667.23498	-1490.75142	1556.16753	1
55	C	84.05723	65.53622	78.39729	-714.45746	-175.43074	286.98927	1
56	H	84.46436	65.19000	77.40796	-787.09484	1763.03619	-1922.46060	1
57	O	83.09440	64.53380	78.78999	-429.46514	516.51932	-128.40526	1
58	H	83.16770	63.91123	78.03968	1981.82785	436.16847	-1818.18182	1
59	C	85.24913	65.72034	79.40542	630.79189	-468.94448	76.03230	1
60	H	85.72690	64.74328	79.65040	-1775.71861	2062.30353	131.89849	1
61	H	86.04965	66.38325	78.99587	-1855.14608	88.94118	1993.53760	1
62	H	84.90490	66.16951	80.36600	-1504.82350	-780.94249	-2132.90992	1
63	C	84.57672	68.06165	77.65096	288.57638	618.62814	-397.00270	1
64	O	85.48440	68.41787	78.40153	321.70495	-185.26452	574.37218	1
65	N	84.36384	68.41374	76.40845	-447.05792	-446.53431	367.76425	1
66	H	83.52583	68.04892	75.95785	350.31316	1975.63644	-1843.31522	1
67	C	85.32777	69.08612	75.59456	-511.23061	374.03917	-471.51480	1
68	H	86.30568	68.67255	75.93124	2234.79579	-898.70890	-1273.45190	1
69	C	84.89739	68.69817	74.11026	529.53781	-159.34528	563.72604	1
70	H	85.51429	69.29523	73.39273	654.59388	2347.94251	1217.51488	1

71	H	85.19033	67.62993	73.91960	-1526.55661	2103.42026	817.87394	1
72	O	83.45948	68.77476	73.80585	-554.84278	14.12789	399.58769	1
73	H	83.50456	69.03990	72.87600	1297.06236	2061.84854	1220.68812	1
74	C	85.26148	70.68328	75.88109	-662.15484	-412.13544	123.62687	1
75	O	85.17776	71.48659	74.98549	-540.01537	-317.05804	274.91456	1
76	N	85.42250	70.88468	77.18850	-202.76299	-690.00100	-131.49145	1
77	H	85.56249	70.04034	77.80019	-702.62132	-2617.37191	281.70413	1
78	C	85.28378	72.19202	77.81935	-491.73914	576.34187	222.73509	1
79	H	85.66832	72.02507	78.85346	1977.17978	-1823.58850	-434.68928	1
80	C	86.12716	73.19108	77.04953	-649.50797	-328.66843	306.11224	1
81	H	85.79230	73.16832	75.97882	2075.07803	1452.16490	-1004.45904	1
82	C	85.97231	74.60858	77.56583	-615.18735	-489.99689	-70.96352	1
83	H	86.63331	75.32881	77.00866	-1226.32661	-1724.38906	-1716.47170	1
84	H	84.91228	74.97622	77.46059	2381.64273	-969.84735	900.46860	1
85	H	86.24129	74.68312	78.65569	2122.74991	1702.23946	-141.36228	1
86	C	87.59437	72.79802	77.07504	-501.86074	-479.61276	-376.42482	1
87	H	88.22363	73.48369	76.44432	993.79261	-2246.95401	-1177.81305	1
88	H	88.01230	72.82625	78.11863	42.71279	-626.15391	-2651.37258	1
89	H	87.74264	71.75283	76.68691	-2026.39012	-1590.33709	-887.82922	1
90	C	83.66550	72.59762	77.87142	-672.89153	382.57394	-156.34072	1
91	O	83.35048	73.62776	78.41602	410.04627	221.86223	500.35950	1
92	N	82.89341	71.69811	77.29347	-378.11782	-443.79414	-441.10984	1
93	H	83.38630	70.87714	76.94218	2404.15973	-568.14894	1149.30085	1
94	C	81.46843	71.77779	77.28969	-544.54484	466.16019	331.29119	1
95	H	81.19445	70.86807	76.70752	-1409.80988	-170.17955	2325.32679	1
96	C	81.00472	71.68728	78.81025	-184.48284	116.78282	-758.89137	1
97	H	81.50564	70.81740	79.29732	1893.78641	1861.14652	611.04528	1
98	H	81.33489	72.59245	79.37068	-2170.79665	-974.19311	1327.50117	1
99	C	79.45588	71.52341	78.85737	389.51668	672.81878	-138.49152	1
100	H	78.96073	72.44317	78.46116	510.64577	1933.03327	1851.02484	1
101	H	79.13716	70.71983	78.15937	-2302.30869	-1105.72939	-948.89774	1
102	C	78.88698	71.20390	80.29109	-559.93427	-126.34590	542.30857	1
103	O	77.70642	71.00716	80.42154	-670.36003	-111.83166	76.36448	1
104	N	79.81699	71.18188	81.26940	-216.06729	-537.07037	446.51379	1
105	H	80.82640	71.36284	81.21903	-1251.96487	1074.12894	-2168.52500	1
106	H	79.60308	71.01338	82.25859	-2451.83023	-720.73851	944.84612	1
107	C	80.93933	73.15590	76.62928	546.24052	-563.88337	-85.11809	1
108	O	80.06017	73.78048	77.20865	71.70702	-307.40463	606.69673	1
109	N	81.45576	73.39880	75.42887	479.90863	-504.50129	222.86849	1
110	C	81.31164	74.69301	74.81193	75.51268	-600.91904	506.73700	1
111	H	81.45773	75.41957	75.64431	-2033.61562	1795.30103	254.89480	1
112	C	82.45104	74.66467	73.70874	523.79067	517.99274	284.45581	1
113	H	82.25275	75.36730	72.86824	1599.61665	-1127.00911	1895.98173	1
114	H	83.43979	74.94546	74.13616	-1881.83093	1275.82488	-1501.55016	1
115	C	82.43119	73.16628	73.27255	-600.05639	-404.05026	316.64485	1
116	H	81.56346	72.95795	72.60651	-2597.05260	496.36221	657.73249	1
117	H	83.34532	72.84686	72.72257	-1666.24518	1294.38985	-1723.90591	1
118	C	82.27297	72.45179	74.68278	493.57570	-129.95376	-602.56394	1
119	H	81.76174	71.46051	74.66916	-1469.08415	-637.84797	2204.22581	1
120	H	83.22672	72.36645	75.26136	-1038.97840	1068.88701	-2280.71789	1
121	C	79.82084	74.80018	74.16747	188.88100	241.05089	-727.87821	1
122	O	79.65870	74.69923	72.98448	531.88613	-49.19943	427.07960	1
123	N	78.91667	75.03239	75.13669	708.14833	26.93417	-179.73509	1
124	H	79.21783	74.91348	76.13368	-2232.69501	-1179.09831	1023.94816	1
125	C	77.49174	75.05373	74.78299	-738.32412	259.92548	104.42456	1
126	H	77.51217	74.66118	73.73796	2028.89123	1260.02983	1311.33324	1
127	C	76.75323	74.16639	75.76120	-258.65678	-345.52513	661.28459	1
128	H	76.90027	74.57331	76.78644	-1826.06090	-1801.46097	-918.64554	1
129	C	75.26479	74.13451	75.46179	-541.23400	531.92970	-218.41428	1
130	H	74.69869	73.53656	76.22722	1311.73218	-2219.18200	882.19023	1
131	H	74.82036	75.16771	75.44664	-1048.71298	1223.58118	-2196.97971	1
132	H	75.05673	73.67371	74.45764	419.06414	1903.92898	1903.44670	1

133	C	77.30957	72.75264	75.77235	-423.86431	152.66566	-648.55262	1
134	H	76.79746	72.10755	76.53781	105.68386	-2342.50080	1387.51238	1
135	H	77.18638	72.25148	74.77370	-1695.63603	-1484.73621	-1531.02793	1
136	H	78.41028	72.74827	76.01188	-1853.57121	-487.39031	1936.59343	1
137	C	77.01371	76.65018	74.79164	539.71428	-510.58232	267.58633	1
138	O	77.27084	77.30942	73.80909	-15.93758	-278.34085	-624.49402	1
139	N	76.41205	77.03191	75.90038	-676.81886	12.05292	276.17960	1
140	H	76.33515	76.33954	76.64080	-1694.44250	-373.84189	-2100.66098	1
141	C	75.88941	78.34553	76.05460	412.33078	-664.70360	108.35451	1
142	H	75.77799	78.43856	77.15827	1765.77476	1294.44366	1621.76594	1
143	C	76.89656	79.37120	75.39575	-179.66635	-721.95667	-264.73915	1
144	H	77.94429	79.13663	75.69294	-607.34922	2587.87032	-598.10018	1
145	H	76.86929	79.27859	74.27692	-359.69332	-1479.13954	-2259.74260	1
146	C	76.49528	80.82302	75.82560	-240.01076	616.02425	431.85322	1
147	H	75.44590	81.04238	75.52036	-1359.17131	782.54425	2227.99181	1
148	H	76.52881	80.94556	76.93141	-820.36667	85.81767	-2596.78715	1
149	C	77.50575	81.80476	75.10808	-513.07015	236.18570	-551.87280	1
150	H	78.54296	81.65143	75.48542	1816.11944	-1183.11722	-1650.94321	1
151	H	77.54840	81.59333	74.01464	-1800.04429	-1361.53473	1526.34643	1
152	C	77.03634	83.25687	75.35692	726.08972	-253.19732	-179.64713	1
153	H	76.06206	83.51179	74.89413	1224.27271	-456.51798	-2390.90304	1
154	H	77.04460	83.57125	76.41952	1206.40339	-1150.93514	-2154.90344	1
155	N	78.06850	84.20160	74.65242	329.70796	-633.68968	-155.67358	1
156	H	77.86340	85.24028	74.71709	1348.31305	1938.76845	1359.00643	1
157	H	79.07041	84.16531	75.00093	2096.92035	1446.54551	-966.48890	1
158	H	78.19730	84.07899	73.60591	-1197.07217	-2303.53719	827.28733	1
159	C	74.45514	78.50705	75.27071	-378.01186	-556.17301	-413.96481	1
160	O	74.28348	79.38737	74.45752	-409.44433	-307.55053	-453.30833	1
161	N	73.58061	77.59971	75.69411	-429.02477	524.70884	274.08502	1
162	H	73.88043	76.97031	76.43731	1706.34263	-1425.96036	1574.38926	1
163	C	72.21445	77.79769	75.34272	-45.25864	-626.22952	478.93267	1
164	H	72.25856	78.40538	74.40882	1988.63164	570.90773	1772.87287	1
165	C	71.54696	76.37417	75.21162	551.77128	-20.49526	-564.54996	1
166	H	72.18212	75.69592	74.59825	1434.61535	-1753.10253	1513.99471	1
167	H	71.46563	75.89178	76.21223	-714.67738	1819.09770	1898.36494	1
168	C	70.13151	76.55651	74.56678	446.99263	-555.77305	338.97221	1
169	H	69.47967	77.21454	75.19187	1953.68466	1892.25957	-161.67766	1
170	H	70.20090	77.05093	73.57167	-403.03785	2688.07032	-188.43591	1
171	C	69.52425	75.10226	74.43938	567.86262	335.74681	434.04421	1
172	H	70.18435	74.45156	73.82075	-1080.02275	1568.26081	-1948.78900	1
173	H	69.46593	74.61101	75.43801	-919.54108	2111.34692	1456.13463	1
174	C	68.11890	75.21535	73.80463	195.81897	173.33862	-745.11536	1
175	H	67.37103	75.74201	74.43072	1405.67949	-2301.21089	-390.08113	1
176	H	68.10723	75.62683	72.77553	-940.37328	-1118.32446	2299.72133	1
177	N	67.57287	73.75494	73.65824	319.26422	656.36007	-42.02424	1
178	H	66.60144	73.66268	73.24292	1961.03633	619.91968	1787.09422	1
179	H	68.12704	73.09322	73.04006	854.14343	-2156.80752	1429.08711	1
180	H	67.47325	73.18727	74.54969	1237.02905	-1378.50857	-1998.28500	1
181	C	71.47788	78.57976	76.59854	532.53319	-268.57236	517.55729	1
182	O	70.95130	77.97607	77.50299	266.16714	-290.73804	-558.88002	1
183	N	71.58541	79.88823	76.41501	-226.25352	640.49678	-270.32839	1
184	H	72.10613	80.22404	75.60554	2007.69063	-1035.27229	1523.50231	1
185	C	70.98358	80.74783	77.36945	-540.76542	-573.33303	49.50000	1
186	H	70.83289	80.09814	78.26262	-2374.20950	-1036.76023	843.75774	1
187	C	71.95721	81.99531	77.57724	-77.09082	666.87422	-415.84136	1
188	H	72.06491	82.52925	76.59334	-985.81834	617.19825	2463.91927	1
189	O	73.29541	81.69158	78.01273	293.29899	-391.65602	-477.80926	1
190	H	73.82064	82.00894	77.25115	2528.72714	-681.76262	-751.27122	1
191	C	71.09260	82.87218	78.55633	252.47363	-605.14473	440.05134	1
192	H	71.56452	83.86370	78.74691	-2052.65063	1456.49051	-1043.51830	1
193	H	70.07591	83.05975	78.13680	-2152.98800	-1661.97574	-161.70652	1
194	H	70.95825	82.37313	79.54406	-473.12726	-1584.27339	2165.61725	1

195	C	69.56336	81.28022	76.70608	360.36307	488.46713	505.10056	1
196	O	69.53820	82.29610	76.05019	-200.08817	-528.03552	-385.82850	1
197	N	68.58541	80.47029	77.06831	-597.54095	-226.44775	355.20479	1
198	H	68.86189	79.65856	77.62121	2179.23655	-1300.70981	-991.33835	1
199	C	67.27427	80.53830	76.52946	-687.68921	297.39807	-249.45179	1
200	H	66.71364	79.93774	77.27926	-349.16256	-2467.37713	-1101.72831	1
201	C	66.75316	82.04510	76.40490	672.47345	361.54328	-201.62880	1
202	H	67.41099	82.61250	75.70080	1541.41502	582.18425	2169.97026	1
203	H	65.72260	82.05117	75.97596	-2534.67717	60.25153	997.72295	1
204	C	66.75228	82.72413	77.78320	574.26774	-389.43119	-377.02542	1
205	C	65.76304	82.41160	78.76286	688.82679	-287.33580	-257.96133	1
206	H	64.96653	81.67604	78.54883	331.14182	1470.38163	2269.80013	1
207	C	67.76953	83.68484	78.06129	-383.52382	-675.04808	144.24917	1
208	H	68.52780	83.92769	77.29168	4.09847	1517.59662	2262.86397	1
209	C	65.82672	83.05718	79.99774	-134.76730	428.45285	-649.50303	1
210	H	65.06187	82.81974	80.75756	-903.23433	1600.49020	2011.53387	1
211	C	67.79593	84.29944	79.31544	-335.53281	-615.00040	-364.39058	1
212	H	68.59396	85.03382	79.52227	1596.45398	-1369.33862	1732.02659	1
213	C	66.83335	84.01115	80.32633	585.48547	-340.24194	-406.23938	1
214	O	66.84976	84.62730	81.60504	-419.15649	-173.04408	-511.94141	1
215	H	67.62876	85.22170	81.49310	-1071.84350	1559.71507	-1960.13012	1
216	C	67.27743	79.78305	75.08773	291.41878	-183.13091	710.72246	1
217	O	67.82526	78.71397	74.93039	379.87695	523.47396	-222.23622	1
218	N	66.55465	80.46489	74.19952	564.30591	373.09380	277.24371	1
219	H	66.12453	81.34934	74.47144	-120.59931	-2436.07824	-1214.35098	1
220	C	66.18348	79.78004	73.00479	404.07514	-299.37480	608.84009	1
221	H	66.25055	78.69979	73.27206	-1071.07882	-841.69025	2359.66467	1
222	C	64.74483	80.30465	72.60238	-683.12807	68.71770	-390.13096	1
223	H	64.02396	80.17032	73.43992	2068.88918	1596.58590	770.89603	1
224	H	64.77759	81.40103	72.41166	1379.86429	2342.49779	-179.85638	1
225	C	64.26637	79.54527	71.32616	-176.39967	537.49466	550.97268	1
226	H	65.04158	79.58197	70.52556	-396.28051	1942.22168	1869.33314	1
227	H	64.10249	78.46499	71.53545	-94.44700	586.00678	-2659.20016	1
228	C	62.91794	80.26556	70.86059	-291.69381	-718.18079	-150.72929	1
229	H	62.07552	80.20861	71.59624	-2303.38776	1089.76242	964.62032	1
230	H	63.02081	81.33389	70.54148	884.16729	2568.80533	-207.74283	1
231	N	62.54277	79.51714	69.73625	-594.49522	-252.81478	342.29276	1
232	H	63.05543	78.66545	69.56839	-1735.17426	2084.05705	-263.71605	1
233	C	61.60623	79.83438	68.93754	595.23177	-271.52487	442.22352	1
234	N	60.89622	81.01232	69.19594	585.53813	-424.79750	-105.81303	1
235	H	60.99024	81.66642	69.97180	959.88797	1327.56823	-2177.11905	1
236	H	60.10916	81.35301	68.64293	1578.48647	16.27378	-2220.76233	1
237	N	61.47827	78.88865	67.91077	-452.17763	-390.33541	-421.51853	1
238	H	61.98917	78.02687	67.72527	470.26107	1974.25629	-1817.92087	1
239	H	60.77399	78.95911	67.17517	1856.67307	-1573.97321	-1224.35416	1
240	C	67.19100	80.15544	71.76501	-531.47271	-581.45780	-55.06206	1
241	O	67.29740	79.38559	70.84297	-243.00837	192.73507	609.52485	1
242	N	67.64126	81.44573	71.81616	343.49288	-644.25607	38.09164	1
243	H	67.35350	81.73492	72.75791	-1691.16043	-1535.97525	-1484.73099	1
244	C	69.00879	81.77569	71.34527	542.66492	350.14337	454.42563	1
245	H	69.05384	82.85480	71.61808	1209.57979	-2396.95920	463.86744	1
246	C	70.02799	80.94549	72.08023	-737.14309	145.93010	242.71942	1
247	H	69.81622	79.87316	71.86650	-1050.18303	159.36419	-2509.06125	1
248	C	71.44171	81.26004	71.61777	-706.77696	-252.88343	-245.16230	1
249	H	72.20893	80.66429	72.18404	-1624.64039	-1665.49085	1417.86935	1
250	H	71.57800	81.02932	70.52358	2566.10521	598.51109	693.22305	1
251	H	71.69138	82.34671	71.76174	-1972.69758	107.10018	-1876.34312	1
252	C	69.95182	81.15080	73.58505	412.85148	672.58832	-27.69222	1
253	H	70.69406	80.51137	74.13439	1447.02277	1762.76533	-1490.78944	1
254	H	70.16228	82.22089	73.86516	1320.77379	-145.20455	2378.68491	1
255	H	68.93622	80.89727	73.99380	-1512.10848	1470.52031	1724.75147	1
256	C	69.06875	81.54056	69.71649	-607.11113	499.56689	73.73769	1

257	O	69.78182	80.69616	69.22311	357.97126	460.81534	356.68785	1
258	N	68.29440	82.42086	69.09649	536.55407	-368.62270	332.76306	1
259	H	67.76055	83.08291	69.65753	524.38866	2297.69985	1367.20941	1
260	C	68.21247	82.35382	67.68707	46.50277	-774.29190	-147.97904	1
261	H	68.92216	81.54378	67.39460	1676.51875	1883.29066	1032.55549	1
262	C	66.67892	82.06963	67.26249	-559.41456	-34.19198	-556.30433	1
263	H	66.06777	82.98317	67.45561	-64.66664	395.18769	2695.05373	1
264	H	66.61380	81.88993	66.16300	-2703.44278	-60.40056	333.79418	1
265	C	66.12564	80.90350	68.03639	-519.76435	377.31045	459.42366	1
266	H	66.18073	81.14141	69.12392	-1746.74323	1667.50644	-1261.73691	1
267	C	64.66864	80.67104	67.65562	570.95554	16.46261	-545.27700	1
268	H	64.23653	79.78626	68.18845	2391.58273	28.05277	-1305.07271	1
269	H	64.02583	81.55282	67.91093	175.75588	917.63458	2559.43867	1
270	H	64.55243	80.48334	66.55717	-1063.97851	-2155.34650	1283.00462	1
271	C	66.93608	79.63665	67.80218	193.76014	2.62946	-765.53141	1
272	H	66.47554	78.75307	68.31575	507.39394	-846.55087	2539.60089	1
273	H	67.01779	79.38815	66.71228	1337.57841	1818.19054	1526.01994	1
274	H	67.98015	79.74035	68.20842	1100.88635	-1172.91350	-2199.08909	1
275	C	68.57759	83.81822	67.10204	-549.21115	475.64486	-309.38218	1
276	O	68.41965	84.84001	67.71625	556.06106	-390.37755	-78.24250	1
277	O	68.96281	83.84552	65.74134	-572.27940	-310.19032	-209.75862	1
278	H	68.98129	82.86313	65.56712	-1380.08193	2212.14486	790.85944	1

Listing 85: C00085.xmolout

1		276								
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7480	10992	
		0.2500	300.00	0.00	0.00	0.00	-1293.4847	0.0000	300.0000	
3	H	81.91957	72.42649	65.31007	-2043.14101	-1757.64893	399.89339			1
4	N	82.37937	72.97459	66.03181	426.75047	490.45733	-334.42467			1
5	H	81.61328	73.53777	66.39241	442.25559	-1110.30854	-2448.52907			1
6	C	83.53188	73.68346	65.62944	415.32972	-666.39213	83.73172			1
7	H	84.02239	73.01856	64.88549	879.32219	2491.00447	667.35213			1
8	C	83.08740	75.09406	64.97522	31.35357	477.41777	628.23362			1
9	H	82.57787	75.71136	65.75253	1168.38489	2240.25337	-1019.71136			1
10	H	83.99548	75.67146	64.67806	-360.43770	2534.90498	931.67112			1
11	C	82.17904	74.88695	63.79458	463.18208	512.70242	-382.34388			1
12	H	81.35459	74.20094	64.09193	1725.29117	1863.52247	-987.07854			1
13	C	81.56386	76.21380	63.36464	710.42801	-144.27427	-313.15367			1
14	H	80.87220	76.08629	62.49251	364.20195	-1033.13725	2494.72524			1
15	H	80.97270	76.68402	64.19216	2567.61904	335.80679	847.48802			1
16	H	82.34993	76.95134	63.05899	-2587.99029	680.92867	-512.16411			1
17	C	82.92725	74.27128	62.61954	268.17616	741.64379	-40.42634			1
18	H	82.26120	74.14186	61.72777	1283.54314	-1945.37420	-1411.27812			1
19	H	83.78852	74.91270	62.29937	-1258.57796	1317.15249	-2026.02085			1
20	H	83.34203	73.26199	62.87262	-2502.84526	909.80597	575.92391			1
21	C	84.48504	74.04371	66.87049	619.36578	-458.64843	-172.09273			1
22	O	85.53023	74.65606	66.64857	-81.40433	433.87611	522.34594			1
23	N	83.99502	73.68740	68.03364	175.23996	-622.20190	341.55523			1
24	H	83.08748	73.19017	68.12510	-876.57256	-303.22879	-2561.90213			1
25	C	84.85114	73.59035	69.18355	-571.88214	-534.10783	-106.15033			1
26	H	85.84873	73.22563	68.84825	-2713.20841	-16.25800	-248.80809			1
27	C	84.93797	75.07686	69.76775	166.60354	288.16399	-716.09568			1
28	H	83.90224	75.52595	69.77619	-2097.85574	1636.78449	-586.18044			1
29	O	85.64677	76.02655	68.94793	-317.80580	-363.38227	484.43082			1
30	H	85.65068	75.52746	68.05334	1863.74748	-1451.84923	1357.29467			1
31	C	85.43684	74.90793	71.24008	503.80731	517.99032	318.51606			1
32	H	85.43306	75.88220	71.78432	640.61020	-2157.10410	-1536.29104			1
33	H	84.79341	74.20244	71.82047	1687.88455	465.60692	2087.56452			1
34	H	86.48126	74.51321	71.27709	-1293.07895	-1899.88581	-1463.57452			1
35	C	83.98975	72.54970	70.06870	-153.07550	-733.68902	248.70981			1
36	O	82.81996	72.38963	69.77718	186.15459	-480.78787	-449.34387			1

37	N	84.71165	71.95274	71.01619	-487.53139	543.18517	42.03850	1
38	C	84.07599	71.21031	72.06972	-699.35871	69.34393	360.10701	1
39	H	83.20086	70.70761	71.59775	2.81126	-221.99807	-2715.58072	1
40	C	85.25124	70.26757	72.56706	-507.46439	-592.59194	122.07761	1
41	H	85.10299	69.90298	73.60816	-1975.08116	525.87560	-1801.71556	1
42	H	85.36081	69.36691	71.92230	1588.27743	-1913.22100	1113.83566	1
43	C	86.47082	71.22888	72.41880	-613.62442	-457.55993	-194.14490	1
44	H	86.45494	72.00175	73.22385	1707.54637	-721.27992	1996.92523	1
45	H	87.45827	70.71758	72.47279	758.23357	2100.81767	1560.55011	1
46	C	86.16652	71.86661	70.99572	-352.41524	704.96076	49.21465	1
47	H	86.59404	72.88316	70.82621	1714.76886	-2070.42778	443.35792	1
48	H	86.42025	71.21343	70.12747	1224.15040	1801.50881	1636.97633	1
49	C	83.64459	72.27262	73.23358	566.85117	537.05831	117.62814	1
50	O	84.43955	72.62050	74.10395	-550.26779	-406.08867	4.21666	1
51	N	82.41030	72.67442	73.03440	566.34832	-425.77725	180.18749	1
52	H	81.94790	72.33251	72.19224	644.44502	2646.80550	-52.73430	1
53	C	81.62518	73.07269	74.17061	612.34801	-281.48662	411.56221	1
54	H	81.99150	72.45768	75.02365	1667.23498	-1490.75142	1556.16753	1
55	C	81.90525	74.62191	74.38725	-714.45746	-175.43074	286.98927	1
56	H	81.57647	75.21052	73.48156	-787.09484	1763.03619	-1922.46060	1
57	O	83.28390	75.02823	74.50841	-429.46514	516.51932	-128.40526	1
58	H	83.74964	74.13151	74.39228	1981.82785	436.16847	-1818.18182	1
59	C	80.95790	74.95637	75.59091	630.79189	-468.94448	76.03230	1
60	H	80.96434	76.04772	75.82140	-1775.71861	2062.30353	131.89849	1
61	H	79.90023	74.66629	75.38141	-1855.14608	88.94118	1993.53760	1
62	H	81.27045	74.42124	76.51846	-1504.82350	-780.94249	-2132.90992	1
63	C	80.07465	72.81005	73.74261	288.57638	618.62814	-397.00270	1
64	O	79.54863	73.46867	72.85050	321.70495	-185.26452	574.37218	1
65	N	79.55310	71.84862	74.47333	-447.05792	-446.53431	367.76425	1
66	H	80.10785	71.42913	75.21626	350.31316	1975.63644	-1843.31522	1
67	C	78.29608	71.30539	74.06822	-511.23061	374.03917	-471.51480	1
68	H	78.31482	71.54109	72.97810	2234.79579	-898.70890	-1273.45190	1
69	C	78.33856	69.73999	74.40408	529.53781	-159.34528	563.72604	1
70	H	77.35440	69.31528	74.06688	654.59388	2347.94251	1217.51488	1
71	H	79.13008	69.29573	73.74215	-1526.55661	2103.42026	817.87394	1
72	O	78.55859	69.35312	75.78224	-554.84278	14.12789	399.58769	1
73	H	79.53443	69.36094	75.80122	1297.06236	2061.84854	1220.68812	1
74	C	77.10245	72.16645	74.76527	-662.15484	-412.13544	123.62687	1
75	O	76.31181	71.69755	75.57096	-540.01537	-317.05804	274.91456	1
76	N	77.15601	73.35309	74.21197	-202.76299	-690.00100	-131.49145	1
77	H	77.92612	73.54340	73.52715	-702.62132	-2617.37191	281.70413	1
78	C	76.19770	74.37399	74.42339	-491.73914	576.34187	222.73509	1
79	H	76.47988	75.13577	73.66235	1977.17978	-1823.58850	-434.68928	1
80	C	74.73056	73.79074	74.21443	-649.50797	-328.66843	306.11224	1
81	H	74.52495	72.97992	74.95044	2075.07803	1452.16490	-1004.45904	1
82	C	73.76096	75.00734	74.39326	-615.18735	-489.99689	-70.96352	1
83	H	72.69506	74.68242	74.31295	-1226.32661	-1724.38906	-1716.47170	1
84	H	73.89799	75.49455	75.38796	2381.64273	-969.84735	900.46860	1
85	H	73.93354	75.78989	73.61726	2122.74991	1702.23946	-141.36228	1
86	C	74.51977	73.26933	72.75276	-501.86074	-479.61276	-376.42482	1
87	H	73.46243	72.95456	72.58307	993.79261	-2246.95401	-1177.81305	1
88	H	74.75878	74.05525	71.99820	42.71279	-626.15391	-2651.37258	1
89	H	75.16992	72.38955	72.53593	-2026.39012	-1590.33709	-887.82922	1
90	C	76.27444	74.98909	75.94122	-672.89153	382.57394	-156.34072	1
91	O	76.32234	76.18593	76.07692	410.04627	221.86223	500.35950	1
92	N	76.15640	74.05623	76.88625	-378.11782	-443.79414	-441.10984	1
93	H	76.09723	73.04009	76.62217	2404.15973	-568.14894	1149.30085	1
94	C	76.69936	74.46478	78.16642	-544.54484	466.16019	331.29119	1
95	H	77.57239	75.08913	77.87298	-1409.80988	-170.17955	2325.32679	1
96	C	75.58143	75.38023	78.80084	-184.48284	116.78282	-758.89137	1
97	H	75.40617	76.28418	78.16916	1893.78641	1861.14652	611.04528	1
98	H	74.60201	74.84137	78.80897	-2170.79665	-974.19311	1327.50117	1

99	C	76.04450	75.76980	80.24863	389.51668	672.81878	-138.49152	1
100	H	76.54283	74.90695	80.74652	510.64577	1933.03327	1851.02484	1
101	H	76.84935	76.53707	80.19644	-2302.30869	-1105.72939	-948.89774	1
102	C	74.88607	76.27877	81.15849	-559.93427	-126.34590	542.30857	1
103	O	75.07338	76.49364	82.36002	-670.36003	-111.83166	76.36448	1
104	N	73.74188	76.45557	80.50828	-216.06729	-537.07037	446.51379	1
105	H	73.44435	76.21473	79.51645	-1251.96487	1074.12894	-2168.52500	1
106	H	72.92165	76.82882	81.00864	-2451.83023	-720.73851	944.84612	1
107	C	77.16095	73.12288	78.96663	546.24052	-563.88337	-85.11809	1
108	O	78.34671	72.91255	78.90071	71.70702	-307.40463	606.69673	1
109	N	76.22963	72.38849	79.60912	479.90863	-504.50129	222.86849	1
110	C	76.65842	71.24606	80.34310	75.51268	-600.91904	506.73700	1
111	H	77.77443	71.22832	80.32203	-2033.61562	1795.30103	254.89480	1
112	C	75.96102	71.51421	81.74995	523.79067	517.99274	284.45581	1
113	H	75.92531	70.60765	82.39711	1599.61665	-1127.00911	1895.98173	1
114	H	76.48968	72.30695	82.32507	-1881.83093	1275.82488	-1501.55016	1
115	C	74.55218	71.99447	81.28224	-600.05639	-404.05026	316.64485	1
116	H	73.89319	71.13181	81.03242	-2597.05260	496.36221	657.73249	1
117	H	74.01588	72.57805	82.06598	-1666.24518	1294.38985	-1723.90591	1
118	C	74.90236	72.85463	79.99178	493.57570	-129.95376	-602.56394	1
119	H	74.22751	72.68183	79.11985	-1469.08415	-637.84797	2204.22581	1
120	H	74.97966	73.94808	80.19376	-1038.97840	1068.88701	-2280.71789	1
121	C	75.92001	69.84781	79.85921	188.88100	241.05089	-727.87821	1
122	O	75.51444	69.10826	80.73034	531.88613	-49.19943	427.07960	1
123	N	75.85357	69.71835	78.54580	708.14833	26.93417	-179.73509	1
124	H	76.27046	70.47479	78.00085	-2232.69501	-1179.09831	1023.94816	1
125	C	75.41020	68.52988	77.91211	-738.32412	259.92548	104.42456	1
126	H	75.75161	68.64384	76.85882	2028.89123	1260.02983	1311.33324	1
127	C	76.07284	67.28280	78.64512	-258.65678	-345.52513	661.28459	1
128	H	75.81312	67.29804	79.73271	-1826.06090	-1801.46097	-918.64554	1
129	C	75.61620	65.93461	77.99261	-541.23400	531.92970	-218.41428	1
130	H	76.10536	65.05703	78.47809	1311.73218	-2219.18200	882.19023	1
131	H	74.51172	65.79069	78.08198	-1048.71298	1223.58118	-2196.97971	1
132	H	75.86739	65.89827	76.90672	419.06414	1903.92898	1903.44670	1
133	C	77.62412	67.38928	78.44883	-423.86431	152.66566	-648.55262	1
134	H	78.16225	66.54154	78.93458	105.68386	-2342.50080	1387.51238	1
135	H	77.90091	67.38927	77.36795	-1695.63603	-1484.73621	-1531.02793	1
136	H	78.02187	68.33455	78.88788	-1853.57121	-487.39031	1936.59343	1
137	C	73.78006	68.39961	78.01077	539.71428	-510.58232	267.58633	1
138	O	73.21146	67.53557	77.38168	-15.93758	-278.34085	-624.49402	1
139	N	73.24363	69.30708	78.81601	-676.81886	12.05292	276.17960	1
140	H	73.88500	69.90521	79.33690	-1694.44250	-373.84189	-2100.66098	1
141	C	71.82555	69.28488	79.03074	412.33078	-664.70360	108.35451	1
142	H	71.43476	69.23986	77.99013	1765.77476	1294.44366	1621.76594	1
143	C	71.47168	67.96572	79.82220	-179.66635	-721.95667	-264.73915	1
144	H	71.89156	67.07557	79.29748	-607.34922	2587.87032	-598.10018	1
145	H	71.93995	67.97597	80.83246	-359.69332	-1479.13954	-2259.74260	1
146	C	69.91063	67.88896	79.92511	-240.01076	616.02425	431.85322	1
147	H	69.51401	68.81969	80.39411	-1359.17131	782.54425	2227.99181	1
148	H	69.45077	67.83443	78.91307	-820.36667	85.81767	-2596.78715	1
149	C	69.50096	66.63229	80.79206	-513.07015	236.18570	-551.87280	1
150	H	69.82254	65.68424	80.30275	1816.11944	-1183.11722	-1650.94321	1
151	H	70.00755	66.65119	81.78445	-1800.04429	-1361.53473	1526.34643	1
152	C	67.96389	66.68189	80.96045	726.08972	-253.19732	-179.64713	1
153	H	67.59194	67.55796	81.52860	1224.27271	-456.51798	-2390.90304	1
154	H	67.39261	66.57399	80.01695	1206.40339	-1150.93514	-2154.90344	1
155	N	67.53249	65.44948	81.82420	329.70796	-633.68968	-155.67358	1
156	H	66.49256	65.37197	82.01936	1348.31305	1938.76845	1359.00643	1
157	H	67.74313	64.48505	81.43412	2096.92035	1446.54551	-966.48890	1
158	H	67.93227	65.38382	82.80531	-1197.07217	-2303.53719	827.28733	1
159	C	71.40811	70.63192	79.85455	-378.01186	-556.17301	-413.96481	1
160	O	70.83918	70.55947	80.92210	-409.44433	-307.55053	-453.30833	1

161	N	71.77236	71.72052	79.18835	-429.02477	524.70884	274.08502	1
162	H	72.24179	71.59396	78.29245	1706.34263	-1425.96036	1574.38926	1
163	C	71.24548	72.99011	79.62776	-45.25864	-626.22952	478.93267	1
164	H	70.15010	72.80182	79.67986	1988.63164	570.90773	1772.87287	1
165	C	71.86012	73.27854	81.04996	551.77128	-20.49526	-564.54996	1
166	H	71.64430	72.43501	81.75016	1434.61535	-1753.10253	1513.99471	1
167	H	72.97046	73.33156	80.96618	-714.67738	1819.09770	1898.36494	1
168	C	71.30897	74.63173	81.61352	446.99263	-555.77305	338.97221	1
169	H	71.34326	75.42045	80.82545	1953.68466	1892.25957	-161.67766	1
170	H	70.24659	74.54834	81.93642	-403.03785	2688.07032	-188.43591	1
171	C	72.27576	74.97467	82.81412	567.86262	335.74681	434.04421	1
172	H	72.25093	74.16571	83.57958	-1080.02275	1568.26081	-1948.78900	1
173	H	73.33241	75.01707	82.45407	-919.54108	2111.34692	1456.13463	1
174	C	71.89746	76.34037	83.44666	195.81897	173.33862	-745.11536	1
175	H	71.71169	77.15337	82.71487	1405.67949	-2301.21089	-390.08113	1
176	H	71.07509	76.30471	84.19064	-940.37328	-1118.32446	2299.72133	1
177	N	73.16429	76.79962	84.20533	319.26422	656.36007	-42.02424	1
178	H	73.13433	77.78372	84.59483	1961.03633	619.91968	1787.09422	1
179	H	73.40220	76.25519	85.08198	854.14343	-2156.80752	1429.08711	1
180	H	74.11171	76.77146	83.58819	1237.02905	-1378.50857	-1998.28500	1
181	C	71.67820	74.10607	78.53139	532.53319	-268.57236	517.55729	1
182	O	72.44877	75.02558	78.81401	266.16714	-290.73804	-558.88002	1
183	N	71.08835	73.84824	77.38469	-226.25352	640.49678	-270.32839	1
184	H	70.45707	73.04903	77.36272	2007.69063	-1035.27229	1523.50231	1
185	C	71.08170	74.86784	76.38333	-540.76542	-573.33303	49.50000	1
186	H	72.14741	75.15751	76.26643	-2374.20950	-1036.76023	843.75774	1
187	C	70.42590	74.21249	75.08889	-77.09082	666.87422	-415.84136	1
188	H	69.42977	73.77825	75.37618	-985.81834	617.19825	2463.91927	1
189	O	71.17082	73.10997	74.51558	293.29899	-391.65602	-477.80926	1
190	H	70.53550	72.37942	74.62811	2528.72714	-681.76262	-751.27122	1
191	C	70.18590	75.43359	74.12985	252.47363	-605.14473	440.05134	1
192	H	69.68760	75.10723	73.18875	-2052.65063	1456.49051	-1043.51830	1
193	H	69.52692	76.21861	74.59658	-2152.98800	-1661.97574	-161.70652	1
194	H	71.13974	75.93247	73.84015	-473.12726	-1584.27339	2165.61725	1
195	C	70.21369	76.12496	76.97835	360.36307	488.46713	505.10056	1
196	O	69.27548	76.00483	77.72930	-200.08817	-528.03552	-385.82850	1
197	N	70.72280	77.22588	76.43344	-597.54095	-226.44775	355.20479	1
198	H	71.51058	77.14046	75.79262	2179.23655	-1300.70981	-991.33835	1
199	C	70.02260	78.44987	76.60097	-687.68921	297.39807	-249.45179	1
200	H	69.49082	78.27522	77.56496	-349.16256	-2467.37713	-1101.72831	1
201	C	71.08627	79.64578	76.60384	672.47345	361.54328	-201.62880	1
202	H	71.70316	79.60807	75.67685	1541.41502	582.18425	2169.97026	1
203	H	70.54345	80.62099	76.60187	-2534.67717	60.25153	997.72295	1
204	C	71.98975	79.57289	77.84300	574.26774	-389.43119	-377.02542	1
205	C	71.48383	80.07818	79.07882	688.82679	-287.33580	-257.96133	1
206	H	70.44333	80.44195	79.15607	331.14182	1470.38163	2269.80013	1
207	C	73.32289	79.06606	77.76219	-383.52382	-675.04808	144.24917	1
208	H	73.70988	78.64467	76.81669	4.09847	1517.59662	2262.86397	1
209	C	72.33706	80.12607	80.17996	-134.76730	428.45285	-649.50303	1
210	H	71.95050	80.53147	81.13106	-903.23433	1600.49020	2011.53387	1
211	C	74.13867	79.13417	78.89527	-335.53281	-615.00040	-364.39058	1
212	H	75.17166	78.75146	78.81875	1596.45398	-1369.33862	1732.02659	1
213	C	73.68986	79.67967	80.13411	585.48547	-340.24194	-406.23938	1
214	O	74.51238	79.79072	81.28556	-419.15649	-173.04408	-511.94141	1
215	H	75.30038	79.28401	80.97820	-1071.84350	1559.71507	-1960.13012	1
216	C	68.97491	78.59505	75.36173	291.41878	-183.13091	710.72246	1
217	O	68.19441	77.71112	75.06885	379.87695	523.47396	-222.23622	1
218	N	69.09201	79.78074	74.77647	564.30591	373.09380	277.24371	1
219	H	69.79721	80.44921	75.08638	-120.59931	-2436.07824	-1214.35098	1
220	C	68.14065	80.08256	73.75184	404.07514	-299.37480	608.84009	1
221	H	67.22802	79.53802	74.09076	-1071.07882	-841.69025	2359.66467	1
222	C	68.00146	81.65856	73.69677	-683.12807	68.71770	-390.13096	1

223	H	67.89205	82.07536	74.72378	2068.88918	1596.58590	770.89603	1
224	H	68.92640	82.11954	73.27672	1379.86429	2342.49779	-179.85638	1
225	C	66.76898	82.02691	72.81494	-176.39967	537.49466	550.97268	1
226	H	66.91610	81.67148	71.76774	-396.28051	1942.22168	1869.33314	1
227	H	65.84480	81.52580	73.17996	-94.44700	586.00678	-2659.20016	1
228	C	66.62618	83.61888	72.87338	-291.69381	-718.18079	-150.72929	1
229	H	66.48042	84.06746	73.88854	-2303.38776	1089.76242	964.62032	1
230	H	67.45453	84.16508	72.35213	884.16729	2568.80533	-207.74283	1
231	N	65.45349	83.80809	72.12977	-594.49522	-252.81478	342.29276	1
232	H	65.22171	83.08215	71.46874	-1735.17426	2084.05705	-263.71605	1
233	C	64.69338	84.82567	72.19965	595.23177	-271.52487	442.22352	1
234	N	65.02779	85.84533	73.09632	585.53813	-424.79750	-105.81303	1
235	H	65.83984	85.93094	73.70605	959.88797	1327.56823	-2177.11905	1
236	H	64.50537	86.71414	73.21398	1578.48647	16.27378	-2220.76233	1
237	N	63.61807	84.70623	71.30876	-452.17763	-390.33541	-421.51853	1
238	H	63.37642	83.96824	70.64911	470.26107	1974.25629	-1817.92087	1
239	H	62.89742	85.42136	71.20334	1856.67307	-1573.97321	-1224.35416	1
240	C	68.64886	79.50762	72.30430	-531.47271	-581.45780	-55.06206	1
241	O	67.95260	79.70219	71.33012	-243.00837	192.73507	609.52485	1
242	N	69.78396	78.83301	72.39921	343.49288	-644.25607	38.09164	1
243	H	70.15716	78.73324	73.34163	-1691.16043	-1535.97525	-1484.73099	1
244	C	70.48793	78.37375	71.25392	542.66492	350.14337	454.42563	1
245	H	71.23486	77.66440	71.67507	1209.57979	-2396.95920	463.86744	1
246	C	69.46340	77.68793	70.25361	-737.14309	145.93010	242.71942	1
247	H	68.68514	78.42833	69.92955	-1050.18303	159.36419	-2509.06125	1
248	C	70.23376	77.10522	69.02009	-706.77696	-252.88343	-245.16230	1
249	H	69.54247	76.60330	68.30262	-1624.64039	-1665.49085	1417.86935	1
250	H	70.77119	77.91694	68.46006	2566.10521	598.51109	693.22305	1
251	H	70.99625	76.35223	69.32973	-1972.69758	107.10018	-1876.34312	1
252	C	68.80328	76.47785	71.00102	412.85148	672.58832	-27.69222	1
253	H	68.00464	75.99868	70.38814	1447.02277	1762.76533	-1490.78944	1
254	H	69.55445	75.69080	71.24336	1320.77379	-145.20455	2378.68491	1
255	H	68.33789	76.80406	71.96184	-1512.10848	1470.52031	1724.75147	1
256	C	71.21523	79.67017	70.55785	-607.11113	499.56689	73.73769	1
257	O	71.43060	79.68959	69.36353	357.97126	460.81534	356.68785	1
258	N	71.66053	80.47716	71.50682	536.55407	-368.62270	332.76306	1
259	H	71.37594	80.22265	72.45099	524.38866	2297.69985	1367.20941	1
260	C	72.26421	81.73866	71.26164	46.50277	-774.29190	-147.97904	1
261	H	72.95820	81.84972	72.12184	1676.51875	1883.29066	1032.55549	1
262	C	73.00670	81.78196	69.83472	-559.41456	-34.19198	-556.30433	1
263	H	72.25044	81.62646	69.02039	-64.66664	395.18769	2695.05373	1
264	H	73.45165	82.79057	69.65307	-2703.44278	-60.40056	333.79418	1
265	C	74.06450	80.70887	69.77504	-519.76435	377.31045	459.42366	1
266	H	73.59275	79.75164	70.09979	-1746.74323	1667.50644	-1261.73691	1
267	C	74.56683	80.52628	68.34855	570.95554	16.46261	-545.27700	1
268	H	75.33429	79.71234	68.28080	2391.58273	28.05277	-1305.07271	1
269	H	73.73180	80.25411	67.65191	175.75588	917.63458	2559.43867	1
270	H	75.04010	81.46155	67.95281	-1063.97851	-2155.34650	1283.00462	1
271	C	75.23745	81.02034	70.69353	193.76014	2.62946	-765.53141	1
272	H	76.01919	80.21835	70.65108	507.39394	-846.55087	2539.60089	1
273	H	75.73655	81.98326	70.41189	1337.57841	1818.19054	1526.01994	1
274	H	74.91609	81.11270	71.76258	1100.88635	-1172.91350	-2199.08909	1
275	C	71.12794	82.87575	71.35114	-549.21115	475.64486	-309.38218	1
276	O	69.95095	82.69146	71.18456	556.06106	-390.37755	-78.24250	1
277	O	71.61491	84.18244	71.61240	-572.27940	-310.19032	-209.75862	1
278	H	72.58534	83.97196	71.68342	-1380.08193	2212.14486	790.85944	1

Listing 86: C00086.xmolout

1	276								
2	150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100	
	0.2500	300.00	0.00	0.00	0.00	-1293.4830	0.0000	300.0000	

3	H	81.65603	70.80945	71.56068	-2043.14101	-1757.64893	399.89339	1
4	N	82.32176	70.21833	71.06671	426.75047	490.45733	-334.42467	1
5	H	81.70164	69.62099	70.52464	442.25559	-1110.30854	-2448.52907	1
6	C	83.28614	70.90440	70.29191	415.32972	-666.39213	83.73172	1
7	H	83.33682	71.92297	70.73844	879.32219	2491.00447	667.35213	1
8	C	84.70174	70.12353	70.40267	31.35357	477.41777	628.23362	1
9	H	84.67180	69.21815	69.75206	1168.38489	2240.25337	-1019.71136	1
10	H	85.52403	70.75804	69.99488	-360.43770	2534.90498	931.67112	1
11	C	84.97913	69.73018	71.82494	463.18208	512.70242	-382.34388	1
12	H	84.12467	69.11131	72.18299	1725.29117	1863.52247	-987.07854	1
13	C	86.25603	68.90156	71.90811	710.42801	-144.27427	-313.15367	1
14	H	86.45416	68.55044	72.95328	364.20195	-1033.13725	2494.72524	1
15	H	86.20416	67.99220	71.25592	2567.61904	335.80679	847.48802	1
16	H	87.15098	69.49165	71.58241	-2587.99029	680.92867	-512.16411	1
17	C	85.10607	70.94735	72.73212	268.17616	741.64379	-40.42634	1
18	H	85.32585	70.65214	73.79041	1283.54314	-1945.37420	-1411.27812	1
19	H	85.93078	71.62805	72.39797	-1258.57796	1317.15249	-2026.02085	1
20	H	84.16143	71.54956	72.74586	-2502.84526	909.80597	575.92391	1
21	C	82.78242	70.88612	68.76557	619.36578	-458.64843	-172.09273	1
22	O	81.74466	70.32691	68.37968	-81.40433	433.87611	522.34594	1
23	N	83.65509	71.59500	68.11979	175.23996	-622.20190	341.55523	1
24	H	84.45647	72.04638	68.60892	-876.57256	-303.22879	-2561.90213	1
25	C	83.71147	71.76004	66.69260	-571.88214	-534.10783	-106.15033	1
26	H	84.03644	70.77675	66.28314	-2713.20841	-16.25800	-248.80809	1
27	C	82.21090	72.08025	66.22326	166.60354	288.16399	-716.09568	1
28	H	81.69480	72.43386	67.16681	-2097.85574	1636.78449	-586.18044	1
29	O	81.46241	70.91719	65.85521	-317.80580	-363.38227	484.43082	1
30	H	81.32358	70.50718	66.78739	1863.74748	-1451.84923	1357.29467	1
31	C	82.29998	73.26180	65.19989	503.80731	517.99032	318.51606	1
32	H	81.29869	73.70337	64.99005	640.61020	-2157.10410	-1536.29104	1
33	H	82.94155	74.08577	65.59274	1687.88455	465.60692	2087.56452	1
34	H	82.72726	72.93941	64.22276	-1293.07895	-1899.88581	-1463.57452	1
35	C	84.85236	72.88601	66.58855	-153.07550	-733.68902	248.70981	1
36	O	85.48552	73.14537	67.59931	186.15459	-480.78787	-449.34387	1
37	N	85.07425	73.31467	65.34324	-487.53139	543.18517	42.03850	1
38	C	85.76731	74.55608	65.12546	-699.35871	69.34393	360.10701	1
39	H	86.58595	74.52237	65.87950	2.81126	-221.99807	-2715.58072	1
40	C	86.24107	74.46301	63.62162	-507.46439	-592.59194	122.07761	1
41	H	86.17594	75.44255	63.09451	-1975.08116	525.87560	-1801.71556	1
42	H	87.31027	74.15753	63.56459	1588.27743	-1913.22100	1113.83566	1
43	C	85.31846	73.37392	62.98284	-613.62442	-457.55993	-194.14490	1
44	H	84.35619	73.80883	62.63330	1707.54637	-721.27992	1996.92523	1
45	H	85.77326	72.87340	62.09859	758.23357	2100.81767	1560.55011	1
46	C	85.10904	72.39251	64.21271	-352.41524	704.96076	49.21465	1
47	H	84.16834	71.79465	64.19696	1714.76886	-2070.42778	443.35792	1
48	H	85.96869	71.70980	64.41121	1224.15040	1801.50881	1636.97633	1
49	C	84.80644	75.84993	65.41179	566.85117	537.05831	117.62814	1
50	O	85.11962	76.61895	66.29011	-550.26779	-406.08867	4.21666	1
51	N	83.72641	75.91706	64.61397	566.34832	-425.77725	180.18749	1
52	H	83.72557	75.21674	63.87265	644.44502	2646.80550	-52.73430	1
53	C	83.26492	77.26100	64.38115	612.34801	-281.48662	411.56221	1
54	H	84.12103	77.90655	64.68601	1667.23498	-1490.75142	1556.16753	1
55	C	82.86484	77.35155	62.84399	-714.45746	-175.43074	286.98927	1
56	H	82.03751	76.61711	62.63978	-787.09484	1763.03619	-1922.46060	1
57	O	83.91653	77.02401	61.91277	-429.46514	516.51932	-128.40526	1
58	H	83.50074	76.30249	61.40160	1981.82785	436.16847	-1818.18182	1
59	C	82.28278	78.81072	62.74807	630.79189	-468.94448	76.03230	1
60	H	81.87883	79.02414	61.73140	-1775.71861	2062.30353	131.89849	1
61	H	81.45129	78.97608	63.47555	-1855.14608	88.94118	1993.53760	1
62	H	83.06428	79.57626	62.96209	-1504.82350	-780.94249	-2132.90992	1
63	C	81.93248	77.56092	65.27342	288.57638	618.62814	-397.00270	1
64	O	81.72626	78.66467	65.72333	321.70495	-185.26452	574.37218	1

65	N	81.01025	76.53607	65.17538	-447.05792	-446.53431	367.76425	1
66	H	81.63994	75.76606	64.90541	350.31316	1975.63644	-1843.31522	1
67	C	80.20427	76.40299	66.38651	-511.23061	374.03917	-471.51480	1
68	H	80.94389	76.51830	67.20940	2234.79579	-898.70890	-1273.45190	1
69	C	79.14677	77.56728	66.36112	529.53781	-159.34528	563.72604	1
70	H	78.56234	77.54238	67.31249	654.59388	2347.94251	1217.51488	1
71	H	79.68877	78.55026	66.33845	-1526.55661	2103.42026	817.87394	1
72	O	78.13500	77.50472	65.23332	-554.84278	14.12789	399.58769	1
73	H	78.71031	77.83618	64.53481	1297.06236	2061.84854	1220.68812	1
74	C	79.58022	74.91160	66.33786	-662.15484	-412.13544	123.62687	1
75	O	80.20700	74.06046	66.96330	-540.01537	-317.05804	274.91456	1
76	N	78.49925	74.81391	65.60272	-202.76299	-690.00100	-131.49145	1
77	H	78.13523	75.68814	65.17262	-702.62132	-2617.37191	281.70413	1
78	C	77.93852	73.58573	65.17381	-491.73914	576.34187	222.73509	1
79	H	77.19689	73.90279	64.40793	1977.17978	-1823.58850	-434.68928	1
80	C	79.07563	72.63953	64.59030	-649.50797	-328.66843	306.11224	1
81	H	79.88401	72.48566	65.34240	2075.07803	1452.16490	-1004.45904	1
82	C	78.43217	71.26523	64.20180	-615.18735	-489.99689	-70.96352	1
83	H	79.18954	70.56614	63.77465	-1226.32661	-1724.38906	-1716.47170	1
84	H	77.98226	70.76216	65.09081	2381.64273	-969.84735	900.46860	1
85	H	77.62217	71.38775	63.44485	2122.74991	1702.23946	-141.36228	1
86	C	79.64056	73.28443	63.27832	-501.86074	-479.61276	-376.42482	1
87	H	80.47895	72.68298	62.85464	993.79261	-2246.95401	-1177.81305	1
88	H	78.85496	73.36173	62.49082	42.71279	-626.15391	-2651.37258	1
89	H	80.02502	74.31542	63.46234	-2026.39012	-1590.33709	-887.82922	1
90	C	77.21553	72.77706	66.40982	-672.89153	382.57394	-156.34072	1
91	O	76.05880	72.44567	66.31962	410.04627	221.86223	500.35950	1
92	N	78.08025	72.53091	67.38429	-378.11782	-443.79414	-441.10984	1
93	H	79.07791	72.87140	67.32194	2404.15973	-568.14894	1149.30085	1
94	C	77.57662	72.13164	68.65159	-544.54484	466.16019	331.29119	1
95	H	76.51298	71.84579	68.47358	-1409.80988	-170.17955	2325.32679	1
96	C	78.56263	70.94983	69.04537	-184.48284	116.78282	-758.89137	1
97	H	78.58086	70.19197	68.22943	1893.78641	1861.14652	611.04528	1
98	H	79.60957	71.32574	69.12238	-2170.79665	-974.19311	1327.50117	1
99	C	78.12067	70.29245	70.38598	389.51668	672.81878	-138.49152	1
100	H	78.24974	71.01369	71.22812	510.64577	1933.03327	1851.02484	1
101	H	77.03052	70.06978	70.37883	-2302.30869	-1105.72939	-948.89774	1
102	C	78.93149	68.96196	70.64699	-559.93427	-126.34590	542.30857	1
103	O	78.59888	68.23878	71.55139	-670.36003	-111.83166	76.36448	1
104	N	79.95685	68.74801	69.79619	-216.06729	-537.07037	446.51379	1
105	H	80.39378	69.33919	69.04866	-1251.96487	1074.12894	-2168.52500	1
106	H	80.53431	67.90238	69.90197	-2451.83023	-720.73851	944.84612	1
107	C	77.78549	73.35164	69.72725	546.24052	-563.88337	-85.11809	1
108	O	78.59933	73.18268	70.59730	71.70702	-307.40463	606.69673	1
109	N	76.99507	74.41540	69.50187	479.90863	-504.50129	222.86849	1
110	C	76.95387	75.52846	70.39331	75.51268	-600.91904	506.73700	1
111	H	77.91826	75.55396	70.95114	-2033.61562	1795.30103	254.89480	1
112	C	76.67422	76.74483	69.40676	523.79067	517.99274	284.45581	1
113	H	76.26113	77.63721	69.92835	1599.61665	-1127.00911	1895.98173	1
114	H	77.60170	77.07465	68.89178	-1881.83093	1275.82488	-1501.55016	1
115	C	75.66613	76.09286	68.41061	-600.05639	-404.05026	316.64485	1
116	H	74.64538	76.03418	68.85136	-2597.05260	496.36221	657.73249	1
117	H	75.56684	76.64483	67.44818	-1666.24518	1294.38985	-1723.90591	1
118	C	76.30612	74.64969	68.23753	493.57570	-129.95376	-602.56394	1
119	H	75.57292	73.82246	68.07924	-1469.08415	-637.84797	2204.22581	1
120	H	77.10284	74.58980	67.45690	-1038.97840	1068.88701	-2280.71789	1
121	C	75.63483	75.45858	71.36557	188.88100	241.05089	-727.87821	1
122	O	75.31349	76.42410	72.01949	531.88613	-49.19943	427.07960	1
123	N	74.99508	74.29500	71.25590	708.14833	26.93417	-179.73509	1
124	H	75.44804	73.56450	70.70858	-2232.69501	-1179.09831	1023.94816	1
125	C	73.95823	74.05468	72.20361	-738.32412	259.92548	104.42456	1
126	H	73.52581	75.05792	72.42682	2028.89123	1260.02983	1311.33324	1

127	C	72.95521	72.99740	71.57713	-258.65678	-345.52513	661.28459	1
128	H	73.49419	72.06418	71.30462	-1826.06090	-1801.46097	-918.64554	1
129	C	71.83746	72.71084	72.63808	-541.23400	531.92970	-218.41428	1
130	H	71.09476	71.96784	72.26373	1311.73218	-2219.18200	882.19023	1
131	H	72.26629	72.30370	73.58614	-1048.71298	1223.58118	-2196.97971	1
132	H	71.27659	73.63749	72.90344	419.06414	1903.92898	1903.44670	1
133	C	72.28362	73.63232	70.31091	-423.86431	152.66566	-648.55262	1
134	H	71.56123	72.93104	69.83123	105.68386	-2342.50080	1387.51238	1
135	H	71.72475	74.56248	70.56794	-1695.63603	-1484.73621	-1531.02793	1
136	H	73.04475	73.90601	69.54259	-1853.57121	-487.39031	1936.59343	1
137	C	74.65701	73.35156	73.52056	539.71428	-510.58232	267.58633	1
138	O	75.42511	72.42309	73.44767	-15.93758	-278.34085	-624.49402	1
139	N	74.11823	73.92563	74.58634	-676.81886	12.05292	276.17960	1
140	H	73.46645	74.69747	74.45468	-1694.44250	-373.84189	-2100.66098	1
141	C	74.51246	73.50822	75.88763	412.33078	-664.70360	108.35451	1
142	H	75.12832	72.60095	75.68121	1765.77476	1294.44366	1621.76594	1
143	C	75.34381	74.70865	76.50352	-179.66635	-721.95667	-264.73915	1
144	H	76.11727	75.06088	75.78461	-607.34922	2587.87032	-598.10018	1
145	H	74.68416	75.58890	76.67356	-359.69332	-1479.13954	-2259.74260	1
146	C	76.00178	74.22795	77.83824	-240.01076	616.02425	431.85322	1
147	H	75.28061	73.64593	78.45526	-1359.17131	782.54425	2227.99181	1
148	H	76.85754	73.54404	77.64174	-820.36667	85.81767	-2596.78715	1
149	C	76.46512	75.52959	78.60906	-513.07015	236.18570	-551.87280	1
150	H	77.21163	76.10281	78.01245	1816.11944	-1183.11722	-1650.94321	1
151	H	75.60453	76.22057	78.76866	-1800.04429	-1361.53473	1526.34643	1
152	C	77.05871	75.08565	79.96541	726.08972	-253.19732	-179.64713	1
153	H	76.32723	74.60979	80.65075	1224.27271	-456.51798	-2390.90304	1
154	H	77.96761	74.45600	79.88942	1206.40339	-1150.93514	-2154.90344	1
155	N	77.54055	76.37956	80.70467	329.70796	-633.68968	-155.67358	1
156	H	78.01654	76.23089	81.64123	1348.31305	1938.76845	1359.00643	1
157	H	78.27359	76.95290	80.19690	2096.92035	1446.54551	-966.48890	1
158	H	76.81362	77.11696	80.93898	-1197.07217	-2303.53719	827.28733	1
159	C	73.11524	73.19651	76.69051	-378.01186	-556.17301	-413.96481	1
160	O	72.38211	72.32852	76.28833	-409.44433	-307.55053	-453.30833	1
161	N	72.96613	73.97158	77.75251	-429.02477	524.70884	274.08502	1
162	H	73.60865	74.71596	78.08442	1706.34263	-1425.96036	1574.38926	1
163	C	71.81945	73.76431	78.59252	-45.25864	-626.22952	478.93267	1
164	H	70.91890	73.66999	77.94495	1988.63164	570.90773	1772.87287	1
165	C	72.11435	72.43962	79.40777	551.77128	-20.49526	-564.54996	1
166	H	72.27278	71.59731	78.69634	1434.61535	-1753.10253	1513.99471	1
167	H	73.06845	72.53446	79.97320	-714.67738	1819.09770	1898.36494	1
168	C	70.92676	72.12089	80.37342	446.99263	-555.77305	338.97221	1
169	H	70.83367	72.89173	81.19722	1953.68466	1892.25957	-161.67766	1
170	H	69.95596	72.12924	79.82801	-403.03785	2688.07032	-188.43591	1
171	C	71.23371	70.68029	80.95099	567.86262	335.74681	434.04421	1
172	H	71.36518	69.94755	80.12160	-1080.02275	1568.26081	-1948.78900	1
173	H	72.19755	70.67763	81.51019	-919.54108	2111.34692	1456.13463	1
174	C	70.06902	70.24560	81.86937	195.81897	173.33862	-745.11536	1
175	H	69.98461	70.81999	82.81345	1405.67949	-2301.21089	-390.08113	1
176	H	69.08153	70.18975	81.36933	-940.37328	-1118.32446	2299.72133	1
177	N	70.36466	68.77212	82.31372	319.26422	656.36007	-42.02424	1
178	H	69.64517	68.33085	82.95590	1961.03633	619.91968	1787.09422	1
179	H	70.43114	68.04253	81.54541	854.14343	-2156.80752	1429.08711	1
180	H	71.26110	68.60038	82.85531	1237.02905	-1378.50857	-1998.28500	1
181	C	71.93323	75.11679	79.49309	532.53319	-268.57236	517.55729	1
182	O	72.99488	75.72719	79.49423	266.16714	-290.73804	-558.88002	1
183	N	70.79878	75.37220	80.12040	-226.25352	640.49678	-270.32839	1
184	H	70.02620	74.72147	79.97835	2007.69063	-1035.27229	1523.50231	1
185	C	70.75810	76.33172	81.16626	-540.76542	-573.33303	49.50000	1
186	H	71.81713	76.68481	81.17934	-2374.20950	-1036.76023	843.75774	1
187	C	69.70601	77.48866	80.79799	-77.09082	666.87422	-415.84136	1
188	H	68.73885	77.27035	81.32919	-985.81834	617.19825	2463.91927	1

189	O	69.37292	77.66279	79.41299	293.29899	-391.65602	-477.80926	1
190	H	68.39843	77.57873	79.44243	2528.72714	-681.76262	-751.27122	1
191	C	70.39109	78.74125	81.46008	252.47363	-605.14473	440.05134	1
192	H	69.69043	79.60650	81.50894	-2052.65063	1456.49051	-1043.51830	1
193	H	70.75430	78.54630	82.49654	-2152.98800	-1661.97574	-161.70652	1
194	H	71.27390	79.06802	80.86375	-473.12726	-1584.27339	2165.61725	1
195	C	70.29657	75.49573	82.48585	360.36307	488.46713	505.10056	1
196	O	70.38981	74.28592	82.53920	-200.08817	-528.03552	-385.82850	1
197	N	69.82607	76.32419	83.42082	-597.54095	-226.44775	355.20479	1
198	H	69.83627	77.32140	83.21431	2179.23655	-1300.70981	-991.33835	1
199	C	69.91779	75.88750	84.76760	-687.68921	297.39807	-249.45179	1
200	H	70.00233	74.77686	84.72100	-349.16256	-2467.37713	-1101.72831	1
201	C	71.19654	76.59911	85.42531	672.47345	361.54328	-201.62880	1
202	H	71.09826	77.70567	85.35008	1541.41502	582.18425	2169.97026	1
203	H	71.23363	76.34824	86.51034	-2534.67717	60.25153	997.72295	1
204	C	72.47692	76.12720	84.72620	574.26774	-389.43119	-377.02542	1
205	C	72.99122	74.83399	85.04352	688.82679	-287.33580	-257.96133	1
206	H	72.46779	74.17946	85.76379	331.14182	1470.38163	2269.80013	1
207	C	73.14372	76.95826	83.77492	-383.52382	-675.04808	144.24917	1
208	H	72.73961	77.95291	83.51453	4.09847	1517.59662	2262.86397	1
209	C	74.17036	74.41725	84.42911	-134.76730	428.45285	-649.50303	1
210	H	74.57281	73.42031	84.67983	-903.23433	1600.49020	2011.53387	1
211	C	74.32239	76.49397	83.18545	-335.53281	-615.00040	-364.39058	1
212	H	74.83375	77.14543	82.45519	1596.45398	-1369.33862	1732.02659	1
213	C	74.88378	75.22048	83.49353	585.48547	-340.24194	-406.23938	1
214	O	76.08944	74.73820	82.91897	-419.15649	-173.04408	-511.94141	1
215	H	76.32473	75.50991	82.35332	-1071.84350	1559.71507	-1960.13012	1
216	C	68.69005	76.45120	85.68347	291.41878	-183.13091	710.72246	1
217	O	68.51830	75.98339	86.78820	379.87695	523.47396	-222.23622	1
218	N	68.04109	77.47018	85.12245	564.30591	373.09380	277.24371	1
219	H	68.33639	77.76318	84.19310	-120.59931	-2436.07824	-1214.35098	1
220	C	67.03683	78.11819	85.89871	404.07514	-299.37480	608.84009	1
221	H	66.72363	77.35395	86.64908	-1071.07882	-841.69025	2359.66467	1
222	C	67.71109	79.38851	86.58030	-683.12807	68.71770	-390.13096	1
223	H	68.63629	79.10212	87.12833	2068.88918	1596.58590	770.89603	1
224	H	68.03328	80.12296	85.80897	1379.86429	2342.49779	-179.85638	1
225	C	66.65353	80.01232	87.53987	-176.39967	537.49466	550.97268	1
226	H	65.69794	80.19580	86.99642	-396.28051	1942.22168	1869.33314	1
227	H	66.39811	79.29932	88.35534	-94.44700	586.00678	-2659.20016	1
228	C	67.21076	81.38398	88.13998	-291.69381	-718.18079	-150.72929	1
229	H	68.09715	81.30889	88.81970	-2303.38776	1089.76242	964.62032	1
230	H	67.40677	82.19408	87.39170	884.16729	2568.80533	-207.74283	1
231	N	66.08850	81.75363	88.90204	-594.49522	-252.81478	342.29276	1
232	H	65.25972	81.18900	88.79073	-1735.17426	2084.05705	-263.71605	1
233	C	66.03778	82.73992	89.70339	595.23177	-271.52487	442.22352	1
234	N	67.18430	83.52676	89.84880	585.53813	-424.79750	-105.81303	1
235	H	68.08965	83.43862	89.38914	959.88797	1327.56823	-2177.11905	1
236	H	67.26153	84.34332	90.45615	1578.48647	16.27378	-2220.76233	1
237	N	64.77207	82.83019	90.29963	-452.17763	-390.33541	-421.51853	1
238	H	63.93965	82.25344	90.18729	470.26107	1974.25629	-1817.92087	1
239	H	64.52040	83.55216	90.97552	1856.67307	-1573.97321	-1224.35416	1
240	C	65.83281	78.70522	84.96659	-531.47271	-581.45780	-55.06206	1
241	O	64.73539	78.87073	85.44487	-243.00837	192.73507	609.52485	1
242	N	66.25103	79.06351	83.75256	343.49288	-644.25607	38.09164	1
243	H	67.22514	78.86523	83.52578	-1691.16043	-1535.97525	-1484.73099	1
244	C	65.32927	79.67075	82.79694	542.66492	350.14337	454.42563	1
245	H	64.45391	79.93603	83.44124	1209.57979	-2396.95920	463.86744	1
246	C	66.01843	80.87868	82.18420	-737.14309	145.93010	242.71942	1
247	H	66.94515	80.52505	81.67938	-1050.18303	159.36419	-2509.06125	1
248	C	65.15056	81.56744	81.14866	-706.77696	-252.88343	-245.16230	1
249	H	65.68308	82.43187	80.66342	-1624.64039	-1665.49085	1417.86935	1
250	H	64.84354	80.84983	80.32629	2566.10521	598.51109	693.22305	1

251	H	64.20513	81.97245	81.60496	-1972.69758	107.10018	-1876.34312	1
252	C	66.42634	81.87868	83.25251	412.85148	672.58832	-27.69222	1
253	H	66.99984	82.74446	82.82130	1447.02277	1762.76533	-1490.78944	1
254	H	65.52841	82.30418	83.77971	1320.77379	-145.20455	2378.68491	1
255	H	67.07274	81.40216	84.03948	-1512.10848	1470.52031	1724.75147	1
256	C	64.93353	78.50749	81.68551	-607.11113	499.56689	73.73769	1
257	O	64.58969	78.81446	80.56526	357.97126	460.81534	356.68785	1
258	N	65.01305	77.29321	82.20696	536.55407	-368.62270	332.76306	1
259	H	65.29879	77.22321	83.18235	524.38866	2297.69985	1367.20941	1
260	C	64.34110	76.23484	81.53624	46.50277	-774.29190	-147.97904	1
261	H	63.66151	76.73964	80.81287	1676.51875	1883.29066	1032.55549	1
262	C	65.43763	75.29859	80.80584	-559.41456	-34.19198	-556.30433	1
263	H	66.18255	74.94680	81.55909	-64.66664	395.18769	2695.05373	1
264	H	64.95355	74.38031	80.39578	-2703.44278	-60.40056	333.79418	1
265	C	66.11851	76.07942	79.71435	-519.76435	377.31045	459.42366	1
266	H	66.51856	77.01859	80.15950	-1746.74323	1667.50644	-1261.73691	1
267	C	67.27463	75.26951	79.14022	570.95554	16.46261	-545.27700	1
268	H	67.80953	75.82407	78.32618	2391.58273	28.05277	-1305.07271	1
269	H	68.03235	75.02435	79.92772	175.75588	917.63458	2559.43867	1
270	H	66.92233	74.29974	78.70370	-1063.97851	-2155.34650	1283.00462	1
271	C	65.14948	76.46055	78.60397	193.76014	2.62946	-765.53141	1
272	H	65.68138	76.91743	77.72977	507.39394	-846.55087	2539.60089	1
273	H	64.58248	75.57220	78.22272	1337.57841	1818.19054	1526.01994	1
274	H	64.39764	77.21557	78.95996	1100.88635	-1172.91350	-2199.08909	1
275	C	63.62008	75.32097	82.64984	-549.21115	475.64486	-309.38218	1
276	O	63.97631	75.27379	83.79778	556.06106	-390.37755	-78.24250	1
277	O	62.61875	74.44378	82.16690	-572.27940	-310.19032	-209.75862	1
278	H	62.59561	74.74269	81.21660	-1380.08193	2212.14486	790.85944	1

Listing 87: C00087.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.7275	2910
		0.2500	300.00	0.00	0.00	0.00	-1293.4826	0.0000	300.0000
3	H	66.32904	74.58603	69.75108	-2043.14101	-1757.64893	399.89339		1
4	N	66.32302	75.50505	70.19171	426.75047	490.45733	-334.42467		1
5	H	66.33882	75.26030	71.18535	442.25559	-1110.30854	-2448.52907		1
6	C	67.42834	76.31409	69.83767	415.32972	-666.39213	83.73172		1
7	H	67.97197	75.68191	69.10362	879.32219	2491.00447	667.35213		1
8	C	66.91475	77.68441	69.16752	31.35357	477.41777	628.23362		1
9	H	66.32366	78.26181	69.91839	1168.38489	2240.25337	-1019.71136		1
10	H	67.77836	78.33354	68.88490	-360.43770	2534.90498	931.67112		1
11	C	66.07372	77.38263	67.95394	463.18208	512.70242	-382.34388		1
12	H	65.27149	76.67116	68.25328	1725.29117	1863.52247	-987.07854		1
13	C	65.42628	78.65973	67.43229	710.42801	-144.27427	-313.15367		1
14	H	64.77878	78.46093	66.53963	364.20195	-1033.13725	2494.72524		1
15	H	64.78180	79.14573	68.20945	2567.61904	335.80679	847.48802		1
16	H	66.19538	79.41301	67.12112	-2587.99029	680.92867	-512.16411		1
17	C	66.90053	76.74968	66.84296	268.17616	741.64379	-40.42634		1
18	H	66.29030	76.58419	65.91771	1283.54314	-1945.37420	-1411.27812		1
19	H	67.76877	77.39711	66.55526	-1258.57796	1317.15249	-2026.02085		1
20	H	67.31461	75.75426	67.14691	-2502.84526	909.80597	575.92391		1
21	C	68.24972	76.50378	71.22844	619.36578	-458.64843	-172.09273		1
22	O	68.21645	75.64113	72.08425	-81.40433	433.87611	522.34594		1
23	N	68.90743	77.65431	71.22062	175.23996	-622.20190	341.55523		1
24	H	68.73689	78.26479	70.42461	-876.57256	-303.22879	-2561.90213		1
25	C	69.96491	77.98750	72.11338	-571.88214	-534.10783	-106.15033		1
26	H	70.01561	79.09350	72.00968	-2713.20841	-16.25800	-248.80809		1
27	C	69.59582	77.49671	73.58727	166.60354	288.16399	-716.09568		1
28	H	69.60604	76.36804	73.57797	-2097.85574	1636.78449	-586.18044		1
29	O	68.28487	77.88949	74.04909	-317.80580	-363.38227	484.43082		1
30	H	67.77019	77.09572	73.78322	1863.74748	-1451.84923	1357.29467		1

31	C	70.80213	78.02526	74.44602	503.80731	517.99032	318.51606	1
32	H	70.71818	77.69613	75.50781	640.61020	-2157.10410	-1536.29104	1
33	H	71.78382	77.65839	74.06013	1687.88455	465.60692	2087.56452	1
34	H	70.84289	79.13954	74.44895	-1293.07895	-1899.88581	-1463.57452	1
35	C	71.31934	77.25786	71.57233	-153.07550	-733.68902	248.70981	1
36	O	71.77916	76.33868	72.20711	186.15459	-480.78787	-449.34387	1
37	N	71.79114	77.81660	70.44316	-487.53139	543.18517	42.03850	1
38	C	72.93945	77.29583	69.78510	-699.35871	69.34393	360.10701	1
39	H	72.90973	76.19238	69.92259	2.81126	-221.99807	-2715.58072	1
40	C	72.78021	77.84360	68.31562	-507.46439	-592.59194	122.07761	1
41	H	73.73539	77.83895	67.74193	-1975.08116	525.87560	-1801.71556	1
42	H	72.04175	77.25353	67.72709	1588.27743	-1913.22100	1113.83566	1
43	C	72.25111	79.28077	68.62890	-613.62442	-457.55993	-194.14490	1
44	H	73.08050	79.92427	69.00471	1707.54637	-721.27992	1996.92523	1
45	H	71.80879	79.80036	67.74944	758.23357	2100.81767	1560.55011	1
46	C	71.19432	78.96578	69.77013	-352.41524	704.96076	49.21465	1
47	H	71.04125	79.78078	70.51502	1714.76886	-2070.42778	443.35792	1
48	H	70.20547	78.61640	69.39241	1224.15040	1801.50881	1636.97633	1
49	C	74.28679	77.99593	70.49800	566.85117	537.05831	117.62814	1
50	O	74.98610	78.84938	69.88396	-550.26779	-406.08867	4.21666	1
51	N	74.47388	77.55760	71.67343	566.34832	-425.77725	180.18749	1
52	H	73.78100	76.89884	71.99916	644.44502	2646.80550	-52.73430	1
53	C	76.16032	79.20624	73.12604	612.34801	-281.48662	411.56221	2
54	H	77.10058	78.79218	73.54837	1667.23498	-1490.75142	1556.16753	2
55	C	76.46425	80.28532	72.03725	-714.45746	-175.43074	286.98927	2
56	H	75.47226	80.65565	71.65186	-787.09484	1763.03619	-1922.46060	2
57	O	77.18659	79.82709	70.89454	-429.46514	516.51932	-128.40526	2
58	H	76.37934	79.53251	70.29930	1981.82785	436.16847	-1818.18182	2
59	C	77.16389	81.39862	72.91337	630.79189	-468.94448	76.03230	2
60	H	77.37225	82.31699	72.31870	-1775.71861	2062.30353	131.89849	2
61	H	76.53484	81.70245	73.78239	-1855.14608	88.94118	1993.53760	2
62	H	78.13758	81.04205	73.32127	-1504.82350	-780.94249	-2132.90992	2
63	C	75.24722	79.87297	74.25807	288.57638	618.62814	-397.00270	2
64	O	74.17341	80.38663	74.02542	321.70495	-185.26452	574.37218	2
65	N	75.92338	79.84980	75.41659	-447.05792	-446.53431	367.76425	2
66	H	76.78997	79.31553	75.48723	350.31316	1975.63644	-1843.31522	2
67	C	75.27844	80.29120	76.59634	-511.23061	374.03917	-471.51480	2
68	H	74.27965	80.67748	76.28126	2234.79579	-898.70890	-1273.45190	2
69	C	75.21516	79.00241	77.55057	529.53781	-159.34528	563.72604	2
70	H	74.89560	79.37408	78.55895	654.59388	2347.94251	1217.51488	2
71	H	74.37632	78.35959	77.16505	-1526.55661	2103.42026	817.87394	2
72	O	76.39216	78.19132	77.59984	-554.84278	14.12789	399.58769	2
73	H	76.88133	78.64043	78.38984	1297.06236	2061.84854	1220.68812	2
74	C	76.19120	81.40140	77.37019	-662.15484	-412.13544	123.62687	2
75	O	75.71641	81.93656	78.37520	-540.01537	-317.05804	274.91456	2
76	N	77.37445	81.56741	76.83028	-202.76299	-690.00100	-131.49145	2
77	H	77.49100	80.97081	76.01338	-702.62132	-2617.37191	281.70413	2
78	C	78.36820	82.56105	77.17804	-491.73914	576.34187	222.73509	2
79	H	79.10446	82.49266	76.34177	1977.17978	-1823.58850	-434.68928	2
80	C	77.68822	83.92305	77.27866	-649.50797	-328.66843	306.11224	2
81	H	76.81273	83.81437	77.96157	2075.07803	1452.16490	-1004.45904	2
82	C	78.62123	84.96620	77.86230	-615.18735	-489.99689	-70.96352	2
83	H	78.12132	85.96992	77.95450	-1226.32661	-1724.38906	-1716.47170	2
84	H	78.97713	84.67287	78.88932	2381.64273	-969.84735	900.46860	2
85	H	79.53711	85.10623	77.22394	2122.74991	1702.23946	-141.36228	2
86	C	77.16078	84.38303	75.93277	-501.86074	-479.61276	-376.42482	2
87	H	76.62528	85.36939	76.01038	993.79261	-2246.95401	-1177.81305	2
88	H	77.99069	84.51254	75.18443	42.71279	-626.15391	-2651.37258	2
89	H	76.43509	83.63944	75.50080	-2026.39012	-1590.33709	-887.82922	2
90	C	79.08083	82.17265	78.63777	-672.89153	382.57394	-156.34072	2
91	O	80.27756	82.19090	78.73339	410.04627	221.86223	500.35950	2
92	N	78.17031	82.01709	79.58479	-378.11782	-443.79414	-441.10984	2

93	H	77.15562	82.03261	79.31360	2404.15973	-568.14894	1149.30085	2
94	C	78.59582	81.26846	80.74424	-544.54484	466.16019	331.29119	2
95	H	79.59618	81.68456	81.00340	-1409.80988	-170.17955	2325.32679	2
96	C	77.45009	81.54030	81.81168	-184.48284	116.78282	-758.89137	2
97	H	77.27617	82.63644	81.89565	1893.78641	1861.14652	611.04528	2
98	H	76.48538	81.10895	81.46005	-2170.79665	-974.19311	1327.50117	2
99	C	77.84149	80.94677	83.19796	389.51668	672.81878	-138.49152	2
100	H	77.88555	79.81115	83.15769	510.64577	1933.03327	1851.02484	2
101	H	78.87548	81.25387	83.47024	-2302.30869	-1105.72939	-948.89774	2
102	C	76.86158	81.41320	84.34124	-559.93427	-126.34590	542.30857	2
103	O	77.09405	81.11319	85.48405	-670.36003	-111.83166	76.36448	2
104	N	75.82093	82.15710	83.90720	-216.06729	-537.07037	446.51379	2
105	H	75.55113	82.41423	82.95057	-1251.96487	1074.12894	-2168.52500	2
106	H	75.08854	82.52994	84.52097	-2451.83023	-720.73851	944.84612	2
107	C	78.63047	79.70262	80.37351	546.24052	-563.88337	-85.11809	2
108	O	77.88004	79.24434	79.52264	71.70702	-307.40463	606.69673	2
109	N	79.52317	79.06889	81.12717	479.90863	-504.50129	222.86849	2
110	C	79.55705	77.63569	81.18633	75.51268	-600.91904	506.73700	2
111	H	79.26516	77.26819	80.17599	-2033.61562	1795.30103	254.89480	2
112	C	81.06424	77.37033	81.60333	523.79067	517.99274	284.45581	2
113	H	81.22023	76.36880	82.06261	1599.61665	-1127.00911	1895.98173	2
114	H	81.74445	77.42783	80.72433	-1881.83093	1275.82488	-1501.55016	2
115	C	81.32670	78.54931	82.59192	-600.05639	-404.05026	316.64485	2
116	H	80.84320	78.36367	83.57720	-2597.05260	496.36221	657.73249	2
117	H	82.40588	78.73529	82.79365	-1666.24518	1294.38985	-1723.90591	2
118	C	80.62130	79.74090	81.81757	493.57570	-129.95376	-602.56394	2
119	H	80.20413	80.53967	82.47154	-1469.08415	-637.84797	2204.22581	2
120	H	81.23852	80.20829	81.01382	-1038.97840	1068.88701	-2280.71789	2
121	C	78.53721	77.11374	82.35624	188.88100	241.05089	-727.87821	2
122	O	77.97997	77.88430	83.11848	531.88613	-49.19943	427.07960	2
123	N	78.51764	75.79397	82.33395	708.14833	26.93417	-179.73509	2
124	H	79.11221	75.42156	81.59414	-2232.69501	-1179.09831	1023.94816	2
125	C	77.77281	74.91174	83.20271	-738.32412	259.92548	104.42456	2
126	H	78.41351	74.00030	83.27065	2028.89123	1260.02983	1311.33324	2
127	C	77.49302	75.56599	84.54258	-258.65678	-345.52513	661.28459	2
128	H	76.99901	76.55400	84.34505	-1826.06090	-1801.46097	-918.64554	2
129	C	76.55496	74.71544	85.38025	-541.23400	531.92970	-218.41428	2
130	H	76.30259	75.21033	86.35766	1311.73218	-2219.18200	882.19023	2
131	H	75.58571	74.52070	84.84321	-1048.71298	1223.58118	-2196.97971	2
132	H	77.00669	73.71360	85.61919	419.06414	1903.92898	1903.44670	2
133	C	78.76486	75.84219	85.32356	-423.86431	152.66566	-648.55262	2
134	H	78.54978	76.38182	86.28693	105.68386	-2342.50080	1387.51238	2
135	H	79.30821	74.89311	85.58592	-1695.63603	-1484.73621	-1531.02793	2
136	H	79.47477	76.48416	84.73270	-1853.57121	-487.39031	1936.59343	2
137	C	76.28752	74.55862	82.48196	539.71428	-510.58232	267.58633	2
138	O	75.55909	75.41001	82.03669	-15.93758	-278.34085	-624.49402	2
139	N	76.07738	73.26385	82.64171	-676.81886	12.05292	276.17960	2
140	H	76.84738	72.76536	83.08166	-1694.44250	-373.84189	-2100.66098	2
141	C	74.93843	72.57037	82.15116	412.33078	-664.70360	108.35451	2
142	H	75.23861	71.51815	82.35155	1765.77476	1294.44366	1621.76594	2
143	C	73.67688	72.99015	83.00793	-179.66635	-721.95667	-264.73915	2
144	H	73.89869	72.94253	84.09741	-607.34922	2587.87032	-598.10018	2
145	H	73.38932	74.04813	82.81439	-359.69332	-1479.13954	-2259.74260	2
146	C	72.53912	71.98646	82.61831	-240.01076	616.02425	431.85322	2
147	H	72.36384	71.99646	81.51860	-1359.17131	782.54425	2227.99181	2
148	H	72.83500	70.94108	82.85896	-820.36667	85.81767	-2596.78715	2
149	C	71.21907	72.38316	83.39101	-513.07015	236.18570	-551.87280	2
150	H	71.30077	72.13952	84.47535	1816.11944	-1183.11722	-1650.94321	2
151	H	71.03834	73.48133	83.33875	-1800.04429	-1361.53473	1526.34643	2
152	C	70.05806	71.60693	82.72470	726.08972	-253.19732	-179.64713	2
153	H	69.81840	71.93673	81.69382	1224.27271	-456.51798	-2390.90304	2
154	H	70.16004	70.50337	82.75216	1206.40339	-1150.93514	-2154.90344	2

155	N	68.75972	71.90254	83.54681	329.70796	-633.68968	-155.67358	2
156	H	67.86763	71.48050	83.15777	1348.31305	1938.76845	1359.00643	2
157	H	68.73370	71.55548	84.54975	2096.92035	1446.54551	-966.48890	2
158	H	68.47749	72.91968	83.65847	-1197.07217	-2303.53719	827.28733	2
159	C	74.79002	72.85541	80.53794	-378.01186	-556.17301	-413.96481	2
160	O	75.69011	72.47905	79.81797	-409.44433	-307.55053	-453.30833	2
161	N	73.65143	73.44234	80.22215	-429.02477	524.70884	274.08502	2
162	H	73.04748	73.73062	80.98819	1706.34263	-1425.96036	1574.38926	2
163	C	73.26977	73.73259	78.88424	-45.25864	-626.22952	478.93267	2
164	H	72.51579	74.54520	78.98891	1988.63164	570.90773	1772.87287	2
165	C	74.59260	74.18525	78.14895	551.77128	-20.49526	-564.54996	2
166	H	75.12155	74.92769	78.79066	1434.61535	-1753.10253	1513.99471	2
167	H	75.30324	73.31871	78.04418	-714.67738	1819.09770	1898.36494	2
168	C	74.30648	74.79052	76.72706	446.99263	-555.77305	338.97221	2
169	H	74.02141	73.97452	75.99562	1953.68466	1892.25957	-161.67766	2
170	H	73.47751	75.53582	76.74423	-403.03785	2688.07032	-188.43591	2
171	C	75.66539	75.44634	76.32976	567.86262	335.74681	434.04421	2
172	H	75.97979	76.19255	77.09919	-1080.02275	1568.26081	-1948.78900	2
173	H	76.47439	74.68320	76.30863	-919.54108	2111.34692	1456.13463	2
174	C	75.52888	76.16456	74.90414	195.81897	173.33862	-745.11536	2
175	H	75.39335	75.45645	74.04873	1405.67949	-2301.21089	-390.08113	2
176	H	74.74527	76.96333	74.88238	-940.37328	-1118.32446	2299.72133	2
177	N	76.79033	76.82296	74.73884	319.26422	656.36007	-42.02424	2
178	H	75.61367	78.33715	72.65056	1961.03633	619.91968	1787.09422	2
179	H	77.03334	77.40800	75.53653	854.14343	-2156.80752	1429.08711	2
180	H	77.59136	76.20170	74.67854	1237.02905	-1378.50857	-1998.28500	2
181	C	72.60369	72.39608	78.19415	532.53319	-268.57236	517.55729	2
182	O	72.54680	71.30697	78.71189	266.16714	-290.73804	-558.88002	2
183	N	72.07721	72.79325	77.03714	-226.25352	640.49678	-270.32839	2
184	H	72.22801	73.76794	76.78901	2007.69063	-1035.27229	1523.50231	2
185	C	71.78242	71.82250	76.03470	-540.76542	-573.33303	49.50000	2
186	H	71.34044	70.95385	76.57241	-2374.20950	-1036.76023	843.75774	2
187	C	70.80586	72.54603	74.99999	-77.09082	666.87422	-415.84136	2
188	H	71.31736	73.46323	74.59720	-985.81834	617.19825	2463.91927	2
189	O	69.56289	73.01219	75.56637	293.29899	-391.65602	-477.80926	2
190	H	69.59139	73.95963	75.33106	2528.72714	-681.76262	-751.27122	2
191	C	70.65761	71.50332	73.83319	252.47363	-605.14473	440.05134	2
192	H	69.98417	71.89331	73.03420	-2052.65063	1456.49051	-1043.51830	2
193	H	71.64644	71.25814	73.33756	-2152.98800	-1661.97574	-161.70652	2
194	H	70.21593	70.54586	74.19565	-473.12726	-1584.27339	2165.61725	2
195	C	73.18097	71.43916	75.28078	360.36307	488.46713	505.10056	2
196	O	74.08771	72.23216	75.12521	-200.08817	-528.03552	-385.82850	2
197	N	73.05720	70.20890	74.81275	-597.54095	-226.44775	355.20479	2
198	H	72.20806	69.68277	75.00816	2179.23655	-1300.70981	-991.33835	2
199	C	74.09896	69.68071	73.99070	-687.68921	297.39807	-249.45179	2
200	H	75.04079	69.83093	74.56311	-349.16256	-2467.37713	-1101.72831	2
201	C	73.74445	68.16329	73.65431	672.47345	361.54328	-201.62880	2
202	H	72.82934	68.12264	73.02023	1541.41502	582.18425	2169.97026	2
203	H	74.57125	67.71803	73.05366	-2534.67717	60.25153	997.72295	2
204	C	73.52204	67.36223	74.94664	574.26774	-389.43119	-377.02542	2
205	C	74.63196	67.00657	75.76949	688.82679	-287.33580	-257.96133	2
206	H	75.65822	67.31310	75.49705	331.14182	1470.38163	2269.80013	2
207	C	72.19628	66.97967	75.31229	-383.52382	-675.04808	144.24917	2
208	H	71.33397	67.26400	74.68233	4.09847	1517.59662	2262.86397	2
209	C	74.39193	66.26390	76.92572	-134.76730	428.45285	-649.50303	2
210	H	75.24933	65.98716	77.56364	-903.23433	1600.49020	2011.53387	2
211	C	72.00844	66.23431	76.47881	-335.53281	-615.00040	-364.39058	2
212	H	70.97975	65.93868	76.74946	1596.45398	-1369.33862	1732.02659	2
213	C	73.08905	65.84570	77.32337	585.48547	-340.24194	-406.23938	2
214	O	72.90850	65.08214	78.50615	-419.15649	-173.04408	-511.94141	2
215	H	71.92874	64.97173	78.48525	-1071.84350	1559.71507	-1960.13012	2
216	C	74.10108	70.48250	72.57079	291.41878	-183.13091	710.72246	2

217	O	73.10166	70.89684	72.01788	379.87695	523.47396	-222.23622	2
218	N	75.35218	70.47698	72.13249	564.30591	373.09380	277.24371	2
219	H	76.07918	70.03394	72.69226	-120.59931	-2436.07824	-1214.35098	2
220	C	75.64418	71.07602	70.87951	404.07514	-299.37480	608.84009	2
221	H	74.71284	71.60730	70.57035	-1071.07882	-841.69025	2359.66467	2
222	C	76.91342	71.99576	71.13674	-683.12807	68.71770	-390.13096	2
223	H	76.78335	72.56689	72.08320	2068.88918	1596.58590	770.89603	2
224	H	77.81948	71.36664	71.28883	1379.86429	2342.49779	-179.85638	2
225	C	77.11815	72.96849	69.93699	-176.39967	537.49466	550.97268	2
226	H	77.34793	72.42000	68.99717	-396.28051	1942.22168	1869.33314	2
227	H	76.19781	73.55735	69.72660	-94.44700	586.00678	-2659.20016	2
228	C	78.32553	73.91772	70.38365	-291.69381	-718.18079	-150.72929	2
229	H	78.07131	74.64145	71.19976	-2303.38776	1089.76242	964.62032	2
230	H	79.27209	73.39732	70.67697	884.16729	2568.80533	-207.74283	2
231	N	78.58484	74.66861	69.22926	-594.49522	-252.81478	342.29276	2
232	H	77.90791	74.60365	68.48516	-1735.17426	2084.05705	-263.71605	2
233	C	79.59017	75.43110	69.07663	595.23177	-271.52487	442.22352	2
234	N	80.51145	75.51277	70.12686	585.53813	-424.79750	-105.81303	2
235	H	80.48816	75.07408	71.04646	959.88797	1327.56823	-2177.11905	2
236	H	81.33466	76.11580	70.13039	1578.48647	16.27378	-2220.76233	2
237	N	79.56521	76.05479	67.82093	-452.17763	-390.33541	-421.51853	2
238	H	78.87363	76.02808	67.07334	470.26107	1974.25629	-1817.92087	2
239	H	80.26140	76.74325	67.53219	1856.67307	-1573.97321	-1224.35416	2
240	C	76.11773	69.86621	69.87618	-531.47271	-581.45780	-55.06206	2
241	O	77.11473	69.18757	70.08592	-243.00837	192.73507	609.52485	2
242	N	75.28840	69.80584	68.85674	343.49288	-644.25607	38.09164	2
243	H	74.52025	70.47201	68.88596	-1691.16043	-1535.97525	-1484.73099	2
244	C	75.33596	68.69562	67.90345	542.66492	350.14337	454.42563	2
245	H	75.55407	67.82512	68.56711	1209.57979	-2396.95920	463.86744	2
246	C	74.01319	68.61216	67.16228	-737.14309	145.93010	242.71942	2
247	H	73.80806	69.61205	66.71893	-1050.18303	159.36419	-2509.06125	2
248	C	74.06717	67.60012	66.03275	-706.77696	-252.88343	-245.16230	2
249	H	73.09262	67.54730	65.47323	-1624.64039	-1665.49085	1417.86935	2
250	H	74.86913	67.86144	65.28458	2566.10521	598.51109	693.22305	2
251	H	74.29127	66.56510	66.41254	-1972.69758	107.10018	-1876.34312	2
252	C	72.86686	68.27433	68.09841	412.85148	672.58832	-27.69222	2
253	H	71.87513	68.29526	67.56813	1447.02277	1762.76533	-1490.78944	2
254	H	72.98577	67.24672	68.54032	1320.77379	-145.20455	2378.68491	2
255	H	72.80485	68.99756	68.95788	-1512.10848	1470.52031	1724.75147	2
256	C	76.62154	69.01606	66.90003	-607.11113	499.56689	73.73769	2
257	O	76.45957	69.41085	65.77445	357.97126	460.81534	356.68785	2
258	N	77.74777	68.77643	67.55208	536.55407	-368.62270	332.76306	2
259	H	77.74400	68.52121	68.56698	524.38866	2297.69985	1367.20941	2
260	C	78.93947	68.77971	66.79132	46.50277	-774.29190	-147.97904	2
261	H	78.64720	69.16046	65.78442	1676.51875	1883.29066	1032.55549	2
262	C	80.03811	69.68240	67.56202	-559.41456	-34.19198	-556.30433	2
263	H	80.31944	69.18734	68.52248	-64.66664	395.18769	2695.05373	2
264	H	80.97786	69.74750	66.96376	-2703.44278	-60.40056	333.79418	2
265	C	79.46400	71.04683	67.82880	-519.76435	377.31045	459.42366	2
266	H	78.52319	70.91314	68.41003	-1746.74323	1667.50644	-1261.73691	2
267	C	80.43427	71.88558	68.65154	570.95554	16.46261	-545.27700	2
268	H	80.06682	72.93677	68.77555	2391.58273	28.05277	-1305.07271	2
269	H	80.58354	71.45932	69.67703	175.75588	917.63458	2559.43867	2
270	H	81.44208	71.94567	68.16592	-1063.97851	-2155.34650	1283.00462	2
271	C	79.13279	71.78089	66.53635	193.76014	2.62946	-765.53141	2
272	H	78.77973	72.82617	66.73390	507.39394	-846.55087	2539.60089	2
273	H	80.02536	71.85389	65.86275	1337.57841	1818.19054	1526.01994	2
274	H	78.32226	71.25938	65.96299	1100.88635	-1172.91350	-2199.08909	2
275	C	79.51337	67.26454	66.77826	-549.21115	475.64486	-309.38218	2
276	O	79.26178	66.44608	67.62246	556.06106	-390.37755	-78.24250	2
277	O	80.45933	66.98695	65.76425	-572.27940	-310.19032	-209.75862	2
278	H	80.41747	67.85549	65.27428	-1380.08193	2212.14486	790.85944	2

Listing 88: C00088.xmolout

1	276							
2	150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
	0.2500	300.00	0.00	0.00	0.00	-1293.4725	0.0000	300.0000
3	H	79.32990	71.39819	90.43648	-2043.14101	-1757.64893	399.89339	1
4	N	79.34998	71.48243	89.42115	426.75047	490.45733	-334.42467	1
5	H	78.50753	72.03664	89.26914	442.25559	-1110.30854	-2448.52907	1
6	C	80.52376	72.11840	88.94053	415.32972	-666.39213	83.73172	1
7	H	80.70185	72.95846	89.64551	879.32219	2491.00447	667.35213	1
8	C	81.73913	71.06387	88.94335	31.35357	477.41777	628.23362	1
9	H	81.57258	70.32446	88.12303	1168.38489	2240.25337	-1019.71136	1
10	H	82.68966	71.59061	88.68657	-360.43770	2534.90498	931.67112	1
11	C	81.86383	70.34550	90.26361	463.18208	512.70242	-382.34388	1
12	H	80.89704	69.83637	90.47623	1725.29117	1863.52247	-987.07854	1
13	C	82.95807	69.28804	90.18597	710.42801	-144.27427	-313.15367	1
14	H	83.04593	68.71165	91.14300	364.20195	-1033.13725	2494.72524	1
15	H	82.76206	68.54732	89.36814	2567.61904	335.80679	847.48802	1
16	H	83.96012	69.74713	89.98343	-2587.99029	680.92867	-512.16411	1
17	C	82.16907	71.30708	91.40334	268.17616	741.64379	-40.42634	1
18	H	82.28131	70.76753	92.37938	1283.54314	-1945.37420	-1411.27812	1
19	H	83.12177	71.86924	91.22383	-1258.57796	1317.15249	-2026.02085	1
20	H	81.35588	72.06625	91.53638	-2502.84526	909.80597	575.92391	1
21	C	80.28871	72.62004	87.41562	619.36578	-458.64843	-172.09273	1
22	O	80.98493	73.49178	86.94231	-81.40433	433.87611	522.34594	1
23	N	79.37715	71.87032	86.77518	175.23996	-622.20190	341.55523	1
24	H	78.86081	71.21411	87.36049	-876.57256	-303.22879	-2561.90213	1
25	C	78.80719	72.45759	85.59646	-571.88214	-534.10783	-106.15033	1
26	H	79.68490	72.87780	85.05952	-2713.20841	-16.25800	-248.80809	1
27	C	78.02663	71.30239	84.82261	166.60354	288.16399	-716.09568	1
28	H	77.16137	70.97262	85.46019	-2097.85574	1636.78449	-586.18044	1
29	O	78.78637	70.11252	84.53085	-317.80580	-363.38227	484.43082	1
30	H	78.29610	69.44284	85.04578	1863.74748	-1451.84923	1357.29467	1
31	C	77.48659	72.07360	83.56273	503.80731	517.99032	318.51606	1
32	H	76.81702	71.42635	82.94945	640.61020	-2157.10410	-1536.29104	1
33	H	76.89589	73.00396	83.83432	1687.88455	465.60692	2087.56452	1
34	H	78.32252	72.39691	82.89956	-1293.07895	-1899.88581	-1463.57452	1
35	C	77.74019	73.58338	86.10677	-153.07550	-733.68902	248.70981	1
36	O	76.92027	73.28640	86.93317	186.15459	-480.78787	-449.34387	1
37	N	77.91652	74.74175	85.45473	-487.53139	543.18517	42.03850	1
38	C	76.95489	75.79844	85.53664	-699.35871	69.34393	360.10701	1
39	H	76.48748	75.69800	86.54418	2.81126	-221.99807	-2715.58072	1
40	C	77.87134	77.08215	85.32852	-507.46439	-592.59194	122.07761	1
41	H	77.30444	77.97812	84.99149	-1975.08116	525.87560	-1801.71556	1
42	H	78.38836	77.36901	86.27135	1588.27743	-1913.22100	1113.83566	1
43	C	78.88738	76.56675	84.26383	-613.62442	-457.55993	-194.14490	1
44	H	78.43354	76.57245	83.24702	1707.54637	-721.27992	1996.92523	1
45	H	79.81340	77.18117	84.19978	758.23357	2100.81767	1560.55011	1
46	C	79.15504	75.08420	84.76874	-352.41524	704.96076	49.21465	1
47	H	79.32401	74.34309	83.95292	1714.76886	-2070.42778	443.35792	1
48	H	79.96041	74.97812	85.53917	1224.15040	1801.50881	1636.97633	1
49	C	75.86059	75.61679	84.33927	566.85117	537.05831	117.62814	1
50	O	75.76605	74.59072	83.69536	-550.26779	-406.08867	4.21666	1
51	N	75.11708	76.70858	84.25054	566.34832	-425.77725	180.18749	1
52	H	75.31217	77.49744	84.86296	644.44502	2646.80550	-52.73430	1
53	C	73.98815	76.67322	83.38192	612.34801	-281.48662	411.56221	1
54	H	73.72784	75.59220	83.29902	1667.23498	-1490.75142	1556.16753	1
55	C	72.87345	77.61772	84.03389	-714.45746	-175.43074	286.98927	1
56	H	73.19640	78.68792	83.90933	-787.09484	1763.03619	-1922.46060	1
57	O	72.63163	77.43790	85.44043	-429.46514	516.51932	-128.40526	1

58	H	72.85909	78.32419	85.78758	1981.82785	436.16847	-1818.18182	1
59	C	71.64354	77.32932	83.09677	630.79189	-468.94448	76.03230	1
60	H	70.77932	77.98820	83.34423	-1775.71861	2062.30353	131.89849	1
61	H	71.88646	77.48799	82.01770	-1855.14608	88.94118	1993.53760	1
62	H	71.29318	76.27611	83.20289	-1504.82350	-780.94249	-2132.90992	1
63	C	74.43611	77.34224	81.95635	288.57638	618.62814	-397.00270	1
64	O	75.10127	78.34313	81.88831	321.70495	-185.26452	574.37218	1
65	N	73.88731	76.63555	80.96477	-447.05792	-446.53431	367.76425	1
66	H	73.20513	75.88055	81.13793	350.31316	1975.63644	-1843.31522	1
67	C	73.75843	77.30673	79.70588	-511.23061	374.03917	-471.51480	1
68	H	73.96296	78.38614	79.90426	2234.79579	-898.70890	-1273.45190	1
69	C	74.80608	76.65424	78.67928	529.53781	-159.34528	563.72604	1
70	H	74.70360	77.19272	77.69573	654.59388	2347.94251	1217.51488	1
71	H	75.83119	76.89619	79.06929	-1526.55661	2103.42026	817.87394	1
72	O	74.62578	75.23895	78.38536	-554.84278	14.12789	399.58769	1
73	H	74.98339	74.86946	79.21475	1297.06236	2061.84854	1220.68812	1
74	C	72.23630	76.90838	79.32930	-662.15484	-412.13544	123.62687	1
75	O	71.59304	76.24534	80.12218	-540.01537	-317.05804	274.91456	1
76	N	71.85880	77.41431	78.15540	-202.76299	-690.00100	-131.49145	1
77	H	72.58195	77.92340	77.64416	-702.62132	-2617.37191	281.70413	1
78	C	70.61969	76.99674	77.50434	-491.73914	576.34187	222.73509	1
79	H	69.90696	76.85658	78.35191	1977.17978	-1823.58850	-434.68928	1
80	C	70.21336	78.08498	76.52684	-649.50797	-328.66843	306.11224	1
81	H	71.03412	78.19596	75.78263	2075.07803	1452.16490	-1004.45904	1
82	C	68.94360	77.73911	75.77114	-615.18735	-489.99689	-70.96352	1
83	H	68.62668	78.57311	75.08604	-1226.32661	-1724.38906	-1716.47170	1
84	H	69.07607	76.81817	75.13490	2381.64273	-969.84735	900.46860	1
85	H	68.08692	77.53823	76.47187	2122.74991	1702.23946	-141.36228	1
86	C	70.03995	79.42576	77.21909	-501.86074	-479.61276	-376.42482	1
87	H	69.80504	80.24644	76.48708	993.79261	-2246.95401	-1177.81305	1
88	H	69.20101	79.39707	77.96731	42.71279	-626.15391	-2651.37258	1
89	H	70.96923	79.72657	77.77599	-2026.39012	-1590.33709	-887.82922	1
90	C	70.87932	75.56031	76.70299	-672.89153	382.57394	-156.34072	1
91	O	69.94199	75.02521	76.16270	410.04627	221.86223	500.35950	1
92	N	72.13285	75.16238	76.76929	-378.11782	-443.79414	-441.10984	1
93	H	72.78477	75.72219	77.31757	2404.15973	-568.14894	1149.30085	1
94	C	72.57970	73.97970	76.09875	-544.54484	466.16019	331.29119	1
95	H	73.60855	73.89411	76.51732	-1409.80988	-170.17955	2325.32679	1
96	C	71.61419	72.81943	76.60922	-184.48284	116.78282	-758.89137	1
97	H	70.82229	73.24287	77.26794	1893.78641	1861.14652	611.04528	1
98	H	71.08256	72.31142	75.77220	-2170.79665	-974.19311	1327.50117	1
99	C	72.52332	71.83345	77.40408	389.51668	672.81878	-138.49152	1
100	H	73.25487	71.34037	76.72784	510.64577	1933.03327	1851.02484	1
101	H	73.15476	72.41194	78.11491	-2302.30869	-1105.72939	-948.89774	1
102	C	71.72865	70.73547	78.20883	-559.93427	-126.34590	542.30857	1
103	O	72.32076	69.77972	78.63754	-670.36003	-111.83166	76.36448	1
104	N	70.41867	71.01276	78.38862	-216.06729	-537.07037	446.51379	1
105	H	69.88338	71.84494	78.11646	-1251.96487	1074.12894	-2168.52500	1
106	H	69.79452	70.45305	78.98011	-2451.83023	-720.73851	944.84612	1
107	C	72.62682	74.31257	74.51627	546.24052	-563.88337	-85.11809	1
108	O	72.99537	75.41461	74.18628	71.70702	-307.40463	606.69673	1
109	N	72.45235	73.23773	73.72403	479.90863	-504.50129	222.86849	1
110	C	72.44209	73.47531	72.31328	75.51268	-600.91904	506.73700	1
111	H	72.80986	74.52389	72.19762	-2033.61562	1795.30103	254.89480	1
112	C	73.43836	72.35525	71.79459	523.79067	517.99274	284.45581	1
113	H	73.28242	72.10416	70.70770	1599.61665	-1127.00911	1895.98173	1
114	H	74.49588	72.69090	71.88434	-1881.83093	1275.82488	-1501.55016	1
115	C	73.16255	71.15583	72.75410	-600.05639	-404.05026	316.64485	1
116	H	72.26738	70.57617	72.43433	-2597.05260	496.36221	657.73249	1
117	H	74.00222	70.42661	72.80172	-1666.24518	1294.38985	-1723.90591	1
118	C	72.92159	71.91436	74.12717	493.57570	-129.95376	-602.56394	1
119	H	72.14145	71.44536	74.77146	-1469.08415	-637.84797	2204.22581	1

120	H	73.84001	72.09144	74.73286	-1038.97840	1068.88701	-2280.71789	1
121	C	70.96779	73.28650	71.60878	188.88100	241.05089	-727.87821	1
122	O	70.67009	74.02153	70.65227	531.88613	-49.19943	427.07960	1
123	N	70.30637	72.26712	72.08753	708.14833	26.93417	-179.73509	1
124	H	70.87508	71.89319	72.85260	-2232.69501	-1179.09831	1023.94816	1
125	C	68.90005	71.94632	71.97282	-738.32412	259.92548	104.42456	1
126	H	68.83986	70.99367	72.55200	2028.89123	1260.02983	1311.33324	1
127	C	68.08844	73.06974	72.60907	-258.65678	-345.52513	661.28459	1
128	H	68.32149	74.01098	72.06398	-1826.06090	-1801.46097	-918.64554	1
129	C	66.60080	72.80050	72.47914	-541.23400	531.92970	-218.41428	1
130	H	65.98298	73.62744	72.92500	1311.73218	-2219.18200	882.19023	1
131	H	66.29276	72.69467	71.40169	-1048.71298	1223.58118	-2196.97971	1
132	H	66.30630	71.84699	72.99836	419.06414	1903.92898	1903.44670	1
133	C	68.46141	73.27886	74.06447	-423.86431	152.66566	-648.55262	1
134	H	67.85467	74.09863	74.53861	105.68386	-2342.50080	1387.51238	1
135	H	68.29299	72.34749	74.67247	-1695.63603	-1484.73621	-1531.02793	1
136	H	69.54509	73.56271	74.18316	-1853.57121	-487.39031	1936.59343	1
137	C	68.35774	71.72693	70.40615	539.71428	-510.58232	267.58633	1
138	O	67.74131	70.72227	70.17010	-15.93758	-278.34085	-624.49402	1
139	N	68.57015	72.77412	69.63450	-676.81886	12.05292	276.17960	1
140	H	69.15487	73.57704	69.97169	-1694.44250	-373.84189	-2100.66098	1
141	C	68.11926	72.69354	68.28726	412.33078	-664.70360	108.35451	1
142	H	67.44317	71.80620	68.23353	1765.77476	1294.44366	1621.76594	1
143	C	67.42390	74.08392	67.95580	-179.66635	-721.95667	-264.73915	1
144	H	66.55785	74.25812	68.63207	-607.34922	2587.87032	-598.10018	1
145	H	68.12820	74.92156	68.15675	-359.69332	-1479.13954	-2259.74260	1
146	C	66.97146	74.09781	66.46033	-240.01076	616.02425	431.85322	1
147	H	67.83816	73.89660	65.78945	-1359.17131	782.54425	2227.99181	1
148	H	66.23584	73.28731	66.25797	-820.36667	85.81767	-2596.78715	1
149	C	66.35315	75.51832	66.13706	-513.07015	236.18570	-551.87280	1
150	H	65.41271	75.68496	66.71074	1816.11944	-1183.11722	-1650.94321	1
151	H	67.04652	76.33284	66.44878	-1800.04429	-1361.53473	1526.34643	1
152	C	66.09486	75.57950	64.61387	726.08972	-253.19732	-179.64713	1
153	H	67.00813	75.51600	63.98900	1224.27271	-456.51798	-2390.90304	1
154	H	65.33454	74.86292	64.24437	1206.40339	-1150.93514	-2154.90344	1
155	N	65.49819	76.99111	64.28973	329.70796	-633.68968	-155.67358	1
156	H	65.28620	77.17430	63.26659	1348.31305	1938.76845	1359.00643	1
157	H	64.56976	77.23795	64.74087	2096.92035	1446.54551	-966.48890	1
158	H	66.09202	77.83650	64.53346	-1197.07217	-2303.53719	827.28733	1
159	C	69.40691	72.57910	67.28238	-378.01186	-556.17301	-413.96481	1
160	O	69.24943	72.14640	66.16404	-409.44433	-307.55053	-453.30833	1
161	N	70.50826	73.10377	67.80376	-429.02477	524.70884	274.08502	1
162	H	70.55136	73.43979	68.77496	1706.34263	-1425.96036	1574.38926	1
163	C	71.66410	73.08085	66.94324	-45.25864	-626.22952	478.93267	1
164	H	71.63541	72.03354	66.56755	1988.63164	570.90773	1772.87287	1
165	C	71.40818	74.09956	65.76504	551.77128	-20.49526	-564.54996	1
166	H	70.43848	73.87666	65.26066	1434.61535	-1753.10253	1513.99471	1
167	H	71.30656	75.13822	66.15269	-714.67738	1819.09770	1898.36494	1
168	C	72.60505	73.97215	64.76182	446.99263	-555.77305	338.97221	1
169	H	73.57698	73.99033	65.30427	1953.68466	1892.25957	-161.67766	1
170	H	72.57835	72.99576	64.22868	-403.03785	2688.07032	-188.43591	1
171	C	72.52286	75.17839	63.74613	567.86262	335.74681	434.04421	1
172	H	71.68533	75.04128	63.02430	-1080.02275	1568.26081	-1948.78900	1
173	H	72.31245	76.13483	64.27752	-919.54108	2111.34692	1456.13463	1
174	C	73.89245	75.25064	63.02336	195.81897	173.33862	-745.11536	1
175	H	74.73788	75.54352	63.67979	1405.67949	-2301.21089	-390.08113	1
176	H	74.16443	74.34562	62.44260	-940.37328	-1118.32446	2299.72133	1
177	N	73.81016	76.38968	61.97275	319.26422	656.36007	-42.02424	1
178	H	74.79136	76.72439	61.59620	1961.03633	619.91968	1787.09422	1
179	H	73.24943	76.18148	61.09548	854.14343	-2156.80752	1429.08711	1
180	H	73.34642	77.28755	62.29909	1237.02905	-1378.50857	-1998.28500	1
181	C	72.94402	73.40153	67.91190	532.53319	-268.57236	517.55729	1

182	O	73.19815	72.58038	68.77010	266.16714	-290.73804	-558.88002	1
183	N	73.53923	74.53710	67.59781	-226.25352	640.49678	-270.32839	1
184	H	73.10649	75.07586	66.84863	2007.69063	-1035.27229	1523.50231	1
185	C	74.55053	75.17356	68.35917	-540.76542	-573.33303	49.50000	1
186	H	74.59407	76.20941	67.95580	-2374.20950	-1036.76023	843.75774	1
187	C	74.01879	75.15336	69.86879	-77.09082	666.87422	-415.84136	1
188	H	73.72807	74.09511	70.12886	-985.81834	617.19825	2463.91927	1
189	O	72.85621	75.96533	70.09685	293.29899	-391.65602	-477.80926	1
190	H	72.16053	75.28490	70.27429	2528.72714	-681.76262	-751.27122	1
191	C	75.30171	75.53436	70.68530	252.47363	-605.14473	440.05134	1
192	H	75.09852	75.54715	71.78117	-2052.65063	1456.49051	-1043.51830	1
193	H	76.13124	74.80743	70.51487	-2152.98800	-1661.97574	-161.70652	1
194	H	75.67971	76.54617	70.40919	-473.12726	-1584.27339	2165.61725	1
195	C	75.97194	74.39873	68.10977	360.36307	488.46713	505.10056	1
196	O	76.09808	73.19752	68.10335	-200.08817	-528.03552	-385.82850	1
197	N	76.93464	75.31704	68.00456	-597.54095	-226.44775	355.20479	1
198	H	76.69671	76.30776	68.03614	2179.23655	-1300.70981	-991.33835	1
199	C	78.19332	74.84101	67.53868	-687.68921	297.39807	-249.45179	1
200	H	77.96653	73.89889	66.98743	-349.16256	-2467.37713	-1101.72831	1
201	C	78.92810	75.97312	66.69170	672.47345	361.54328	-201.62880	1
202	H	79.03900	76.89374	67.30778	1541.41502	582.18425	2169.97026	1
203	H	79.95814	75.62462	66.44789	-2534.67717	60.25153	997.72295	1
204	C	78.16642	76.29652	65.38955	574.26774	-389.43119	-377.02542	1
205	C	78.25042	75.40155	64.28593	688.82679	-287.33580	-257.96133	1
206	H	78.80264	74.44987	64.37192	331.14182	1470.38163	2269.80013	1
207	C	77.44148	77.51647	65.28008	-383.52382	-675.04808	144.24917	1
208	H	77.36315	78.20448	66.13908	4.09847	1517.59662	2262.86397	1
209	C	77.63962	75.77734	63.07203	-134.76730	428.45285	-649.50303	1
210	H	77.71744	75.10171	62.20018	-903.23433	1600.49020	2011.53387	1
211	C	76.85586	77.84312	64.03814	-335.53281	-615.00040	-364.39058	1
212	H	76.31379	78.80242	63.94443	1596.45398	-1369.33862	1732.02659	1
213	C	76.94448	76.99458	62.91542	585.48547	-340.24194	-406.23938	1
214	O	76.33128	77.34857	61.58193	-419.15649	-173.04408	-511.94141	1
215	H	76.11293	78.26718	61.80309	-1071.84350	1559.71507	-1960.13012	1
216	C	79.21521	74.58141	68.79134	291.41878	-183.13091	710.72246	1
217	O	80.26590	74.00702	68.60625	379.87695	523.47396	-222.23622	1
218	N	78.77946	75.15778	69.90752	564.30591	373.09380	277.24371	1
219	H	77.87637	75.62343	69.86230	-120.59931	-2436.07824	-1214.35098	1
220	C	79.55435	75.00257	71.09102	404.07514	-299.37480	608.84009	1
221	H	80.23644	74.14841	70.87011	-1071.07882	-841.69025	2359.66467	1
222	C	80.33245	76.37454	71.26586	-683.12807	68.71770	-390.13096	1
223	H	80.78475	76.68817	70.29814	2068.88918	1596.58590	770.89603	1
224	H	79.63431	77.19343	71.55007	1379.86429	2342.49779	-179.85638	1
225	C	81.42901	76.19351	72.35807	-176.39967	537.49466	550.97268	1
226	H	80.97779	75.85347	73.31991	-396.28051	1942.22168	1869.33314	1
227	H	82.16434	75.40962	72.06905	-94.44700	586.00678	-2659.20016	1
228	C	82.13405	77.62040	72.52685	-291.69381	-718.18079	-150.72929	1
229	H	82.60397	78.05331	71.60814	-2303.38776	1089.76242	964.62032	1
230	H	81.47079	78.39380	72.99229	884.16729	2568.80533	-207.74283	1
231	N	83.14718	77.31808	73.44603	-594.49522	-252.81478	342.29276	1
232	H	82.98092	76.52339	74.04477	-1735.17426	2084.05705	-263.71605	1
233	C	84.22475	77.97686	73.59879	595.23177	-271.52487	442.22352	1
234	N	84.44135	79.09545	72.78848	585.53813	-424.79750	-105.81303	1
235	H	83.84503	79.50530	72.07095	959.88797	1327.56823	-2177.11905	1
236	H	85.26341	79.69850	72.83605	1578.48647	16.27378	-2220.76233	1
237	N	85.01203	77.41346	74.61237	-452.17763	-390.33541	-421.51853	1
238	H	84.86022	76.59570	75.20078	470.26107	1974.25629	-1817.92087	1
239	H	85.91982	77.79026	74.88762	1856.67307	-1573.97321	-1224.35416	1
240	C	78.54716	74.76648	72.36415	-531.47271	-581.45780	-55.06206	1
241	O	78.68998	73.79471	73.06815	-243.00837	192.73507	609.52485	1
242	N	77.57952	75.70104	72.42155	343.49288	-644.25607	38.09164	1
243	H	77.75071	76.38320	71.68017	-1691.16043	-1535.97525	-1484.73099	1

244	C	76.98254	76.14981	73.68458	542.66492	350.14337	454.42563	1
245	H	76.07426	76.71609	73.37196	1209.57979	-2396.95920	463.86744	1
246	C	76.67194	74.96479	74.57168	-737.14309	145.93010	242.71942	1
247	H	77.64378	74.50896	74.88049	-1050.18303	159.36419	-2509.06125	1
248	C	75.91698	75.39219	75.81824	-706.77696	-252.88343	-245.16230	1
249	H	75.75763	74.53493	76.53016	-1624.64039	-1665.49085	1417.86935	1
250	H	76.46855	76.19142	76.38662	2566.10521	598.51109	693.22305	1
251	H	74.89831	75.80126	75.56249	-1972.69758	107.10018	-1876.34312	1
252	C	75.87998	73.89288	73.84339	412.85148	672.58832	-27.69222	1
253	H	75.72409	72.98200	74.48238	1447.02277	1762.76533	-1490.78944	1
254	H	74.86219	74.26572	73.53710	1320.77379	-145.20455	2378.68491	1
255	H	76.42078	73.56107	72.91193	-1512.10848	1470.52031	1724.75147	1
256	C	78.09654	77.13504	74.42028	-607.11113	499.56689	73.73769	1
257	O	79.28950	76.95805	74.35884	357.97126	460.81534	356.68785	1
258	N	77.43555	78.07538	75.08237	536.55407	-368.62270	332.76306	1
259	H	76.41747	78.06142	75.05893	524.38866	2297.69985	1367.20941	1
260	C	78.16079	78.90944	75.96439	46.50277	-774.29190	-147.97904	1
261	H	79.23423	78.66583	75.79034	1676.51875	1883.29066	1032.55549	1
262	C	77.75653	80.44290	75.66017	-559.41456	-34.19198	-556.30433	1
263	H	76.67787	80.59217	75.90499	-64.66664	395.18769	2695.05373	1
264	H	78.32185	81.13864	76.32523	-2703.44278	-60.40056	333.79418	1
265	C	78.01460	80.74479	74.20753	-519.76435	377.31045	459.42366	1
266	H	77.56561	79.92740	73.59873	-1746.74323	1667.50644	-1261.73691	1
267	C	77.35311	82.05892	73.81215	570.95554	16.46261	-545.27700	1
268	H	77.51582	82.29556	72.72909	2391.58273	28.05277	-1305.07271	1
269	H	76.24595	82.03292	73.98370	175.75588	917.63458	2559.43867	1
270	H	77.75973	82.91914	74.40386	-1063.97851	-2155.34650	1283.00462	1
271	C	79.50614	80.80428	73.90795	193.76014	2.62946	-765.53141	1
272	H	79.70272	81.03630	72.82939	507.39394	-846.55087	2539.60089	1
273	H	80.01757	81.59496	74.51534	1337.57841	1818.19054	1526.01994	1
274	H	80.01173	79.83037	74.13537	1100.88635	-1172.91350	-2199.08909	1
275	C	77.61594	78.55195	77.44847	-549.21115	475.64486	-309.38218	1
276	O	76.45527	78.65590	77.75275	556.06106	-390.37755	-78.24250	1
277	O	78.57773	78.13285	78.39079	-572.27940	-310.19032	-209.75862	1
278	H	79.39486	78.17573	77.81827	-1380.08193	2212.14486	790.85944	1

Listing 89: C00089.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.7727	3091
		0.2500	300.00	0.00	0.00	0.00	-1293.4702	0.0000	300.0000
3	H	79.87832	74.05051	80.38166	-2043.14101	-1757.64893	399.89339		1
4	N	80.77122	73.82749	79.94591	426.75047	490.45733	-334.42467		1
5	H	80.45720	73.28652	79.14176	442.25559	-1110.30854	-2448.52907		1
6	C	81.55764	74.96260	79.63522	415.32972	-666.39213	83.73172		1
7	H	80.98019	75.84915	79.97780	879.32219	2491.00447	667.35213		1
8	C	82.97750	74.81574	80.38938	31.35357	477.41777	628.23362		1
9	H	83.47163	73.87085	80.05943	1168.38489	2240.25337	-1019.71136		1
10	H	83.66525	75.64271	80.08964	-360.43770	2534.90498	931.67112		1
11	C	82.76718	74.80521	81.88045	463.18208	512.70242	-382.34388		1
12	H	81.92224	74.11700	82.10929	1725.29117	1863.52247	-987.07854		1
13	C	84.01498	74.28979	82.58711	710.42801	-144.27427	-313.15367		1
14	H	83.88121	74.26546	83.69939	364.20195	-1033.13725	2494.72524		1
15	H	84.27633	73.25007	82.26072	2567.61904	335.80679	847.48802		1
16	H	84.90495	74.93674	82.37462	-2587.99029	680.92867	-512.16411		1
17	C	82.42650	76.19527	82.40030	268.17616	741.64379	-40.42634		1
18	H	82.28405	76.19750	83.51188	1283.54314	-1945.37420	-1411.27812		1
19	H	83.23976	76.93114	82.16971	-1258.57796	1317.15249	-2026.02085		1
20	H	81.48273	76.59072	81.94418	-2502.84526	909.80597	575.92391		1
21	C	81.82033	74.93683	78.04007	619.36578	-458.64843	-172.09273		1
22	O	81.69744	75.96221	77.34804	-81.40433	433.87611	522.34594		1
23	N	82.18575	73.73265	77.68260	175.23996	-622.20190	341.55523		1

24	H	82.21372	73.02083	78.41040	-876.57256	-303.22879	-2561.90213	1
25	C	82.32072	73.41956	76.29567	-571.88214	-534.10783	-106.15033	1
26	H	82.79208	74.31865	75.83654	-2713.20841	-16.25800	-248.80809	1
27	C	83.15571	72.06113	76.16758	166.60354	288.16399	-716.09568	1
28	H	82.55241	71.23176	76.62906	-2097.85574	1636.78449	-586.18044	1
29	O	84.43406	72.04067	76.82382	-317.80580	-363.38227	484.43082	1
30	H	84.30946	71.30869	77.46165	1863.74748	-1451.84923	1357.29467	1
31	C	83.18166	71.88126	74.60425	503.80731	517.99032	318.51606	1
32	H	83.60944	70.89297	74.31665	640.61020	-2157.10410	-1536.29104	1
33	H	82.15799	71.94961	74.14344	1687.88455	465.60692	2087.56452	1
34	H	83.81135	72.66268	74.11913	-1293.07895	-1899.88581	-1463.57452	1
35	C	80.80977	73.12214	75.75033	-153.07550	-733.68902	248.70981	1
36	O	80.17196	72.21909	76.24009	186.15459	-480.78787	-449.34387	1
37	N	80.50331	73.94418	74.74895	-487.53139	543.18517	42.03850	1
38	C	79.31267	73.78723	73.95868	-699.35871	69.34393	360.10701	1
39	H	78.49339	73.50177	74.65274	2.81126	-221.99807	-2715.58072	1
40	C	79.15331	75.22746	73.30498	-507.46439	-592.59194	122.07761	1
41	H	78.56252	75.21369	72.36208	-1975.08116	525.87560	-1801.71556	1
42	H	78.62609	75.91828	73.99502	1588.27743	-1913.22100	1113.83566	1
43	C	80.63658	75.66235	73.09233	-613.62442	-457.55993	-194.14490	1
44	H	81.05720	75.19661	72.17296	1707.54637	-721.27992	1996.92523	1
45	H	80.76740	76.76191	72.97673	758.23357	2100.81767	1560.55011	1
46	C	81.33873	75.08424	74.39429	-352.41524	704.96076	49.21465	1
47	H	82.38320	74.71893	74.24081	1714.76886	-2070.42778	443.35792	1
48	H	81.31051	75.75074	75.29787	1224.15040	1801.50881	1636.97633	1
49	C	79.57469	72.67695	72.80464	566.85117	537.05831	117.62814	1
50	O	80.67791	72.13979	72.65429	-550.26779	-406.08867	4.21666	1
51	N	78.44731	72.45130	72.17895	566.34832	-425.77725	180.18749	1
52	H	77.67186	73.02167	72.51735	644.44502	2646.80550	-52.73430	1
53	C	78.36851	72.00355	70.81380	612.34801	-281.48662	411.56221	1
54	H	78.48947	72.94415	70.23529	1667.23498	-1490.75142	1556.16753	1
55	C	79.56135	70.99723	70.52136	-714.45746	-175.43074	286.98927	1
56	H	79.73146	70.42863	71.48047	-787.09484	1763.03619	-1922.46060	1
57	O	80.81037	71.62775	70.21721	-429.46514	516.51932	-128.40526	1
58	H	81.18581	71.71489	71.16936	1981.82785	436.16847	-1818.18182	1
59	C	79.05754	70.02148	69.39774	630.79189	-468.94448	76.03230	1
60	H	79.84511	69.28030	69.12585	-1775.71861	2062.30353	131.89849	1
61	H	78.15388	69.43996	69.71647	-1855.14608	88.94118	1993.53760	1
62	H	78.79246	70.57461	68.46678	-1504.82350	-780.94249	-2132.90992	1
63	C	76.84162	71.45022	70.69539	288.57638	618.62814	-397.00270	1
64	O	76.58284	70.24581	70.80282	321.70495	-185.26452	574.37218	1
65	N	76.04705	72.45827	70.43612	-447.05792	-446.53431	367.76425	1
66	H	76.52427	73.35797	70.37500	350.31316	1975.63644	-1843.31522	1
67	C	74.63129	72.43678	70.42164	-511.23061	374.03917	-471.51480	1
68	H	74.36406	73.41273	69.95775	2234.79579	-898.70890	-1273.45190	1
69	C	74.13792	71.18399	69.55872	529.53781	-159.34528	563.72604	1
70	H	73.10293	71.39807	69.16743	654.59388	2347.94251	1217.51488	1
71	H	74.82249	71.14823	68.66935	-1526.55661	2103.42026	817.87394	1
72	O	74.06368	69.91132	70.20855	-554.84278	14.12789	399.58769	1
73	H	75.05318	69.82654	70.50766	1297.06236	2061.84854	1220.68812	1
74	C	74.06100	72.32523	71.94593	-662.15484	-412.13544	123.62687	1
75	O	74.64684	71.77322	72.85121	-540.01537	-317.05804	274.91456	1
76	N	72.88255	72.93910	71.99506	-202.76299	-690.00100	-131.49145	1
77	H	72.45378	73.35085	71.16377	-702.62132	-2617.37191	281.70413	1
78	C	72.25122	72.97061	73.28090	-491.73914	576.34187	222.73509	1
79	H	72.42397	71.93523	73.65388	1977.17978	-1823.58850	-434.68928	1
80	C	72.89437	74.07547	74.22234	-649.50797	-328.66843	306.11224	1
81	H	72.62606	75.09152	73.85627	2075.07803	1452.16490	-1004.45904	1
82	C	72.30228	73.80918	75.64897	-615.18735	-489.99689	-70.96352	1
83	H	72.80595	74.46865	76.43044	-1226.32661	-1724.38906	-1716.47170	1
84	H	71.20444	74.01589	75.68218	2381.64273	-969.84735	900.46860	1
85	H	72.45400	72.74927	75.96800	2122.74991	1702.23946	-141.36228	1

86	C	74.44972	73.92288	74.35598	-501.86074	-479.61276	-376.42482	1
87	H	74.89423	74.70710	75.01247	993.79261	-2246.95401	-1177.81305	1
88	H	74.71561	72.92583	74.78618	42.71279	-626.15391	-2651.37258	1
89	H	74.95408	73.98246	73.36071	-2026.39012	-1590.33709	-887.82922	1
90	C	70.69264	73.45048	73.12725	-672.89153	382.57394	-156.34072	1
91	O	70.37719	74.52898	73.61525	410.04627	221.86223	500.35950	1
92	N	69.96730	72.54941	72.50840	-378.11782	-443.79414	-441.10984	1
93	H	70.50211	71.74964	72.16864	2404.15973	-568.14894	1149.30085	1
94	C	68.54912	72.56224	72.39548	-544.54484	466.16019	331.29119	1
95	H	68.30184	71.47783	72.38567	-1409.80988	-170.17955	2325.32679	1
96	C	67.90096	73.33411	73.61712	-184.48284	116.78282	-758.89137	1
97	H	68.13233	72.82496	74.58063	1893.78641	1861.14652	611.04528	1
98	H	68.33636	74.36014	73.71991	-2170.79665	-974.19311	1327.50117	1
99	C	66.36107	73.41022	73.36894	389.51668	672.81878	-138.49152	1
100	H	66.15297	73.63709	72.29948	510.64577	1933.03327	1851.02484	1
101	H	65.89191	72.41354	73.52106	-2302.30869	-1105.72939	-948.89774	1
102	C	65.65085	74.48931	74.26911	-559.93427	-126.34590	542.30857	1
103	O	64.46834	74.68031	74.14514	-670.36003	-111.83166	76.36448	1
104	N	66.47637	75.13270	75.12371	-216.06729	-537.07037	446.51379	1
105	H	67.48121	75.01181	75.29580	-1251.96487	1074.12894	-2168.52500	1
106	H	66.16426	75.86369	75.77237	-2451.83023	-720.73851	944.84612	1
107	C	68.11430	73.14829	70.92607	546.24052	-563.88337	-85.11809	1
108	O	67.42948	72.40170	70.27502	71.70702	-307.40463	606.69673	1
109	N	68.45378	74.41795	70.65457	479.90863	-504.50129	222.86849	1
110	C	68.72397	74.83331	69.31344	75.51268	-600.91904	506.73700	1
111	H	68.16244	74.11844	68.66772	-2033.61562	1795.30103	254.89480	1
112	C	68.17309	76.32393	69.34020	523.79067	517.99274	284.45581	1
113	H	68.53526	76.94717	68.49045	1599.61665	-1127.00911	1895.98173	1
114	H	67.06101	76.34924	69.30163	-1881.83093	1275.82488	-1501.55016	1
115	C	68.69758	76.79572	70.73163	-600.05639	-404.05026	316.64485	1
116	H	69.79116	77.00489	70.69844	-2597.05260	496.36221	657.73249	1
117	H	68.20705	77.72208	71.10715	-1666.24518	1294.38985	-1723.90591	1
118	C	68.37243	75.51462	71.61119	493.57570	-129.95376	-602.56394	1
119	H	69.13467	75.28635	72.42212	-1469.08415	-637.84797	2204.22581	1
120	H	67.34326	75.48594	72.04159	-1038.97840	1068.88701	-2280.71789	1
121	C	70.35064	74.72134	69.11977	188.88100	241.05089	-727.87821	1
122	O	70.97096	73.74716	69.47728	531.88613	-49.19943	427.07960	1
123	N	70.80092	75.79549	68.48699	708.14833	26.93417	-179.73509	1
124	H	70.16635	76.54615	68.21632	-2232.69501	-1179.09831	1023.94816	1
125	C	72.17967	75.84461	68.15010	-738.32412	259.92548	104.42456	1
126	H	72.67597	75.08030	68.79149	2028.89123	1260.02983	1311.33324	1
127	C	72.25292	75.50895	66.59613	-258.65678	-345.52513	661.28459	1
128	H	71.55062	76.15984	66.03178	-1826.06090	-1801.46097	-918.64554	1
129	C	73.72283	75.69897	66.09232	-541.23400	531.92970	-218.41428	1
130	H	73.82446	75.42638	65.01537	1311.73218	-2219.18200	882.19023	1
131	H	74.05280	76.75974	66.19876	-1048.71298	1223.58118	-2196.97971	1
132	H	74.43941	75.06579	66.66634	419.06414	1903.92898	1903.44670	1
133	C	71.87868	73.99838	66.41073	-423.86431	152.66566	-648.55262	1
134	H	71.76733	73.72675	65.33491	105.68386	-2342.50080	1387.51238	1
135	H	72.65477	73.32742	66.84793	-1695.63603	-1484.73621	-1531.02793	1
136	H	70.91521	73.75538	66.91855	-1853.57121	-487.39031	1936.59343	1
137	C	72.64066	77.40231	68.41402	539.71428	-510.58232	267.58633	1
138	O	72.35021	78.28344	67.64003	-15.93758	-278.34085	-624.49402	1
139	N	73.27119	77.48297	69.58194	-676.81886	12.05292	276.17960	1
140	H	73.42794	76.61849	70.09949	-1694.44250	-373.84189	-2100.66098	1
141	C	74.06233	78.66077	69.81530	412.33078	-664.70360	108.35451	1
142	H	74.64685	78.79081	68.87861	1765.77476	1294.44366	1621.76594	1
143	C	73.05233	79.85467	70.01883	-179.66635	-721.95667	-264.73915	1
144	H	72.33136	79.89709	69.16709	-607.34922	2587.87032	-598.10018	1
145	H	72.43348	79.70359	70.93251	-359.69332	-1479.13954	-2259.74260	1
146	C	73.88556	81.17692	70.11803	-240.01076	616.02425	431.85322	1
147	H	74.49819	81.18635	71.04835	-1359.17131	782.54425	2227.99181	1

148	H	74.60649	81.25721	69.27370	-820.36667	85.81767	-2596.78715	1
149	C	72.86134	82.38134	70.09308	-513.07015	236.18570	-551.87280	1
150	H	72.26862	82.37637	69.14917	1816.11944	-1183.11722	-1650.94321	1
151	H	72.11848	82.28531	70.91813	-1800.04429	-1361.53473	1526.34643	1
152	C	73.66217	83.69713	70.22888	726.08972	-253.19732	-179.64713	1
153	H	74.17442	83.82577	71.20322	1224.27271	-456.51798	-2390.90304	1
154	H	74.37015	83.89583	69.39960	1206.40339	-1150.93514	-2154.90344	1
155	N	72.63506	84.87781	70.16220	329.70796	-633.68968	-155.67358	1
156	H	73.04586	85.85043	70.26406	1348.31305	1938.76845	1359.00643	1
157	H	72.07376	84.98188	69.26720	2096.92035	1446.54551	-966.48890	1
158	H	71.87424	84.89543	70.90206	-1197.07217	-2303.53719	827.28733	1
159	C	74.99323	78.43321	71.14453	-378.01186	-556.17301	-413.96481	1
160	O	76.14181	78.81578	71.08338	-409.44433	-307.55053	-453.30833	1
161	N	74.34433	77.84264	72.13313	-429.02477	524.70884	274.08502	1
162	H	73.37334	77.60585	71.93338	1706.34263	-1425.96036	1574.38926	1
163	C	74.85370	77.69805	73.45807	-45.25864	-626.22952	478.93267	1
164	H	74.52666	76.68565	73.78197	1988.63164	570.90773	1772.87287	1
165	C	76.41420	77.92625	73.45551	551.77128	-20.49526	-564.54996	1
166	H	76.90244	77.33256	72.64741	1434.61535	-1753.10253	1513.99471	1
167	H	76.63403	78.99457	73.21058	-714.67738	1819.09770	1898.36494	1
168	C	76.99928	77.56330	74.86308	446.99263	-555.77305	338.97221	1
169	H	76.39775	78.01454	75.68317	1953.68466	1892.25957	-161.67766	1
170	H	76.97242	76.46508	75.03394	-403.03785	2688.07032	-188.43591	1
171	C	78.47528	78.12569	74.87675	567.86262	335.74681	434.04421	1
172	H	79.00489	77.88100	73.92783	-1080.02275	1568.26081	-1948.78900	1
173	H	78.47676	79.23821	74.93634	-919.54108	2111.34692	1456.13463	1
174	C	79.20865	77.49697	76.08966	195.81897	173.33862	-745.11536	1
175	H	78.82353	77.80803	77.08278	1405.67949	-2301.21089	-390.08113	1
176	H	79.28940	76.39086	76.05040	-940.37328	-1118.32446	2299.72133	1
177	N	80.67816	77.98061	76.04617	319.26422	656.36007	-42.02424	1
178	H	81.35035	77.39370	76.73140	1961.03633	619.91968	1787.09422	1
179	H	81.15567	77.92097	75.10205	854.14343	-2156.80752	1429.08711	1
180	H	80.85674	78.99484	76.29406	1237.02905	-1378.50857	-1998.28500	1
181	C	74.23666	78.88000	74.41685	532.53319	-268.57236	517.55729	1
182	O	74.22444	80.04667	74.10515	266.16714	-290.73804	-558.88002	1
183	N	73.97719	78.33187	75.60369	-226.25352	640.49678	-270.32839	1
184	H	74.05371	77.31968	75.69884	2007.69063	-1035.27229	1523.50231	1
185	C	73.18609	79.07536	76.52725	-540.76542	-573.33303	49.50000	1
186	H	73.34139	80.12785	76.19183	-2374.20950	-1036.76023	843.75774	1
187	C	71.66454	78.59292	76.41145	-77.09082	666.87422	-415.84136	1
188	H	71.56645	77.60994	76.94863	-985.81834	617.19825	2463.91927	1
189	O	71.14569	78.38445	75.08862	293.29899	-391.65602	-477.80926	1
190	H	70.94905	77.42511	75.10712	2528.72714	-681.76262	-751.27122	1
191	C	70.94882	79.72274	77.24085	252.47363	-605.14473	440.05134	1
192	H	69.86056	79.51424	77.35888	-2052.65063	1456.49051	-1043.51830	1
193	H	71.38065	79.82610	78.26520	-2152.98800	-1661.97574	-161.70652	1
194	H	71.04089	80.71414	76.73931	-473.12726	-1584.27339	2165.61725	1
195	C	73.74502	78.71854	78.02309	360.36307	488.46713	505.10056	1
196	O	72.97274	78.36666	78.91535	-200.08817	-528.03552	-385.82850	1
197	N	75.04334	78.91429	78.06544	-597.54095	-226.44775	355.20479	1
198	H	75.42426	79.21064	77.16648	2179.23655	-1300.70981	-991.33835	1
199	C	75.86471	78.74043	79.19805	-687.68921	297.39807	-249.45179	1
200	H	76.83471	79.19546	78.90215	-349.16256	-2467.37713	-1101.72831	1
201	C	75.18401	79.40628	80.48598	672.47345	361.54328	-201.62880	1
202	H	74.14073	79.02278	80.60471	1541.41502	582.18425	2169.97026	1
203	H	75.75080	79.09726	81.39437	-2534.67717	60.25153	997.72295	1
204	C	75.16217	80.93668	80.38189	574.26774	-389.43119	-377.02542	1
205	C	76.34064	81.68389	80.68253	688.82679	-287.33580	-257.96133	1
206	H	77.28357	81.17101	80.94532	331.14182	1470.38163	2269.80013	1
207	C	73.94726	81.60175	80.03393	-383.52382	-675.04808	144.24917	1
208	H	73.03887	81.02058	79.79118	4.09847	1517.59662	2262.86397	1
209	C	76.26789	83.07591	80.65467	-134.76730	428.45285	-649.50303	1

210	H	77.17469	83.65705	80.89693	-903.23433	1600.49020	2011.53387	1
211	C	73.92587	82.99834	80.02420	-335.53281	-615.00040	-364.39058	1
212	H	72.97880	83.50490	79.76837	1596.45398	-1369.33862	1732.02659	1
213	C	75.07335	83.78505	80.33615	585.48547	-340.24194	-406.23938	1
214	O	75.06204	85.20410	80.33451	-419.15649	-173.04408	-511.94141	1
215	H	74.11631	85.36304	80.10460	-1071.84350	1559.71507	-1960.13012	1
216	C	76.01937	77.15659	79.59210	291.41878	-183.13091	710.72246	1
217	O	77.10176	76.62921	79.63145	379.87695	523.47396	-222.23622	1
218	N	74.83333	76.66911	79.95802	564.30591	373.09380	277.24371	1
219	H	73.96437	77.22616	79.76373	-120.59931	-2436.07824	-1214.35098	1
220	C	74.75519	75.25206	80.15657	404.07514	-299.37480	608.84009	1
221	H	75.70401	74.93938	80.64980	-1071.07882	-841.69025	2359.66467	1
222	C	73.43249	75.04904	81.00614	-683.12807	68.71770	-390.13096	1
223	H	73.45071	75.70019	81.90881	2068.88918	1596.58590	770.89603	1
224	H	72.55338	75.39095	80.41435	1379.86429	2342.49779	-179.85638	1
225	C	73.26003	73.55517	81.41701	-176.39967	537.49466	550.97268	1
226	H	73.30388	72.88094	80.53182	-396.28051	1942.22168	1869.33314	1
227	H	74.07545	73.22060	82.09616	-94.44700	586.00678	-2659.20016	1
228	C	71.83061	73.48966	82.13135	-291.69381	-718.18079	-150.72929	1
229	H	71.69701	74.17512	83.00652	-2303.38776	1089.76242	964.62032	1
230	H	70.95595	73.64364	81.44914	884.16729	2568.80533	-207.74283	1
231	N	71.75512	72.17831	82.61784	-594.49522	-252.81478	342.29276	1
232	H	72.50421	71.55509	82.36023	-1735.17426	2084.05705	-263.71605	1
233	C	70.81191	71.73451	83.34525	595.23177	-271.52487	442.22352	1
234	N	69.77766	72.61537	83.68304	585.53813	-424.79750	-105.81303	1
235	H	69.64482	73.59084	83.41990	959.88797	1327.56823	-2177.11905	1
236	H	68.96726	72.37173	84.25313	1578.48647	16.27378	-2220.76233	1
237	N	71.01481	70.38689	83.67516	-452.17763	-390.33541	-421.51853	1
238	H	71.76758	69.74488	83.43186	470.26107	1974.25629	-1817.92087	1
239	H	70.36728	69.85228	84.25551	1856.67307	-1573.97321	-1224.35416	1
240	C	74.53980	74.58516	78.68867	-531.47271	-581.45780	-55.06206	1
241	O	73.86743	75.11978	77.82648	-243.00837	192.73507	609.52485	1
242	N	75.07866	73.36880	78.66543	343.49288	-644.25607	38.09164	1
243	H	75.60130	73.12015	79.50519	-1691.16043	-1535.97525	-1484.73099	1
244	C	75.35202	72.71966	77.38360	542.66492	350.14337	454.42563	1
245	H	74.73737	73.33771	76.69019	1209.57979	-2396.95920	463.86744	1
246	C	76.84419	72.79193	77.10947	-737.14309	145.93010	242.71942	1
247	H	77.37681	72.34861	77.98117	-1050.18303	159.36419	-2509.06125	1
248	C	77.21618	71.99505	75.87541	-706.77696	-252.88343	-245.16230	1
249	H	78.35861	71.93245	75.77304	-1624.64039	-1665.49085	1417.86935	1
250	H	76.83121	70.94096	75.92246	2566.10521	598.51109	693.22305	1
251	H	76.80456	72.45070	74.93305	-1972.69758	107.10018	-1876.34312	1
252	C	77.34619	74.21916	76.98287	412.85148	672.58832	-27.69222	1
253	H	78.46180	74.25330	76.83516	1447.02277	1762.76533	-1490.78944	1
254	H	76.87650	74.74592	76.10902	1320.77379	-145.20455	2378.68491	1
255	H	77.11092	74.82642	77.90219	-1512.10848	1470.52031	1724.75147	1
256	C	74.78791	71.15760	77.51428	-607.11113	499.56689	73.73769	1
257	O	73.62179	70.93815	77.30042	357.97126	460.81534	356.68785	1
258	N	75.74369	70.30723	77.85226	536.55407	-368.62270	332.76306	1
259	H	76.68688	70.64326	78.03602	524.38866	2297.69985	1367.20941	1
260	C	75.43659	68.93727	78.01272	46.50277	-774.29190	-147.97904	1
261	H	74.32446	68.87724	77.99696	1676.51875	1883.29066	1032.55549	1
262	C	76.14490	68.08829	76.83089	-559.41456	-34.19198	-556.30433	1
263	H	77.24862	68.24238	76.88620	-64.66664	395.18769	2695.05373	1
264	H	75.98185	66.99600	76.99049	-2703.44278	-60.40056	333.79418	1
265	C	75.62830	68.51228	75.48438	-519.76435	377.31045	459.42366	1
266	H	75.70770	69.61975	75.40416	-1746.74323	1667.50644	-1261.73691	1
267	C	76.46434	67.88918	74.37273	570.95554	16.46261	-545.27700	1
268	H	76.12782	68.23515	73.36057	2391.58273	28.05277	-1305.07271	1
269	H	77.54818	68.15647	74.46931	175.75588	917.63458	2559.43867	1
270	H	76.39633	66.77071	74.38194	-1063.97851	-2155.34650	1283.00462	1
271	C	74.16547	68.13257	75.29655	193.76014	2.62946	-765.53141	1

272	H	73.80087	68.40389	74.27163	507.39394	-846.55087	2539.60089	1
273	H	74.00135	67.03194	75.42920	1337.57841	1818.19054	1526.01994	1
274	H	73.50633	68.66315	76.03187	1100.88635	-1172.91350	-2199.08909	1
275	C	76.14647	68.47561	79.38910	-549.21115	475.64486	-309.38218	1
276	O	77.06401	69.07113	79.89018	556.06106	-390.37755	-78.24250	1
277	O	75.70547	67.24424	79.92756	-572.27940	-310.19032	-209.75862	1
278	H	74.98461	67.03814	79.26952	-1380.08193	2212.14486	790.85944	1

Listing 90: C00090.xmolout

1	276								
2	initial	150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	
		11100	0.2500	300.00	0.00	0.00	0.00	300.0000	
3	H	69.32652	74.40636	89.18194	-2043.14101	-1757.64893	399.89339	1	
4	N	70.12955	74.05564	88.66396	426.75047	490.45733	-334.42467	1	
5	H	70.43287	73.27324	89.23954	442.25559	-1110.30854	-2448.52907	1	
6	C	71.13063	75.00978	88.38794	415.32972	-666.39213	83.73172	1	
7	H	70.56368	75.92154	88.10589	879.32219	2491.00447	667.35213	1	
8	C	72.08706	75.19630	89.66629	31.35357	477.41777	628.23362	1	
9	H	72.57367	74.21849	89.90053	1168.38489	2240.25337	-1019.71136	1	
10	H	72.92031	75.89400	89.40945	-360.43770	2534.90498	931.67112	1	
11	C	71.32217	75.70394	90.86475	463.18208	512.70242	-382.34388	1	
12	H	70.47032	75.01619	91.06304	1725.29117	1863.52247	-987.07854	1	
13	C	72.22664	75.71611	92.09055	710.42801	-144.27427	-313.15367	1	
14	H	71.68364	76.07380	93.00325	364.20195	-1033.13725	2494.72524	1	
15	H	72.62760	74.69491	92.32005	2567.61904	335.80679	847.48802	1	
16	H	73.10856	76.39202	91.94376	-2587.99029	680.92867	-512.16411	1	
17	C	70.77270	77.10192	90.61977	268.17616	741.64379	-40.42634	1	
18	H	70.24621	77.50319	91.52424	1283.54314	-1945.37420	-1411.27812	1	
19	H	71.58917	77.82571	90.36317	-1258.57796	1317.15249	-2026.02085	1	
20	H	70.03728	77.11778	89.77449	-2502.84526	909.80597	575.92391	1	
21	C	72.06404	74.39981	87.18668	619.36578	-458.64843	-172.09273	1	
22	O	73.13075	73.88938	87.44062	-81.40433	433.87611	522.34594	1	
23	N	71.44834	74.54427	86.01834	175.23996	-622.20190	341.55523	1	
24	H	70.56084	75.04659	86.01584	-876.57256	-303.22879	-2561.90213	1	
25	C	72.05736	74.13063	84.80112	-571.88214	-534.10783	-106.15033	1	
26	H	71.29355	74.38804	84.03313	-2713.20841	-16.25800	-248.80809	1	
27	C	73.35218	75.07661	84.68093	166.60354	288.16399	-716.09568	1	
28	H	74.00547	74.86975	85.57387	-2097.85574	1636.78449	-586.18044	1	
29	O	73.04471	76.48342	84.71360	-317.80580	-363.38227	484.43082	1	
30	H	73.46854	76.74254	85.55570	1863.74748	-1451.84923	1357.29467	1	
31	C	74.10680	74.61906	83.38264	503.80731	517.99032	318.51606	1	
32	H	74.96397	75.29642	83.15743	640.61020	-2157.10410	-1536.29104	1	
33	H	74.53014	73.58209	83.48134	1687.88455	465.60692	2087.56452	1	
34	H	73.43480	74.63056	82.49269	-1293.07895	-1899.88581	-1463.57452	1	
35	C	72.35799	72.53995	84.84780	-153.07550	-733.68902	248.70981	1	
36	O	73.37944	72.16000	84.31563	186.15459	-480.78787	-449.34387	1	
37	N	71.37421	71.78754	85.36061	-487.53139	543.18517	42.03850	1	
38	C	71.57801	70.39753	85.61901	-699.35871	69.34393	360.10701	1	
39	H	72.65072	70.27355	85.88910	2.81126	-221.99807	-2715.58072	1	
40	C	70.52844	70.15271	86.78099	-507.46439	-592.59194	122.07761	1	
41	H	70.28294	69.07696	86.92625	-1975.08116	525.87560	-1801.71556	1	
42	H	70.90785	70.53138	87.75670	1588.27743	-1913.22100	1113.83566	1	
43	C	69.31639	71.00086	86.28296	-613.62442	-457.55993	-194.14490	1	
44	H	68.77633	70.48205	85.45574	1707.54637	-721.27992	1996.92523	1	
45	H	68.56381	71.21910	87.07435	758.23357	2100.81767	1560.55011	1	
46	C	70.06737	72.29795	85.75928	-352.41524	704.96076	49.21465	1	
47	H	69.60574	72.79938	84.87619	1714.76886	-2070.42778	443.35792	1	
48	H	70.27266	73.05649	86.55054	1224.15040	1801.50881	1636.97633	1	
49	C	71.15566	69.54628	84.26833	566.85117	537.05831	117.62814	1	
50	O	70.02809	69.60263	83.84025	-550.26779	-406.08867	4.21666	1	
51	N	72.18283	68.81464	83.87224	566.34832	-425.77725	180.18749	1	

52	H	73.04212	68.90403	84.41314	644.44502	2646.80550	-52.73430	1
53	C	72.18015	68.05866	82.67055	612.34801	-281.48662	411.56221	1
54	H	73.16200	67.53850	82.73070	1667.23498	-1490.75142	1556.16753	1
55	C	70.94302	67.04945	82.68678	-714.45746	-175.43074	286.98927	1
56	H	69.99293	67.65326	82.68694	-787.09484	1763.03619	-1922.46060	1
57	O	70.88210	66.17378	83.82938	-429.46514	516.51932	-128.40526	1
58	H	70.05156	66.47311	84.24882	1981.82785	436.16847	-1818.18182	1
59	C	71.10035	66.31523	81.30444	630.79189	-468.94448	76.03230	1
60	H	70.27980	65.57863	81.14141	-1775.71861	2062.30353	131.89849	1
61	H	71.07650	67.03203	80.44435	-1855.14608	88.94118	1993.53760	1
62	H	72.06225	65.75479	81.24673	-1504.82350	-780.94249	-2132.90992	1
63	C	72.12754	69.10889	81.41292	288.57638	618.62814	-397.00270	1
64	O	71.23685	69.13221	80.59384	321.70495	-185.26452	574.37218	1
65	N	73.28256	69.77596	81.38758	-447.05792	-446.53431	367.76425	1
66	H	73.88138	69.64993	82.20328	350.31316	1975.63644	-1843.31522	1
67	C	73.28588	71.02487	80.65300	-511.23061	374.03917	-471.51480	1
68	H	72.25359	71.42293	80.79030	2234.79579	-898.70890	-1273.45190	1
69	C	74.42340	71.93707	81.33499	529.53781	-159.34528	563.72604	1
70	H	74.26167	72.98461	80.96789	654.59388	2347.94251	1217.51488	1
71	H	74.18441	71.93043	82.44334	-1526.55661	2103.42026	817.87394	1
72	O	75.78776	71.50550	81.14133	-554.84278	14.12789	399.58769	1
73	H	76.00653	72.00421	80.32921	1297.06236	2061.84854	1220.68812	1
74	C	73.62827	70.82094	79.12074	-662.15484	-412.13544	123.62687	1
75	O	73.54958	71.88277	78.31639	-540.01537	-317.05804	274.91456	1
76	N	73.99563	69.62767	78.83748	-202.76299	-690.00100	-131.49145	1
77	H	74.02213	69.12529	79.74313	-702.62132	-2617.37191	281.70413	1
78	C	73.80224	68.85737	77.65446	-491.73914	576.34187	222.73509	1
79	H	73.45126	67.88554	78.06577	1977.17978	-1823.58850	-434.68928	1
80	C	72.69096	69.48751	76.70917	-649.50797	-328.66843	306.11224	1
81	H	72.71856	70.60248	76.71169	2075.07803	1452.16490	-1004.45904	1
82	C	72.93198	68.92752	75.26416	-615.18735	-489.99689	-70.96352	1
83	H	72.09975	69.18803	74.56835	-1226.32661	-1724.38906	-1716.47170	1
84	H	73.87920	69.32859	74.82589	2381.64273	-969.84735	900.46860	1
85	H	73.03969	67.81584	75.27364	2122.74991	1702.23946	-141.36228	1
86	C	71.30648	68.98716	77.24957	-501.86074	-479.61276	-376.42482	1
87	H	70.45910	69.41672	76.66531	993.79261	-2246.95401	-1177.81305	1
88	H	71.22028	67.87697	77.19204	42.71279	-626.15391	-2651.37258	1
89	H	71.15910	69.27780	78.32139	-2026.39012	-1590.33709	-887.82922	1
90	C	75.22751	68.57820	76.91752	-672.89153	382.57394	-156.34072	1
91	O	75.24587	67.86839	75.93212	410.04627	221.86223	500.35950	1
92	N	76.25368	69.13152	77.55416	-378.11782	-443.79414	-441.10984	1
93	H	76.02212	69.67493	78.38640	2404.15973	-568.14894	1149.30085	1
94	C	77.54034	69.18005	76.96990	-544.54484	466.16019	331.29119	1
95	H	78.18599	69.59919	77.77314	-1409.80988	-170.17955	2325.32679	1
96	C	77.89684	67.69897	76.55619	-184.48284	116.78282	-758.89137	1
97	H	77.58225	66.98427	77.35093	1893.78641	1861.14652	611.04528	1
98	H	77.32628	67.40699	75.63828	-2170.79665	-974.19311	1327.50117	1
99	C	79.43745	67.62806	76.30907	389.51668	672.81878	-138.49152	1
100	H	79.72663	68.36493	75.51608	510.64577	1933.03327	1851.02484	1
101	H	79.99134	67.96594	77.21310	-2302.30869	-1105.72939	-948.89774	1
102	C	79.91755	66.18228	75.90893	-559.93427	-126.34590	542.30857	1
103	O	81.09215	65.96801	75.75452	-670.36003	-111.83166	76.36448	1
104	N	78.91530	65.28637	75.77444	-216.06729	-537.07037	446.51379	1
105	H	77.90035	65.41827	75.85712	-1251.96487	1074.12894	-2168.52500	1
106	H	79.05430	64.31204	75.48639	-2451.83023	-720.73851	944.84612	1
107	C	77.60608	70.09070	75.57924	546.24052	-563.88337	-85.11809	1
108	O	78.58011	70.00097	74.84446	71.70702	-307.40463	606.69673	1
109	N	76.52206	70.81629	75.49964	479.90863	-504.50129	222.86849	1
110	C	76.57071	71.94815	74.73133	75.51268	-600.91904	506.73700	1
111	H	77.18094	71.66513	73.83357	-2033.61562	1795.30103	254.89480	1
112	C	75.03359	72.31133	74.44996	523.79067	517.99274	284.45581	1
113	H	74.94452	73.11960	73.69448	1599.61665	-1127.00911	1895.98173	1

114	H	74.51868	71.43180	74.00936	-1881.83093	1275.82488	-1501.55016	1
115	C	74.32289	72.73433	75.79419	-600.05639	-404.05026	316.64485	1
116	H	74.68411	73.73838	76.12029	-2597.05260	496.36221	657.73249	1
117	H	73.22587	72.83642	75.61741	-1666.24518	1294.38985	-1723.90591	1
118	C	74.56132	71.72106	76.91596	493.57570	-129.95376	-602.56394	1
119	H	75.59507	71.76629	77.30998	-1469.08415	-637.84797	2204.22581	1
120	H	74.40870	70.68099	76.57339	-1038.97840	1068.88701	-2280.71789	1
121	C	77.33504	73.14036	75.62762	188.88100	241.05089	-727.87821	1
122	O	77.99070	72.87678	76.61164	531.88613	-49.19943	427.07960	1
123	N	77.13872	74.30047	75.03551	708.14833	26.93417	-179.73509	1
124	H	76.53716	74.19247	74.22202	-2232.69501	-1179.09831	1023.94816	1
125	C	77.65541	75.59057	75.45101	-738.32412	259.92548	104.42456	1
126	H	76.87161	76.31337	75.11848	2028.89123	1260.02983	1311.33324	1
127	C	77.88745	75.61587	76.95305	-258.65678	-345.52513	661.28459	1
128	H	78.52420	74.72930	77.21975	-1826.06090	-1801.46097	-918.64554	1
129	C	78.61980	76.87009	77.39035	-541.23400	531.92970	-218.41428	1
130	H	78.81856	76.87306	78.49765	1311.73218	-2219.18200	882.19023	1
131	H	79.61460	76.96966	76.86937	-1048.71298	1223.58118	-2196.97971	1
132	H	78.03014	77.79788	77.15320	419.06414	1903.92898	1903.44670	1
133	C	76.58720	75.48218	77.72508	-423.86431	152.66566	-648.55262	1
134	H	76.75435	75.53416	78.83582	105.68386	-2342.50080	1387.51238	1
135	H	75.85920	76.29640	77.45799	-1695.63603	-1484.73621	-1531.02793	1
136	H	76.08505	74.49922	77.51044	-1853.57121	-487.39031	1936.59343	1
137	C	79.06971	75.86797	74.60699	539.71428	-510.58232	267.58633	1
138	O	79.53037	76.98474	74.58511	-15.93758	-278.34085	-624.49402	1
139	N	79.56378	74.77055	74.06338	-676.81886	12.05292	276.17960	1
140	H	79.02051	73.91987	74.19048	-1694.44250	-373.84189	-2100.66098	1
141	C	80.68249	74.87709	73.18673	412.33078	-664.70360	108.35451	1
142	H	81.12193	75.88724	73.36553	1765.77476	1294.44366	1621.76594	1
143	C	81.61940	73.65177	73.56021	-179.66635	-721.95667	-264.73915	1
144	H	81.83986	73.65139	74.65102	-607.34922	2587.87032	-598.10018	1
145	H	81.09778	72.68816	73.36363	-359.69332	-1479.13954	-2259.74260	1
146	C	82.93765	73.75292	72.72689	-240.01076	616.02425	431.85322	1
147	H	82.72023	73.71497	71.63560	-1359.17131	782.54425	2227.99181	1
148	H	83.44909	74.72504	72.90621	-820.36667	85.81767	-2596.78715	1
149	C	83.85859	72.54261	73.16503	-513.07015	236.18570	-551.87280	1
150	H	84.06827	72.58271	74.25860	1816.11944	-1183.11722	-1650.94321	1
151	H	83.34141	71.57061	72.99355	-1800.04429	-1361.53473	1526.34643	1
152	C	85.17366	72.61223	72.35570	726.08972	-253.19732	-179.64713	1
153	H	85.05395	72.45785	71.26484	1224.27271	-456.51798	-2390.90304	1
154	H	85.78645	73.51600	72.54524	1206.40339	-1150.93514	-2154.90344	1
155	N	86.07344	71.41993	72.82917	329.70796	-633.68968	-155.67358	1
156	H	87.01458	71.33410	72.34751	1348.31305	1938.76845	1359.00643	1
157	H	86.36082	71.40916	73.85085	2096.92035	1446.54551	-966.48890	1
158	H	85.68320	70.44108	72.70211	-1197.07217	-2303.53719	827.28733	1
159	C	80.16597	74.63044	71.65601	-378.01186	-556.17301	-413.96481	1
160	O	79.26832	73.81515	71.40696	-409.44433	-307.55053	-453.30833	1
161	N	80.86498	75.37507	70.84291	-429.02477	524.70884	274.08502	1
162	H	81.58186	75.93615	71.30048	1706.34263	-1425.96036	1574.38926	1
163	C	80.73581	75.35212	69.42829	-45.25864	-626.22952	478.93267	1
164	H	81.76739	75.58021	69.07942	1988.63164	570.90773	1772.87287	1
165	C	80.21380	73.93420	68.96739	551.77128	-20.49526	-564.54996	1
166	H	80.73911	73.12409	69.52260	1434.61535	-1753.10253	1513.99471	1
167	H	79.13372	73.82168	69.23331	-714.67738	1819.09770	1898.36494	1
168	C	80.40615	73.78323	67.42067	446.99263	-555.77305	338.97221	1
169	H	79.90476	74.62433	66.88338	1953.68466	1892.25957	-161.67766	1
170	H	81.48152	73.83362	67.13793	-403.03785	2688.07032	-188.43591	1
171	C	79.77047	72.39566	67.00722	567.86262	335.74681	434.04421	1
172	H	80.35247	71.54699	67.43486	-1080.02275	1568.26081	-1948.78900	1
173	H	78.74078	72.29488	67.42178	-919.54108	2111.34692	1456.13463	1
174	C	79.73758	72.32736	65.46276	195.81897	173.33862	-745.11536	1
175	H	79.06841	73.07052	64.98471	1405.67949	-2301.21089	-390.08113	1

176	H	80.73291	72.34578	64.97590	-940.37328	-1118.32446	2299.72133	1
177	N	79.12625	70.94000	65.06989	319.26422	656.36007	-42.02424	1
178	H	79.00582	70.76874	64.03001	1961.03633	619.91968	1787.09422	1
179	H	79.66374	70.07305	65.36343	854.14343	-2156.80752	1429.08711	1
180	H	78.15113	70.72629	65.43068	1237.02905	-1378.50857	-1998.28500	1
181	C	79.68455	76.49298	68.87433	532.53319	-268.57236	517.55729	1
182	O	79.62481	76.64484	67.67081	266.16714	-290.73804	-558.88002	1
183	N	79.03072	77.11699	69.83493	-226.25352	640.49678	-270.32839	1
184	H	79.29231	76.80089	70.76790	2007.69063	-1035.27229	1523.50231	1
185	C	78.15052	78.21604	69.66163	-540.76542	-573.33303	49.50000	1
186	H	78.25316	78.80094	70.60166	-2374.20950	-1036.76023	843.75774	1
187	C	78.53155	79.02995	68.34438	-77.09082	666.87422	-415.84136	1
188	H	78.40396	78.33400	67.46146	-985.81834	617.19825	2463.91927	1
189	O	79.89166	79.51780	68.29614	293.29899	-391.65602	-477.80926	1
190	H	80.29731	78.82318	67.73319	2528.72714	-681.76262	-751.27122	1
191	C	77.41801	80.13893	68.27097	252.47363	-605.14473	440.05134	1
192	H	77.50801	80.74438	67.33911	-2052.65063	1456.49051	-1043.51830	1
193	H	76.38951	79.70485	68.28037	-2152.98800	-1661.97574	-161.70652	1
194	H	77.48628	80.84552	69.13014	-473.12726	-1584.27339	2165.61725	1
195	C	76.62231	77.65755	69.45319	360.36307	488.46713	505.10056	1
196	O	76.32912	76.79263	68.66337	-200.08817	-528.03552	-385.82850	1
197	N	75.81808	78.42821	70.18220	-597.54095	-226.44775	355.20479	1
198	H	76.20309	79.14704	70.79373	2179.23655	-1300.70981	-991.33835	1
199	C	74.43540	78.14453	70.17114	-687.68921	297.39807	-249.45179	1
200	H	74.26725	77.42796	69.33386	-349.16256	-2467.37713	-1101.72831	1
201	C	74.04595	77.56019	71.61707	672.47345	361.54328	-201.62880	1
202	H	74.37343	78.26566	72.41424	1541.41502	582.18425	2169.97026	1
203	H	72.94195	77.44348	71.70718	-2534.67717	60.25153	997.72295	1
204	C	74.75972	76.21020	71.74563	574.26774	-389.43119	-377.02542	1
205	C	74.13577	75.00006	71.32089	688.82679	-287.33580	-257.96133	1
206	H	73.09002	74.99855	70.96481	331.14182	1470.38163	2269.80013	1
207	C	76.11071	76.19827	72.20234	-383.52382	-675.04808	144.24917	1
208	H	76.60845	77.12938	72.52887	4.09847	1517.59662	2262.86397	1
209	C	74.88495	73.82537	71.33608	-134.76730	428.45285	-649.50303	1
210	H	74.39951	72.89457	70.99487	-903.23433	1600.49020	2011.53387	1
211	C	76.80272	74.99017	72.18294	-335.53281	-615.00040	-364.39058	1
212	H	77.85160	75.00846	72.53476	1596.45398	-1369.33862	1732.02659	1
213	C	76.23995	73.76074	71.75104	585.48547	-340.24194	-406.23938	1
214	O	76.95706	72.56281	71.74494	-419.15649	-173.04408	-511.94141	1
215	H	77.93280	72.92992	71.60271	-1071.84350	1559.71507	-1960.13012	1
216	C	73.62437	79.56971	70.08028	291.41878	-183.13091	710.72246	1
217	O	73.77704	80.45310	70.89275	379.87695	523.47396	-222.23622	1
218	N	72.74348	79.47927	69.09218	564.30591	373.09380	277.24371	1
219	H	72.75265	78.64517	68.50646	-120.59931	-2436.07824	-1214.35098	1
220	C	71.99221	80.63107	68.71888	404.07514	-299.37480	608.84009	1
221	H	71.22450	80.20956	68.03195	-1071.07882	-841.69025	2359.66467	1
222	C	71.39254	81.19591	70.07687	-683.12807	68.71770	-390.13096	1
223	H	71.23838	80.34643	70.78002	2068.88918	1596.58590	770.89603	1
224	H	72.12435	81.86609	70.58764	1379.86429	2342.49779	-179.85638	1
225	C	70.04010	81.93608	69.83616	-176.39967	537.49466	550.97268	1
226	H	70.19590	82.95707	69.42025	-396.28051	1942.22168	1869.33314	1
227	H	69.41408	81.39950	69.08922	-94.44700	586.00678	-2659.20016	1
228	C	69.30141	81.99782	71.25209	-291.69381	-718.18079	-150.72929	1
229	H	68.95619	81.01592	71.66504	-2303.38776	1089.76242	964.62032	1
230	H	69.86352	82.52923	72.06179	884.16729	2568.80533	-207.74283	1
231	N	68.16597	82.76467	70.95231	-594.49522	-252.81478	342.29276	1
232	H	68.11337	83.15124	70.02263	-1735.17426	2084.05705	-263.71605	1
233	C	67.21941	83.00854	71.76547	595.23177	-271.52487	442.22352	1
234	N	67.30898	82.46802	73.05297	585.53813	-424.79750	-105.81303	1
235	H	68.03960	81.88676	73.46132	959.88797	1327.56823	-2177.11905	1
236	H	66.61347	82.59407	73.78882	1578.48647	16.27378	-2220.76233	1
237	N	66.23876	83.81217	71.16615	-452.17763	-390.33541	-421.51853	1

238	H	66.17686	84.20327	70.22753	470.26107	1974.25629	-1817.92087	1
239	H	65.39720	84.12175	71.65334	1856.67307	-1573.97321	-1224.35416	1
240	C	73.00950	81.63835	67.93515	-531.47271	-581.45780	-55.06206	1
241	O	73.99283	81.25519	67.34701	-243.00837	192.73507	609.52485	1
242	N	72.47911	82.86529	67.92376	343.49288	-644.25607	38.09164	1
243	H	71.62853	82.96044	68.47661	-1691.16043	-1535.97525	-1484.73099	1
244	C	73.22163	84.04539	67.49082	542.66492	350.14337	454.42563	1
245	H	72.56949	84.89295	67.81150	1209.57979	-2396.95920	463.86744	1
246	C	74.56925	84.05677	68.19173	-737.14309	145.93010	242.71942	1
247	H	75.14187	83.17095	67.82812	-1050.18303	159.36419	-2509.06125	1
248	C	75.35829	85.31102	67.86683	-706.77696	-252.88343	-245.16230	1
249	H	76.37702	85.30043	68.34290	-1624.64039	-1665.49085	1417.86935	1
250	H	75.50353	85.42791	66.75016	2566.10521	598.51109	693.22305	1
251	H	74.83141	86.23620	68.22939	-1972.69758	107.10018	-1876.34312	1
252	C	74.42607	83.91937	69.69736	412.85148	672.58832	-27.69222	1
253	H	75.42325	83.93791	70.21564	1447.02277	1762.76533	-1490.78944	1
254	H	73.80855	84.75257	70.13193	1320.77379	-145.20455	2378.68491	1
255	H	73.92429	82.95188	69.97570	-1512.10848	1470.52031	1724.75147	1
256	C	73.38979	83.99515	65.83926	-607.11113	499.56689	73.73769	1
257	O	74.19743	84.70864	65.28653	357.97126	460.81534	356.68785	1
258	N	72.53338	83.15228	65.28493	536.55407	-368.62270	332.76306	1
259	H	71.93247	82.64206	65.92906	524.38866	2297.69985	1367.20941	1
260	C	72.30314	83.19334	63.88999	46.50277	-774.29190	-147.97904	1
261	H	72.90827	84.05088	63.51674	1676.51875	1883.29066	1032.55549	1
262	C	72.72769	81.77471	63.24243	-559.41456	-34.19198	-556.30433	1
263	H	72.02895	80.98171	63.60053	-64.66664	395.18769	2695.05373	1
264	H	72.61182	81.80481	62.13273	-2703.44278	-60.40056	333.79418	1
265	C	74.14175	81.43691	63.63213	-519.76435	377.31045	459.42366	1
266	H	74.21022	81.44920	64.74517	-1746.74323	1667.50644	-1261.73691	1
267	C	74.50504	80.04277	63.13661	570.95554	16.46261	-545.27700	1
268	H	75.55055	79.75999	63.42382	2391.58273	28.05277	-1305.07271	1
269	H	73.82206	79.26259	63.56171	175.75588	917.63458	2559.43867	1
270	H	74.43632	79.97016	62.02045	-1063.97851	-2155.34650	1283.00462	1
271	C	75.12708	82.45762	63.08075	193.76014	2.62946	-765.53141	1
272	H	76.18787	82.16791	63.29677	507.39394	-846.55087	2539.60089	1
273	H	75.03251	82.56647	61.96910	1337.57841	1818.19054	1526.01994	1
274	H	74.96162	83.47232	63.53618	1100.88635	-1172.91350	-2199.08909	1
275	C	70.70629	83.33060	63.69524	-549.21115	475.64486	-309.38218	1
276	O	69.90781	83.01895	64.53937	556.06106	-390.37755	-78.24250	1
277	O	70.27810	83.72575	62.40595	-572.27940	-310.19032	-209.75862	1
278	H	71.17015	83.88722	61.98996	-1380.08193	2212.14486	790.85944	1

Listing 91: C00091.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.4661	0.0000	300.0000
3	H	84.93286	63.36514	74.49521	-2043.14101	-1757.64893	399.89339		1
4	N	84.70924	63.90716	73.66273	426.75047	490.45733	-334.42467		1
5	H	84.50274	63.18082	72.98041	442.25559	-1110.30854	-2448.52907		1
6	C	85.70254	64.82517	73.25887	415.32972	-666.39213	83.73172		1
7	H	86.05124	65.27355	74.21280	879.32219	2491.00447	667.35213		1
8	C	86.85733	64.05853	72.44592	31.35357	477.41777	628.23362		1
9	H	86.43280	63.68127	71.48418	1168.38489	2240.25337	-1019.71136		1
10	H	87.65858	64.78125	72.15864	-360.43770	2534.90498	931.67112		1
11	C	87.43229	62.91606	73.24716	463.18208	512.70242	-382.34388		1
12	H	86.59845	62.25180	73.56597	1725.29117	1863.52247	-987.07854		1
13	C	88.39062	62.09832	72.39061	710.42801	-144.27427	-313.15367		1
14	H	88.80368	61.22182	72.95385	364.20195	-1033.13725	2494.72524		1
15	H	87.88755	61.69681	71.47315	2567.61904	335.80679	847.48802		1
16	H	89.26332	62.71221	72.04805	-2587.99029	680.92867	-512.16411		1
17	C	88.15809	63.41341	74.48920	268.17616	741.64379	-40.42634		1

18	H	88.59476	62.56610	75.07893	1283.54314	-1945.37420	-1411.27812	1
19	H	89.00168	64.10241	74.22530	-1258.57796	1317.15249	-2026.02085	1
20	H	87.47264	63.97507	75.17477	-2502.84526	909.80597	575.92391	1
21	C	84.95735	65.88841	72.25326	619.36578	-458.64843	-172.09273	1
22	O	84.98209	65.74775	71.05288	-81.40433	433.87611	522.34594	1
23	N	84.33373	66.80474	72.98782	175.23996	-622.20190	341.55523	1
24	H	84.48507	66.76524	73.99583	-876.57256	-303.22879	-2561.90213	1
25	C	83.66699	67.91513	72.40175	-571.88214	-534.10783	-106.15033	1
26	H	83.34995	68.50977	73.28796	-2713.20841	-16.25800	-248.80809	1
27	C	84.79394	68.66961	71.54352	166.60354	288.16399	-716.09568	1
28	H	85.05168	67.99858	70.67638	-2097.85574	1636.78449	-586.18044	1
29	O	86.02392	68.92334	72.24900	-317.80580	-363.38227	484.43082	1
30	H	86.63928	68.34742	71.75290	1863.74748	-1451.84923	1357.29467	1
31	C	84.09009	69.97001	71.01228	503.80731	517.99032	318.51606	1
32	H	84.78177	70.57032	70.37570	640.61020	-2157.10410	-1536.29104	1
33	H	83.17969	69.74073	70.38846	1687.88455	465.60692	2087.56452	1
34	H	83.76526	70.62819	71.85178	-1293.07895	-1899.88581	-1463.57452	1
35	C	82.40549	67.41185	71.51188	-153.07550	-733.68902	248.70981	1
36	O	82.15384	68.04759	70.51490	186.15459	-480.78787	-449.34387	1
37	N	81.68107	66.42302	72.05719	-487.53139	543.18517	42.03850	1
38	C	80.72924	65.68535	71.28821	-699.35871	69.34393	360.10701	1
39	H	81.07433	65.70841	70.22899	2.81126	-221.99807	-2715.58072	1
40	C	80.77514	64.26951	72.00729	-507.46439	-592.59194	122.07761	1
41	H	79.88684	63.63888	71.77946	-1975.08116	525.87560	-1801.71556	1
42	H	81.67377	63.68574	71.70595	1588.27743	-1913.22100	1113.83566	1
43	C	80.86017	64.70658	73.50259	-613.62442	-457.55993	-194.14490	1
44	H	79.87557	65.06725	73.87694	1707.54637	-721.27992	1996.92523	1
45	H	81.18651	63.89355	74.18969	758.23357	2100.81767	1560.55011	1
46	C	81.90939	65.89447	73.39758	-352.41524	704.96076	49.21465	1
47	H	81.77451	66.72291	74.13238	1714.76886	-2070.42778	443.35792	1
48	H	82.97821	65.56848	73.39870	1224.15040	1801.50881	1636.97633	1
49	C	79.20403	66.26388	71.46706	566.85117	537.05831	117.62814	1
50	O	78.28182	65.67405	70.95544	-550.26779	-406.08867	4.21666	1
51	N	79.16369	67.38592	72.18909	566.34832	-425.77725	180.18749	1
52	H	80.06148	67.68871	72.56453	644.44502	2646.80550	-52.73430	1
53	C	77.91765	67.67190	72.84791	612.34801	-281.48662	411.56221	1
54	H	77.49825	66.67894	73.12104	1667.23498	-1490.75142	1556.16753	1
55	C	78.26176	68.60680	74.08425	-714.45746	-175.43074	286.98927	1
56	H	78.73873	69.55277	73.70794	-787.09484	1763.03619	-1922.46060	1
57	O	79.18942	68.04812	75.03909	-429.46514	516.51932	-128.40526	1
58	H	79.89310	68.72513	75.04108	1981.82785	436.16847	-1818.18182	1
59	C	76.81668	68.93204	74.61804	630.79189	-468.94448	76.03230	1
60	H	76.84987	69.64446	75.47422	-1775.71861	2062.30353	131.89849	1
61	H	76.17604	69.39129	73.82867	-1855.14608	88.94118	1993.53760	1
62	H	76.29709	68.01252	74.97378	-1504.82350	-780.94249	-2132.90992	1
63	C	76.99241	68.47845	71.76917	288.57638	618.62814	-397.00270	1
64	O	77.32479	69.53499	71.28228	321.70495	-185.26452	574.37218	1
65	N	75.76741	67.86026	71.63777	-447.05792	-446.53431	367.76425	1
66	H	75.89739	67.03965	72.24382	350.31316	1975.63644	-1843.31522	1
67	C	75.47729	67.51908	70.25367	-511.23061	374.03917	-471.51480	1
68	H	76.40512	67.04124	69.86889	2234.79579	-898.70890	-1273.45190	1
69	C	74.25100	66.51058	70.33639	529.53781	-159.34528	563.72604	1
70	H	74.00126	66.19729	69.28635	654.59388	2347.94251	1217.51488	1
71	H	74.61303	65.59465	70.87334	-1526.55661	2103.42026	817.87394	1
72	O	73.02668	67.01887	70.94503	-554.84278	14.12789	399.58769	1
73	H	73.26898	66.93385	71.88316	1297.06236	2061.84854	1220.68812	1
74	C	75.07066	68.83162	69.41419	-662.15484	-412.13544	123.62687	1
75	O	75.16303	68.84182	68.20849	-540.01537	-317.05804	274.91456	1
76	N	74.51193	69.82807	70.19523	-202.76299	-690.00100	-131.49145	1
77	H	74.56144	69.36855	71.12012	-702.62132	-2617.37191	281.70413	1
78	C	75.07398	71.19892	70.12256	-491.73914	576.34187	222.73509	1
79	H	75.75510	71.17515	71.00759	1977.17978	-1823.58850	-434.68928	1

80	C	75.83365	71.45083	68.84923	-649.50797	-328.66843	306.11224	1
81	H	75.25704	71.00099	68.00402	2075.07803	1452.16490	-1004.45904	1
82	C	76.03408	72.92846	68.55738	-615.18735	-489.99689	-70.96352	1
83	H	76.67039	73.09227	67.64463	-1226.32661	-1724.38906	-1716.47170	1
84	H	75.04766	73.45448	68.37667	2381.64273	-969.84735	900.46860	1
85	H	76.53957	73.45107	69.41539	2122.74991	1702.23946	-141.36228	1
86	C	77.20756	70.79576	68.88987	-501.86074	-479.61276	-376.42482	1
87	H	77.79618	70.99500	67.95305	993.79261	-2246.95401	-1177.81305	1
88	H	77.81744	71.16871	69.76016	42.71279	-626.15391	-2651.37258	1
89	H	77.13414	69.67718	69.00884	-2026.39012	-1590.33709	-887.82922	1
90	C	73.77201	72.16238	70.41326	-672.89153	382.57394	-156.34072	1
91	O	73.58168	73.18609	69.78954	410.04627	221.86223	500.35950	1
92	N	73.06905	71.69809	71.43236	-378.11782	-443.79414	-441.10984	1
93	H	73.35391	70.79672	71.80535	2404.15973	-568.14894	1149.30085	1
94	C	71.95302	72.45513	71.91824	-544.54484	466.16019	331.29119	1
95	H	71.51106	72.85073	70.97487	-1409.80988	-170.17955	2325.32679	1
96	C	71.03677	71.41903	72.69706	-184.48284	116.78282	-758.89137	1
97	H	70.87949	70.50401	72.08188	1893.78641	1861.14652	611.04528	1
98	H	71.53091	71.07157	73.63108	-2170.79665	-974.19311	1327.50117	1
99	C	69.67937	72.11209	73.02727	389.51668	672.81878	-138.49152	1
100	H	69.85740	73.04199	73.61192	510.64577	1933.03327	1851.02484	1
101	H	69.19536	72.47018	72.09205	-2302.30869	-1105.72939	-948.89774	1
102	C	68.68093	71.17776	73.81159	-559.93427	-126.34590	542.30857	1
103	O	67.61884	71.61823	74.16815	-670.36003	-111.83166	76.36448	1
104	N	69.12962	69.91880	74.00381	-216.06729	-537.07037	446.51379	1
105	H	70.00586	69.47957	73.69815	-1251.96487	1074.12894	-2168.52500	1
106	H	68.58624	69.18169	74.46620	-2451.83023	-720.73851	944.84612	1
107	C	72.41860	73.69414	72.85821	546.24052	-563.88337	-85.11809	1
108	O	71.80875	74.74040	72.67589	71.70702	-307.40463	606.69673	1
109	N	73.34541	73.44203	73.78105	479.90863	-504.50129	222.86849	1
110	C	73.67956	74.45192	74.75110	75.51268	-600.91904	506.73700	1
111	H	72.70757	74.93206	75.00662	-2033.61562	1795.30103	254.89480	1
112	C	74.38032	73.60654	75.89982	523.79067	517.99274	284.45581	1
113	H	75.05056	74.22376	76.53954	1599.61665	-1127.00911	1895.98173	1
114	H	73.63455	73.13494	76.57821	-1881.83093	1275.82488	-1501.55016	1
115	C	75.14807	72.53598	75.06375	-600.05639	-404.05026	316.64485	1
116	H	76.08318	72.96697	74.64042	-2597.05260	496.36221	657.73249	1
117	H	75.44983	71.64082	75.65296	-1666.24518	1294.38985	-1723.90591	1
118	C	74.09979	72.20486	73.91585	493.57570	-129.95376	-602.56394	1
119	H	74.55198	71.97275	72.92454	-1469.08415	-637.84797	2204.22581	1
120	H	73.36096	71.41272	74.17769	-1038.97840	1068.88701	-2280.71789	1
121	C	74.70099	75.50730	74.04716	188.88100	241.05089	-727.87821	1
122	O	75.86367	75.54712	74.33618	531.88613	-49.19943	427.07960	1
123	N	74.01179	76.27077	73.18250	708.14833	26.93417	-179.73509	1
124	H	73.01799	76.01379	72.97651	-2232.69501	-1179.09831	1023.94816	1
125	C	74.77201	77.19369	72.32464	-738.32412	259.92548	104.42456	1
126	H	75.83660	76.98560	72.59578	2028.89123	1260.02983	1311.33324	1
127	C	74.42784	76.90241	70.87272	-258.65678	-345.52513	661.28459	1
128	H	73.32046	76.91572	70.76712	-1826.06090	-1801.46097	-918.64554	1
129	C	75.00365	77.95611	69.94569	-541.23400	531.92970	-218.41428	1
130	H	74.74002	77.75670	68.87033	1311.73218	-2219.18200	882.19023	1
131	H	74.61966	78.98346	70.20034	-1048.71298	1223.58118	-2196.97971	1
132	H	76.12607	77.99758	70.01292	419.06414	1903.92898	1903.44670	1
133	C	74.90098	75.52005	70.46354	-423.86431	152.66566	-648.55262	1
134	H	74.52568	75.23833	69.43918	105.68386	-2342.50080	1387.51238	1
135	H	76.02430	75.45399	70.44289	-1695.63603	-1484.73621	-1531.02793	1
136	H	74.53100	74.73199	71.18087	-1853.57121	-487.39031	1936.59343	1
137	C	74.33185	78.73549	72.70901	539.71428	-510.58232	267.58633	1
138	O	75.21402	79.51287	73.08268	-15.93758	-278.34085	-624.49402	1
139	N	73.06850	78.98711	72.49795	-676.81886	12.05292	276.17960	1
140	H	72.50553	78.20395	72.16923	-1694.44250	-373.84189	-2100.66098	1
141	C	72.57411	80.31043	72.67415	412.33078	-664.70360	108.35451	1

142	H	73.48130	80.93204	72.84446	1765.77476	1294.44366	1621.76594	1
143	C	71.78871	80.72615	71.35985	-179.66635	-721.95667	-264.73915	1
144	H	72.37275	80.47730	70.44585	-607.34922	2587.87032	-598.10018	1
145	H	70.83330	80.16267	71.27176	-359.69332	-1479.13954	-2259.74260	1
146	C	71.53337	82.26490	71.47142	-240.01076	616.02425	431.85322	1
147	H	71.04263	82.49763	72.45036	-1359.17131	782.54425	2227.99181	1
148	H	72.49482	82.82711	71.47226	-820.36667	85.81767	-2596.78715	1
149	C	70.61308	82.72730	70.27126	-513.07015	236.18570	-551.87280	1
150	H	71.15166	82.65020	69.29881	1816.11944	-1183.11722	-1650.94321	1
151	H	69.71928	82.06871	70.17738	-1800.04429	-1361.53473	1526.34643	1
152	C	70.18725	84.18500	70.56418	726.08972	-253.19732	-179.64713	1
153	H	69.55975	84.30620	71.46982	1224.27271	-456.51798	-2390.90304	1
154	H	71.02036	84.91559	70.58164	1206.40339	-1150.93514	-2154.90344	1
155	N	69.26781	84.65967	69.38919	329.70796	-633.68968	-155.67358	1
156	H	68.87733	85.64162	69.48233	1348.31305	1938.76845	1359.00643	1
157	H	69.70078	84.69871	68.42092	2096.92035	1446.54551	-966.48890	1
158	H	68.38306	84.10045	69.21265	-1197.07217	-2303.53719	827.28733	1
159	C	71.51698	80.35829	73.92580	-378.01186	-556.17301	-413.96481	1
160	O	71.04793	81.42631	74.26102	-409.44433	-307.55053	-453.30833	1
161	N	71.25760	79.15704	74.42088	-429.02477	524.70884	274.08502	1
162	H	71.78291	78.37046	74.04418	1706.34263	-1425.96036	1574.38926	1
163	C	70.29694	79.04890	75.46446	-45.25864	-626.22952	478.93267	1
164	H	69.72974	80.00767	75.42286	1988.63164	570.90773	1772.87287	1
165	C	69.43994	77.74888	75.17913	551.77128	-20.49526	-564.54996	1
166	H	68.91934	77.83300	74.19911	1434.61535	-1753.10253	1513.99471	1
167	H	70.08399	76.84506	75.09281	-714.67738	1819.09770	1898.36494	1
168	C	68.41408	77.59041	76.34969	446.99263	-555.77305	338.97221	1
169	H	68.94171	77.35137	77.30072	1953.68466	1892.25957	-161.67766	1
170	H	67.87496	78.54700	76.53044	-403.03785	2688.07032	-188.43591	1
171	C	67.39324	76.44351	75.96996	567.86262	335.74681	434.04421	1
172	H	66.88697	76.66617	75.00263	-1080.02275	1568.26081	-1948.78900	1
173	H	67.92053	75.47290	75.81947	-919.54108	2111.34692	1456.13463	1
174	C	66.36024	76.33757	77.11620	195.81897	173.33862	-745.11536	1
175	H	66.76956	75.95161	78.07116	1405.67949	-2301.21089	-390.08113	1
176	H	65.77772	77.26244	77.30035	-940.37328	-1118.32446	2299.72133	1
177	N	65.28948	75.27971	76.68716	319.26422	656.36007	-42.02424	1
178	H	64.52268	75.08067	77.39296	1961.03633	619.91968	1787.09422	1
179	H	64.72312	75.48580	75.81332	854.14343	-2156.80752	1429.08711	1
180	H	65.64921	74.30208	76.48724	1237.02905	-1378.50857	-1998.28500	1
181	C	71.07165	78.87055	76.90774	532.53319	-268.57236	517.55729	1
182	O	70.86726	79.66792	77.79057	266.16714	-290.73804	-558.88002	1
183	N	71.85967	77.79812	76.91597	-226.25352	640.49678	-270.32839	1
184	H	71.86135	77.23820	76.06473	2007.69063	-1035.27229	1523.50231	1
185	C	72.17650	77.22776	78.21287	-540.76542	-573.33303	49.50000	1
186	H	71.26346	77.34245	78.84045	-2374.20950	-1036.76023	843.75774	1
187	C	72.53387	75.69046	77.90005	-77.09082	666.87422	-415.84136	1
188	H	73.31717	75.66653	77.09654	-985.81834	617.19825	2463.91927	1
189	O	71.41904	74.90976	77.44143	293.29899	-391.65602	-477.80926	1
190	H	71.75936	74.57056	76.59163	2528.72714	-681.76262	-751.27122	1
191	C	73.18706	75.21693	79.24737	252.47363	-605.14473	440.05134	1
192	H	73.58901	74.18031	79.16637	-2052.65063	1456.49051	-1043.51830	1
193	H	74.03097	75.87932	79.54803	-2152.98800	-1661.97574	-161.70652	1
194	H	72.45077	75.22152	80.08415	-473.12726	-1584.27339	2165.61725	1
195	C	73.38983	78.06270	78.78981	360.36307	488.46713	505.10056	1
196	O	74.35436	78.58705	78.09827	-200.08817	-528.03552	-385.82850	1
197	N	73.34317	78.12243	80.08701	-597.54095	-226.44775	355.20479	1
198	H	72.56265	77.71793	80.60157	2179.23655	-1300.70981	-991.33835	1
199	C	74.49779	78.71740	80.66090	-687.68921	297.39807	-249.45179	1
200	H	74.20878	79.21616	81.60979	-349.16256	-2467.37713	-1101.72831	1
201	C	75.63108	77.61403	80.80847	672.47345	361.54328	-201.62880	1
202	H	75.80153	77.11004	79.82908	1541.41502	582.18425	2169.97026	1
203	H	76.58942	78.12690	81.06190	-2534.67717	60.25153	997.72295	1

204	C	75.28826	76.57130	81.88838	574.26774	-389.43119	-377.02542	1
205	C	74.97288	76.99222	83.21425	688.82679	-287.33580	-257.96133	1
206	H	74.94676	78.06605	83.47424	331.14182	1470.38163	2269.80013	1
207	C	75.33798	75.18095	81.57031	-383.52382	-675.04808	144.24917	1
208	H	75.60293	74.84498	80.55151	4.09847	1517.59662	2262.86397	1
209	C	74.70403	76.02116	84.17989	-134.76730	428.45285	-649.50303	1
210	H	74.46280	76.34911	85.20600	-903.23433	1600.49020	2011.53387	1
211	C	75.05763	74.24509	82.57007	-335.53281	-615.00040	-364.39058	1
212	H	75.09758	73.17315	82.30874	1596.45398	-1369.33862	1732.02659	1
213	C	74.73172	74.62343	83.90493	585.48547	-340.24194	-406.23938	1
214	O	74.44734	73.68278	84.92981	-419.15649	-173.04408	-511.94141	1
215	H	74.57200	72.84436	84.42652	-1071.84350	1559.71507	-1960.13012	1
216	C	75.16532	79.65881	79.44464	291.41878	-183.13091	710.72246	1
217	O	76.36628	79.72109	79.30607	379.87695	523.47396	-222.23622	1
218	N	74.38443	80.90213	79.50870	564.30591	373.09380	277.24371	1
219	H	74.46713	81.35782	80.42206	-120.59931	-2436.07824	-1214.35098	1
220	C	74.92911	81.81295	78.51868	404.07514	-299.37480	608.84009	1
221	H	76.00493	81.91912	78.78976	-1071.07882	-841.69025	2359.66467	1
222	C	74.72024	81.22710	77.06612	-683.12807	68.71770	-390.13096	1
223	H	75.27888	80.27111	76.92334	2068.88918	1596.58590	770.89603	1
224	H	73.64714	80.97460	76.89975	1379.86429	2342.49779	-179.85638	1
225	C	75.21872	82.32052	76.07327	-176.39967	537.49466	550.97268	1
226	H	74.94530	83.33673	76.43729	-396.28051	1942.22168	1869.33314	1
227	H	76.32880	82.32357	76.00391	-94.44700	586.00678	-2659.20016	1
228	C	74.55034	82.04807	74.63943	-291.69381	-718.18079	-150.72929	1
229	H	74.88973	81.10024	74.10297	-2303.38776	1089.76242	964.62032	1
230	H	73.43127	82.13139	74.66471	884.16729	2568.80533	-207.74283	1
231	N	75.08469	83.18313	74.02316	-594.49522	-252.81478	342.29276	1
232	H	74.87943	84.06636	74.47165	-1735.17426	2084.05705	-263.71605	1
233	C	75.78640	83.22136	72.95243	595.23177	-271.52487	442.22352	1
234	N	76.07028	82.03860	72.28142	585.53813	-424.79750	-105.81303	1
235	H	75.78738	81.07209	72.55723	959.88797	1327.56823	-2177.11905	1
236	H	76.62842	81.98662	71.42198	1578.48647	16.27378	-2220.76233	1
237	N	76.14782	84.54088	72.64428	-452.17763	-390.33541	-421.51853	1
238	H	75.97553	85.40904	73.14802	470.26107	1974.25629	-1817.92087	1
239	H	76.73178	84.79298	71.84664	1856.67307	-1573.97321	-1224.35416	1
240	C	74.09931	83.20900	78.62982	-531.47271	-581.45780	-55.06206	1
241	O	74.66083	84.27165	78.50351	-243.00837	192.73507	609.52485	1
242	N	72.78957	82.97559	78.75279	343.49288	-644.25607	38.09164	1
243	H	72.52270	81.99094	78.78893	-1691.16043	-1535.97525	-1484.73099	1
244	C	71.83707	84.08201	78.74851	542.66492	350.14337	454.42563	1
245	H	72.49060	84.98128	78.62714	1209.57979	-2396.95920	463.86744	1
246	C	70.88911	83.87347	77.57545	-737.14309	145.93010	242.71942	1
247	H	70.31786	82.93669	77.76266	-1050.18303	159.36419	-2509.06125	1
248	C	69.90218	85.01628	77.43508	-706.77696	-252.88343	-245.16230	1
249	H	69.22206	84.87478	76.55032	-1624.64039	-1665.49085	1417.86935	1
250	H	69.24892	85.11626	78.34921	2566.10521	598.51109	693.22305	1
251	H	70.42761	86.00170	77.29795	-1972.69758	107.10018	-1876.34312	1
252	C	71.65100	83.68514	76.27602	412.85148	672.58832	-27.69222	1
253	H	70.97176	83.38162	75.42963	1447.02277	1762.76533	-1490.78944	1
254	H	72.18037	84.62728	75.96381	1320.77379	-145.20455	2378.68491	1
255	H	72.43295	82.88405	76.37651	-1512.10848	1470.52031	1724.75147	1
256	C	71.00556	84.09763	80.18599	-607.11113	499.56689	73.73769	1
257	O	70.13808	84.92103	80.36307	357.97126	460.81534	356.68785	1
258	N	71.40033	83.14025	81.00967	536.55407	-368.62270	332.76306	1
259	H	72.16080	82.53851	80.69968	524.38866	2297.69985	1367.20941	1
260	C	70.98034	83.18451	82.36232	46.50277	-774.29190	-147.97904	1
261	H	70.48975	84.17611	82.49513	1676.51875	1883.29066	1032.55549	1
262	C	69.98510	81.94002	82.62747	-559.41456	-34.19198	-556.30433	1
263	H	70.56021	80.98824	82.53264	-64.66664	395.18769	2695.05373	1
264	H	69.60067	81.96398	83.67506	-2703.44278	-60.40056	333.79418	1
265	C	68.85628	81.96696	81.63168	-519.76435	377.31045	459.42366	1

266	H	69.29548	82.04438	80.61055	-1746.74323	1667.50644	-1261.73691	1
267	C	68.04732	80.67837	81.71125	570.95554	16.46261	-545.27700	1
268	H	67.20548	80.67226	80.97181	2391.58273	28.05277	-1305.07271	1
269	H	68.68194	79.77940	81.49896	175.75588	917.63458	2559.43867	1
270	H	67.59771	80.53572	82.72759	-1063.97851	-2155.34650	1283.00462	1
271	C	67.94510	83.16608	81.85242	193.76014	2.62946	-765.53141	1
272	H	67.05738	83.14248	81.16879	507.39394	-846.55087	2539.60089	1
273	H	67.55480	83.20312	82.90238	1337.57841	1818.19054	1526.01994	1
274	H	68.48638	84.13185	81.65728	1100.88635	-1172.91350	-2199.08909	1
275	C	72.30719	82.92514	83.24722	-549.21115	475.64486	-309.38218	1
276	O	73.16829	82.15102	82.91932	556.06106	-390.37755	-78.24250	1
277	O	72.33068	83.54106	84.51918	-572.27940	-310.19032	-209.75862	1
278	H	71.50228	84.09139	84.44438	-1380.08193	2212.14486	790.85944	1

Listing 92: C00092.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.4631	0.0000	300.0000
3	H	77.48945	78.02532	73.36187	-2043.14101	-1757.64893	399.89339		1
4	N	78.16364	77.95390	74.12454	426.75047	490.45733	-334.42467		1
5	H	78.41065	76.95081	74.13935	442.25559	-1110.30854	-2448.52907		1
6	C	79.30987	78.77037	73.95592	415.32972	-666.39213	83.73172		1
7	H	79.28409	79.07157	72.88579	879.32219	2491.00447	667.35213		1
8	C	79.27274	80.04895	74.93793	31.35357	477.41777	628.23362		1
9	H	79.35621	79.70625	75.99623	1168.38489	2240.25337	-1019.71136		1
10	H	80.15917	80.70287	74.75708	-360.43770	2534.90498	931.67112		1
11	C	77.99737	80.82291	74.74312	463.18208	512.70242	-382.34388		1
12	H	77.14156	80.13032	74.90999	1725.29117	1863.52247	-987.07854		1
13	C	77.91744	81.95931	75.75624	710.42801	-144.27427	-313.15367		1
14	H	76.95764	82.52954	75.66442	364.20195	-1033.13725	2494.72524		1
15	H	77.98189	81.58207	76.80907	2567.61904	335.80679	847.48802		1
16	H	78.75246	82.69325	75.61650	-2587.99029	680.92867	-512.16411		1
17	C	77.89269	81.39646	73.33620	268.17616	741.64379	-40.42634		1
18	H	76.96012	82.00404	73.20723	1283.54314	-1945.37420	-1411.27812		1
19	H	78.75958	82.06495	73.09747	-1258.57796	1317.15249	-2026.02085		1
20	H	77.87044	80.58996	72.55930	-2502.84526	909.80597	575.92391		1
21	C	80.48245	77.72285	74.30777	619.36578	-458.64843	-172.09273		1
22	O	80.23374	76.51614	74.29568	-81.40433	433.87611	522.34594		1
23	N	81.62597	78.33371	74.56467	175.23996	-622.20190	341.55523		1
24	H	81.65558	79.35204	74.52923	-876.57256	-303.22879	-2561.90213		1
25	C	82.79402	77.58414	74.84569	-571.88214	-534.10783	-106.15033		1
26	H	82.49611	76.53439	74.61957	-2713.20841	-16.25800	-248.80809		1
27	C	83.96809	78.20080	73.94425	166.60354	288.16399	-716.09568		1
28	H	84.20678	79.22332	74.34928	-2097.85574	1636.78449	-586.18044		1
29	O	83.65830	78.37494	72.55039	-317.80580	-363.38227	484.43082		1
30	H	83.75455	79.34483	72.45692	1863.74748	-1451.84923	1357.29467		1
31	C	85.17797	77.24425	74.25093	503.80731	517.99032	318.51606		1
32	H	86.11468	77.61354	73.77176	640.61020	-2157.10410	-1536.29104		1
33	H	85.37751	77.16391	75.34672	1687.88455	465.60692	2087.56452		1
34	H	84.99310	76.21502	73.86549	-1293.07895	-1899.88581	-1463.57452		1
35	C	83.23576	77.83757	76.40412	-153.07550	-733.68902	248.70981		1
36	O	84.14036	78.59695	76.62774	186.15459	-480.78787	-449.34387		1
37	N	82.43747	77.18236	77.26998	-487.53139	543.18517	42.03850		1
38	C	82.85572	76.79820	78.57115	-699.35871	69.34393	360.10701		1
39	H	83.80408	77.33505	78.80317	2.81126	-221.99807	-2715.58072		1
40	C	81.58721	77.15159	79.46096	-507.46439	-592.59194	122.07761		1
41	H	81.58772	76.61261	80.43694	-1975.08116	525.87560	-1801.71556		1
42	H	81.52743	78.24044	79.68448	1588.27743	-1913.22100	1113.83566		1
43	C	80.43761	76.69551	78.50797	-613.62442	-457.55993	-194.14490		1
44	H	80.31917	75.58571	78.52566	1707.54637	-721.27992	1996.92523		1
45	H	79.44217	77.12519	78.76295	758.23357	2100.81767	1560.55011		1

46	C	80.98512	77.17952	77.10062	-352.41524	704.96076	49.21465	1
47	H	80.76675	76.48581	76.24449	1714.76886	-2070.42778	443.35792	1
48	H	80.71132	78.22208	76.81418	1224.15040	1801.50881	1636.97633	1
49	C	82.93431	75.14863	78.70640	566.85117	537.05831	117.62814	1
50	O	82.55153	74.65859	79.74533	-550.26779	-406.08867	4.21666	1
51	N	83.44827	74.57870	77.63008	566.34832	-425.77725	180.18749	1
52	H	83.70843	75.25060	76.90790	644.44502	2646.80550	-52.73430	1
53	C	83.91660	73.23350	77.60947	612.34801	-281.48662	411.56221	1
54	H	84.71825	73.29213	76.83974	1667.23498	-1490.75142	1556.16753	1
55	C	84.46679	72.83159	79.05161	-714.45746	-175.43074	286.98927	1
56	H	83.57866	72.74065	79.74124	-787.09484	1763.03619	-1922.46060	1
57	O	85.36553	73.79037	79.65438	-429.46514	516.51932	-128.40526	1
58	H	84.73883	74.25325	80.25124	1981.82785	436.16847	-1818.18182	1
59	C	85.09052	71.40574	78.82783	630.79189	-468.94448	76.03230	1
60	H	85.47227	70.97778	79.78418	-1775.71861	2062.30353	131.89849	1
61	H	84.33898	70.68112	78.41580	-1855.14608	88.94118	1993.53760	1
62	H	85.94945	71.44143	78.11801	-1504.82350	-780.94249	-2132.90992	1
63	C	82.70519	72.26481	77.11692	288.57638	618.62814	-397.00270	1
64	O	82.49500	71.18668	77.63171	321.70495	-185.26452	574.37218	1
65	N	82.07422	72.79503	76.05862	-447.05792	-446.53431	367.76425	1
66	H	82.45224	73.70312	75.78725	350.31316	1975.63644	-1843.31522	1
67	C	81.66970	71.84144	75.03353	-511.23061	374.03917	-471.51480	1
68	H	82.54913	71.16292	74.97325	2234.79579	-898.70890	-1273.45190	1
69	C	80.41231	71.10036	75.56253	529.53781	-159.34528	563.72604	1
70	H	80.14627	70.22475	74.91762	654.59388	2347.94251	1217.51488	1
71	H	80.59576	70.73694	76.59997	-1526.55661	2103.42026	817.87394	1
72	O	78.94212	71.76444	75.50211	-554.84278	14.12789	399.58769	1
73	H	79.12359	72.43562	76.15226	1297.06236	2061.84854	1220.68812	1
74	C	81.46602	72.72846	73.67089	-662.15484	-412.13544	123.62687	1
75	O	82.46161	73.02904	73.05835	-540.01537	-317.05804	274.91456	1
76	N	80.20545	73.08233	73.50945	-202.76299	-690.00100	-131.49145	1
77	H	79.49416	72.74120	74.20781	-702.62132	-2617.37191	281.70413	1
78	C	79.70617	73.65208	72.29924	-491.73914	576.34187	222.73509	1
79	H	78.98881	74.41899	72.66403	1977.17978	-1823.58850	-434.68928	1
80	C	80.84802	74.23265	71.37462	-649.50797	-328.66843	306.11224	1
81	H	81.59549	73.43766	71.13658	2075.07803	1452.16490	-1004.45904	1
82	C	80.18711	74.79199	70.06592	-615.18735	-489.99689	-70.96352	1
83	H	80.94782	75.22702	69.37610	-1226.32661	-1724.38906	-1716.47170	1
84	H	79.64927	73.99038	69.50633	2381.64273	-969.84735	900.46860	1
85	H	79.44441	75.59281	70.29099	2122.74991	1702.23946	-141.36228	1
86	C	81.52687	75.43850	72.11722	-501.86074	-479.61276	-376.42482	1
87	H	82.50031	75.72218	71.65120	993.79261	-2246.95401	-1177.81305	1
88	H	80.87771	76.34678	72.11023	42.71279	-626.15391	-2651.37258	1
89	H	81.72770	75.18907	73.18898	-2026.39012	-1590.33709	-887.82922	1
90	C	78.92284	72.41923	71.54748	-672.89153	382.57394	-156.34072	1
91	O	79.49985	71.52175	70.98033	410.04627	221.86223	500.35950	1
92	N	77.61348	72.58254	71.72273	-378.11782	-443.79414	-441.10984	1
93	H	77.26362	73.42328	72.18132	2404.15973	-568.14894	1149.30085	1
94	C	76.74704	71.75663	70.93671	-544.54484	466.16019	331.29119	1
95	H	77.33395	70.82698	70.74654	-1409.80988	-170.17955	2325.32679	1
96	C	75.43011	71.56227	71.80881	-184.48284	116.78282	-758.89137	1
97	H	75.69648	71.24915	72.84297	1893.78641	1861.14652	611.04528	1
98	H	74.88445	72.52622	71.92206	-2170.79665	-974.19311	1327.50117	1
99	C	74.54425	70.48516	71.11044	389.51668	672.81878	-138.49152	1
100	H	74.14564	70.87806	70.14825	510.64577	1933.03327	1851.02484	1
101	H	75.18290	69.60533	70.85249	-2302.30869	-1105.72939	-948.89774	1
102	C	73.35557	70.00628	72.05114	-559.93427	-126.34590	542.30857	1
103	O	72.19894	70.14494	71.73481	-670.36003	-111.83166	76.36448	1
104	N	73.83303	69.44847	73.17764	-216.06729	-537.07037	446.51379	1
105	H	74.81702	69.30292	73.43305	-1251.96487	1074.12894	-2168.52500	1
106	H	73.26081	69.03022	73.91898	-2451.83023	-720.73851	944.84612	1
107	C	76.36928	72.57777	69.58999	546.24052	-563.88337	-85.11809	1

108	O	76.20893	73.78877	69.62167	71.70702	-307.40463	606.69673	1
109	N	76.21159	71.74637	68.56445	479.90863	-504.50129	222.86849	1
110	C	75.92428	72.25327	67.24549	75.51268	-600.91904	506.73700	1
111	H	76.62793	73.10985	67.13677	-2033.61562	1795.30103	254.89480	1
112	C	76.21511	71.00884	66.30625	523.79067	517.99274	284.45581	1
113	H	75.60664	71.02391	65.37398	1599.61665	-1127.00911	1895.98173	1
114	H	77.28170	70.97696	65.98955	-1881.83093	1275.82488	-1501.55016	1
115	C	75.87003	69.80928	67.24235	-600.05639	-404.05026	316.64485	1
116	H	74.76795	69.67556	67.32748	-2597.05260	496.36221	657.73249	1
117	H	76.28852	68.83627	66.89940	-1666.24518	1294.38985	-1723.90591	1
118	C	76.50358	70.32058	68.60804	493.57570	-129.95376	-602.56394	1
119	H	76.05768	69.87588	69.53132	-1469.08415	-637.84797	2204.22581	1
120	H	77.61605	70.24021	68.65916	-1038.97840	1068.88701	-2280.71789	1
121	C	74.37433	72.74318	67.17404	188.88100	241.05089	-727.87821	1
122	O	73.54586	72.08905	66.60788	531.88613	-49.19943	427.07960	1
123	N	74.24278	73.91807	67.81787	708.14833	26.93417	-179.73509	1
124	H	75.07128	74.26171	68.36648	-2232.69501	-1179.09831	1023.94816	1
125	C	73.26759	74.91398	67.33893	-738.32412	259.92548	104.42456	1
126	H	73.65028	75.86054	67.78893	2028.89123	1260.02983	1311.33324	1
127	C	73.26212	74.95713	65.82501	-258.65678	-345.52513	661.28459	1
128	H	73.00598	73.93571	65.45597	-1826.06090	-1801.46097	-918.64554	1
129	C	72.22688	75.92262	65.27856	-541.23400	531.92970	-218.41428	1
130	H	72.21568	75.93097	64.15385	1311.73218	-2219.18200	882.19023	1
131	H	71.18217	75.64664	65.62667	-1048.71298	1223.58118	-2196.97971	1
132	H	72.42237	76.97679	65.61769	419.06414	1903.92898	1903.44670	1
133	C	74.62680	75.32320	65.26582	-423.86431	152.66566	-648.55262	1
134	H	74.63525	75.30329	64.14181	105.68386	-2342.50080	1387.51238	1
135	H	74.93792	76.35625	65.58203	-1695.63603	-1484.73621	-1531.02793	1
136	H	75.42328	74.61379	65.61991	-1853.57121	-487.39031	1936.59343	1
137	C	71.81218	74.48900	67.98481	539.71428	-510.58232	267.58633	1
138	O	70.77969	74.70851	67.38528	-15.93758	-278.34085	-624.49402	1
139	N	71.94699	74.03765	69.22525	-676.81886	12.05292	276.17960	1
140	H	72.90676	73.90618	69.53772	-1694.44250	-373.84189	-2100.66098	1
141	C	70.77542	73.52807	69.85639	412.33078	-664.70360	108.35451	1
142	H	69.93531	74.01639	69.30651	1765.77476	1294.44366	1621.76594	1
143	C	70.81434	71.95679	69.64949	-179.66635	-721.95667	-264.73915	1
144	H	71.00379	71.69970	68.58216	-607.34922	2587.87032	-598.10018	1
145	H	71.65346	71.49451	70.23189	-359.69332	-1479.13954	-2259.74260	1
146	C	69.43879	71.40306	70.14472	-240.01076	616.02425	431.85322	1
147	H	69.24049	71.73169	71.19061	-1359.17131	782.54425	2227.99181	1
148	H	68.59748	71.79616	69.53086	-820.36667	85.81767	-2596.78715	1
149	C	69.52937	69.82654	70.05927	-513.07015	236.18570	-551.87280	1
150	H	69.66835	69.49266	69.00501	1816.11944	-1183.11722	-1650.94321	1
151	H	70.42480	69.45758	70.61859	-1800.04429	-1361.53473	1526.34643	1
152	C	68.23006	69.24290	70.66064	726.08972	-253.19732	-179.64713	1
153	H	68.11329	69.40605	71.75077	1224.27271	-456.51798	-2390.90304	1
154	H	67.30147	69.53631	70.13166	1206.40339	-1150.93514	-2154.90344	1
155	N	68.31024	67.68811	70.49547	329.70796	-633.68968	-155.67358	1
156	H	67.49416	67.13918	70.89247	1348.31305	1938.76845	1359.00643	1
157	H	68.35584	67.30924	69.50491	2096.92035	1446.54551	-966.48890	1
158	H	69.13344	67.20012	70.95463	-1197.07217	-2303.53719	827.28733	1
159	C	70.76056	73.78662	71.47838	-378.01186	-556.17301	-413.96481	1
160	O	69.71336	74.10500	71.99463	-409.44433	-307.55053	-453.30833	1
161	N	71.91544	73.50724	72.06969	-429.02477	524.70884	274.08502	1
162	H	72.71157	73.23834	71.49423	1706.34263	-1425.96036	1574.38926	1
163	C	71.94408	73.54055	73.48782	-45.25864	-626.22952	478.93267	1
164	H	70.89650	73.75365	73.81243	1988.63164	570.90773	1772.87287	1
165	C	72.52433	72.14981	73.98408	551.77128	-20.49526	-564.54996	1
166	H	71.86485	71.30443	73.67613	1434.61535	-1753.10253	1513.99471	1
167	H	73.50771	71.94211	73.50845	-714.67738	1819.09770	1898.36494	1
168	C	72.67273	72.23652	75.53767	446.99263	-555.77305	338.97221	1
169	H	73.31410	73.10973	75.79177	1953.68466	1892.25957	-161.67766	1

170	H	71.68899	72.41923	76.02643	-403.03785	2688.07032	-188.43591	1
171	C	73.34455	70.91779	76.09363	567.86262	335.74681	434.04421	1
172	H	72.64320	70.05311	76.04718	-1080.02275	1568.26081	-1948.78900	1
173	H	74.22813	70.63031	75.47861	-919.54108	2111.34692	1456.13463	1
174	C	73.76802	71.23481	77.54775	195.81897	173.33862	-745.11536	1
175	H	74.50802	72.05509	77.64000	1405.67949	-2301.21089	-390.08113	1
176	H	72.92545	71.40333	78.24810	-940.37328	-1118.32446	2299.72133	1
177	N	74.51852	69.98380	78.11112	319.26422	656.36007	-42.02424	1
178	H	74.86910	70.06860	79.10896	1961.03633	619.91968	1787.09422	1
179	H	73.98290	69.06811	78.15227	854.14343	-2156.80752	1429.08711	1
180	H	75.40551	69.70005	77.60314	1237.02905	-1378.50857	-1998.28500	1
181	C	73.04907	74.67062	73.96925	532.53319	-268.57236	517.55729	1
182	O	74.17264	74.72876	73.53575	266.16714	-290.73804	-558.88002	1
183	N	72.50045	75.30344	75.00245	-226.25352	640.49678	-270.32839	1
184	H	71.53223	75.08062	75.23159	2007.69063	-1035.27229	1523.50231	1
185	C	73.10272	76.49726	75.48072	-540.76542	-573.33303	49.50000	1
186	H	74.07271	76.53686	74.93211	-2374.20950	-1036.76023	843.75774	1
187	C	72.11300	77.67656	75.04085	-77.09082	666.87422	-415.84136	1
188	H	71.08867	77.45617	75.44760	-985.81834	617.19825	2463.91927	1
189	O	71.95124	77.80331	73.61387	293.29899	-391.65602	-477.80926	1
190	H	71.02012	77.53004	73.50400	2528.72714	-681.76262	-751.27122	1
191	C	72.68135	78.96000	75.74750	252.47363	-605.14473	440.05134	1
192	H	72.20877	79.88294	75.33624	-2052.65063	1456.49051	-1043.51830	1
193	H	72.48759	78.96375	76.85225	-2152.98800	-1661.97574	-161.70652	1
194	H	73.78228	79.05717	75.59678	-473.12726	-1584.27339	2165.61725	1
195	C	73.29416	76.39934	77.10193	360.36307	488.46713	505.10056	1
196	O	73.53764	77.41534	77.72616	-200.08817	-528.03552	-385.82850	1
197	N	73.20849	75.15630	77.54913	-597.54095	-226.44775	355.20479	1
198	H	73.03662	74.47309	76.81450	2179.23655	-1300.70981	-991.33835	1
199	C	73.53465	74.75271	78.86598	-687.68921	297.39807	-249.45179	1
200	H	73.78201	73.67323	78.76892	-349.16256	-2467.37713	-1101.72831	1
201	C	74.70241	75.63454	79.51426	672.47345	361.54328	-201.62880	1
202	H	74.44852	76.72571	79.43806	1541.41502	582.18425	2169.97026	1
203	H	74.78583	75.38852	80.60005	-2534.67717	60.25153	997.72295	1
204	C	76.00643	75.32102	78.76674	574.26774	-389.43119	-377.02542	1
205	C	76.79618	74.19640	79.14965	688.82679	-287.33580	-257.96133	1
206	H	76.48827	73.54513	79.98801	331.14182	1470.38163	2269.80013	1
207	C	76.39234	76.15041	77.67222	-383.52382	-675.04808	144.24917	1
208	H	75.75891	77.00746	77.37056	4.09847	1517.59662	2262.86397	1
209	C	77.96889	73.94404	78.43741	-134.76730	428.45285	-649.50303	1
210	H	78.58894	73.07925	78.73310	-903.23433	1600.49020	2011.53387	1
211	C	77.57567	75.85235	76.98934	-335.53281	-615.00040	-364.39058	1
212	H	77.87594	76.50155	76.14818	1596.45398	-1369.33862	1732.02659	1
213	C	78.40083	74.74820	77.34406	585.48547	-340.24194	-406.23938	1
214	O	79.62063	74.44404	76.67500	-419.15649	-173.04408	-511.94141	1
215	H	79.55729	75.06709	75.91182	-1071.84350	1559.71507	-1960.13012	1
216	C	72.29226	75.01172	79.88932	291.41878	-183.13091	710.72246	1
217	O	72.51306	75.11302	81.07799	379.87695	523.47396	-222.23622	1
218	N	71.13785	75.05430	79.24340	564.30591	373.09380	277.24371	1
219	H	71.14893	74.91385	78.23258	-120.59931	-2436.07824	-1214.35098	1
220	C	69.88735	74.98894	79.95725	404.07514	-299.37480	608.84009	1
221	H	69.98197	74.02949	80.51299	-1071.07882	-841.69025	2359.66467	1
222	C	69.83469	76.21533	80.95451	-683.12807	68.71770	-390.13096	1
223	H	70.84117	76.33590	81.43106	2068.88918	1596.58590	770.89603	1
224	H	69.66061	77.15774	80.38689	1379.86429	2342.49779	-179.85638	1
225	C	68.75625	76.04634	82.07120	-176.39967	537.49466	550.97268	1
226	H	67.72985	75.90362	81.66373	-396.28051	1942.22168	1869.33314	1
227	H	68.95393	75.15192	82.70266	-94.44700	586.00678	-2659.20016	1
228	C	68.86368	77.40103	82.91347	-291.69381	-718.18079	-150.72929	1
229	H	69.76261	77.49382	83.57379	-2303.38776	1089.76242	964.62032	1
230	H	68.79523	78.33117	82.29765	884.16729	2568.80533	-207.74283	1
231	N	67.71706	77.41974	83.71418	-594.49522	-252.81478	342.29276	1

232	H	66.99546	76.75256	83.48938	-1735.17426	2084.05705	-263.71605	1
233	C	67.51883	78.23515	84.66942	595.23177	-271.52487	442.22352	1
234	N	68.52664	79.16449	84.95094	585.53813	-424.79750	-105.81303	1
235	H	69.42871	79.30169	84.49682	959.88797	1327.56823	-2177.11905	1
236	H	68.48241	79.86562	85.69096	1578.48647	16.27378	-2220.76233	1
237	N	66.26763	78.02559	85.26603	-452.17763	-390.33541	-421.51853	1
238	H	65.52566	77.36220	85.04783	470.26107	1974.25629	-1817.92087	1
239	H	65.91706	78.59086	86.04040	1856.67307	-1573.97321	-1224.35416	1
240	C	68.80029	74.94039	78.76520	-531.47271	-581.45780	-55.06206	1
241	O	68.96921	74.26881	77.77697	-243.00837	192.73507	609.52485	1
242	N	67.68890	75.62084	79.11554	343.49288	-644.25607	38.09164	1
243	H	67.76477	76.14646	79.99203	-1691.16043	-1535.97525	-1484.73099	1
244	C	66.88379	76.28026	78.06997	542.66492	350.14337	454.42563	1
245	H	67.49252	76.28848	77.13721	1209.57979	-2396.95920	463.86744	1
246	C	65.61410	75.46305	77.96523	-737.14309	145.93010	242.71942	1
247	H	65.17964	75.39648	78.98852	-1050.18303	159.36419	-2509.06125	1
248	C	64.58981	76.10661	77.04974	-706.77696	-252.88343	-245.16230	1
249	H	63.62824	75.52252	77.02771	-1624.64039	-1665.49085	1417.86935	1
250	H	64.33986	77.15383	77.37893	2566.10521	598.51109	693.22305	1
251	H	64.96372	76.17204	75.99062	-1972.69758	107.10018	-1876.34312	1
252	C	65.91898	74.04976	77.49982	412.85148	672.58832	-27.69222	1
253	H	65.04273	73.35903	77.64091	1447.02277	1762.76533	-1490.78944	1
254	H	66.19581	74.02361	76.41034	1320.77379	-145.20455	2378.68491	1
255	H	66.79535	73.61881	78.06565	-1512.10848	1470.52031	1724.75147	1
256	C	66.66361	77.76081	78.77944	-607.11113	499.56689	73.73769	1
257	O	66.23635	77.84495	79.90709	357.97126	460.81534	356.68785	1
258	N	67.04880	78.73137	77.96271	536.55407	-368.62270	332.76306	1
259	H	67.35460	78.50703	77.01657	524.38866	2297.69985	1367.20941	1
260	C	66.95603	80.05981	78.43805	46.50277	-774.29190	-147.97904	1
261	H	66.68845	79.96384	79.51672	1676.51875	1883.29066	1032.55549	1
262	C	68.34605	80.83373	78.15157	-559.41456	-34.19198	-556.30433	1
263	H	68.50525	80.89588	77.04878	-64.66664	395.18769	2695.05373	1
264	H	68.28237	81.88911	78.50923	-2703.44278	-60.40056	333.79418	1
265	C	69.49649	80.11493	78.80254	-519.76435	377.31045	459.42366	1
266	H	69.42574	79.03389	78.54473	-1746.74323	1667.50644	-1261.73691	1
267	C	70.81953	80.65487	78.27232	570.95554	16.46261	-545.27700	1
268	H	71.69528	80.10876	78.70901	2391.58273	28.05277	-1305.07271	1
269	H	70.88772	80.56015	77.15824	175.75588	917.63458	2559.43867	1
270	H	70.94984	81.74010	78.51871	-1063.97851	-2155.34650	1283.00462	1
271	C	69.45851	80.25637	80.31816	193.76014	2.62946	-765.53141	1
272	H	70.31008	79.71411	80.80506	507.39394	-846.55087	2539.60089	1
273	H	69.52635	81.32966	80.63349	1337.57841	1818.19054	1526.01994	1
274	H	68.50996	79.84288	80.74769	1100.88635	-1172.91350	-2199.08909	1
275	C	65.83330	80.81162	77.54483	-549.21115	475.64486	-309.38218	1
276	O	65.58973	80.52201	76.40333	556.06106	-390.37755	-78.24250	1
277	O	65.25247	81.95536	78.13958	-572.27940	-310.19032	-209.75862	1
278	H	65.67081	81.88865	79.04320	-1380.08193	2212.14486	790.85944	1

Listing 93: C00093.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.8425	3370
		0.2500	300.00	0.00	0.00	0.00	-1293.4467	0.0000	300.0000
3	H	73.11748	65.85716	75.17561	-2043.14101	-1757.64893	399.89339		1
4	N	73.27936	66.60521	75.84514	426.75047	490.45733	-334.42467		1
5	H	72.33554	66.94999	76.00615	442.25559	-1110.30854	-2448.52907		1
6	C	74.21342	67.58584	75.44636	415.32972	-666.39213	83.73172		1
7	H	75.06025	66.98973	75.04303	879.32219	2491.00447	667.35213		1
8	C	73.57056	68.54101	74.31717	31.35357	477.41777	628.23362		1
9	H	72.68897	69.08429	74.73484	1168.38489	2240.25337	-1019.71136		1
10	H	74.31308	69.32878	74.04460	-360.43770	2534.90498	931.67112		1
11	C	73.17486	67.74445	73.10185	463.18208	512.70242	-382.34388		1

12	H	72.40605	66.99538	73.39627	1725.29117	1863.52247	-987.07854	1
13	C	72.56978	68.66426	72.04829	710.42801	-144.27427	-313.15367	1
14	H	72.23452	68.09377	71.14397	364.20195	-1033.13725	2494.72524	1
15	H	71.67799	69.21664	72.44266	2567.61904	335.80679	847.48802	1
16	H	73.30843	69.43189	71.70061	-2587.99029	680.92867	-512.16411	1
17	C	74.37223	67.01041	72.51362	268.17616	741.64379	-40.42634	1
18	H	74.12398	66.53564	71.52947	1283.54314	-1945.37420	-1411.27812	1
19	H	75.23648	67.70497	72.34322	-1258.57796	1317.15249	-2026.02085	1
20	H	74.73344	66.19437	73.19099	-2502.84526	909.80597	575.92391	1
21	C	74.64333	68.53032	76.68286	619.36578	-458.64843	-172.09273	1
22	O	75.12437	69.64286	76.44641	-81.40433	433.87611	522.34594	1
23	N	74.44319	67.94439	77.84088	175.23996	-622.20190	341.55523	1
24	H	73.98425	67.03572	77.80008	-876.57256	-303.22879	-2561.90213	1
25	C	74.87952	68.53359	79.06429	-571.88214	-534.10783	-106.15033	1
26	H	74.58379	69.60232	78.95423	-2713.20841	-16.25800	-248.80809	1
27	C	74.10572	67.76252	80.23422	166.60354	288.16399	-716.09568	1
28	H	74.42988	66.68617	80.24686	-2097.85574	1636.78449	-586.18044	1
29	O	72.67187	67.72583	80.10583	-317.80580	-363.38227	484.43082	1
30	H	72.50998	66.76214	80.06839	1863.74748	-1451.84923	1357.29467	1
31	C	74.65666	68.47172	81.52399	503.80731	517.99032	318.51606	1
32	H	74.26382	67.99329	82.45119	640.61020	-2157.10410	-1536.29104	1
33	H	75.77138	68.43463	81.57792	1687.88455	465.60692	2087.56452	1
34	H	74.35899	69.54597	81.55369	-1293.07895	-1899.88581	-1463.57452	1
35	C	76.49910	68.42519	79.19831	-153.07550	-733.68902	248.70981	1
36	O	77.00706	69.29722	79.85911	186.15459	-480.78787	-449.34387	1
37	N	77.09682	67.33634	78.68483	-487.53139	543.18517	42.03850	1
38	C	78.52344	67.27041	78.72130	-699.35871	69.34393	360.10701	1
39	H	78.84655	67.97555	79.52474	2.81126	-221.99807	-2715.58072	1
40	C	78.76404	65.72268	79.00030	-507.46439	-592.59194	122.07761	1
41	H	79.78908	65.38883	78.72328	-1975.08116	525.87560	-1801.71556	1
42	H	78.62286	65.47160	80.07511	1588.27743	-1913.22100	1113.83566	1
43	C	77.64782	65.08545	78.11689	-613.62442	-457.55993	-194.14490	1
44	H	77.93813	65.10232	77.04150	1707.54637	-721.27992	1996.92523	1
45	H	77.42622	64.02421	78.37067	758.23357	2100.81767	1560.55011	1
46	C	76.43373	66.06662	78.41090	-352.41524	704.96076	49.21465	1
47	H	75.73885	66.21349	77.55266	1714.76886	-2070.42778	443.35792	1
48	H	75.84533	65.81946	79.32365	1224.15040	1801.50881	1636.97633	1
49	C	79.20399	67.61459	77.26518	566.85117	537.05831	117.62814	1
50	O	80.40262	67.77688	77.21751	-550.26779	-406.08867	4.21666	1
51	N	78.33395	67.61175	76.26434	566.34832	-425.77725	180.18749	1
52	H	77.35356	67.47430	76.50349	644.44502	2646.80550	-52.73430	1
53	C	78.83075	67.78206	74.94361	612.34801	-281.48662	411.56221	1
54	H	79.91655	67.97629	75.12855	1667.23498	-1490.75142	1556.16753	1
55	C	78.55487	66.46449	74.07715	-714.45746	-175.43074	286.98927	1
56	H	77.45305	66.38807	73.86996	-787.09484	1763.03619	-1922.46060	1
57	O	78.94895	65.21999	74.67562	-429.46514	516.51932	-128.40526	1
58	H	78.10672	64.72205	74.65270	1981.82785	436.16847	-1818.18182	1
59	C	79.30823	66.84334	72.74831	630.79189	-468.94448	76.03230	1
60	H	79.18927	66.05256	71.97223	-1775.71861	2062.30353	131.89849	1
61	H	78.92670	67.79703	72.31137	-1855.14608	88.94118	1993.53760	1
62	H	80.40193	66.97088	72.92268	-1504.82350	-780.94249	-2132.90992	1
63	C	78.01192	69.04427	74.28427	288.57638	618.62814	-397.00270	1
64	O	77.22965	68.89371	73.38027	321.70495	-185.26452	574.37218	1
65	N	78.35473	70.14148	74.93590	-447.05792	-446.53431	367.76425	1
66	H	79.03722	70.13440	75.71838	350.31316	1975.63644	-1843.31522	1
67	C	78.13895	71.43795	74.34161	-511.23061	374.03917	-471.51480	1
68	H	78.58701	71.35897	73.32493	2234.79579	-898.70890	-1273.45190	1
69	C	76.56444	71.67360	74.24035	529.53781	-159.34528	563.72604	1
70	H	76.43931	72.51573	73.50464	654.59388	2347.94251	1217.51488	1
71	H	76.12925	70.75239	73.76067	-1526.55661	2103.42026	817.87394	1
72	O	75.87331	71.99739	75.45287	-554.84278	14.12789	399.58769	1
73	H	75.65300	71.04566	75.79617	1297.06236	2061.84854	1220.68812	1

74	C	78.96939	72.36096	75.36213	-662.15484	-412.13544	123.62687	1
75	O	79.73694	71.80429	76.13467	-540.01537	-317.05804	274.91456	1
76	N	78.80582	73.67308	75.17399	-202.76299	-690.00100	-131.49145	1
77	H	78.09048	73.91303	74.48288	-702.62132	-2617.37191	281.70413	1
78	C	79.20467	74.63742	76.20001	-491.73914	576.34187	222.73509	1
79	H	78.70469	75.58777	75.89188	1977.17978	-1823.58850	-434.68928	1
80	C	78.69957	74.15088	77.54394	-649.50797	-328.66843	306.11224	1
81	H	79.17932	73.16211	77.74813	2075.07803	1452.16490	-1004.45904	1
82	C	79.06041	75.10334	78.66910	-615.18735	-489.99689	-70.96352	1
83	H	78.66456	74.74708	79.65983	-1226.32661	-1724.38906	-1716.47170	1
84	H	80.17945	75.21703	78.77322	2381.64273	-969.84735	900.46860	1
85	H	78.64137	76.13167	78.48751	2122.74991	1702.23946	-141.36228	1
86	C	77.19609	73.94028	77.53451	-501.86074	-479.61276	-376.42482	1
87	H	76.83113	73.45832	78.48430	993.79261	-2246.95401	-1177.81305	1
88	H	76.64300	74.91237	77.41709	42.71279	-626.15391	-2651.37258	1
89	H	76.86876	73.26982	76.68026	-2026.39012	-1590.33709	-887.82922	1
90	C	80.85951	74.79442	76.17951	-672.89153	382.57394	-156.34072	1
91	O	81.42632	75.41345	77.05360	410.04627	221.86223	500.35950	1
92	N	81.41152	74.21046	75.12686	-378.11782	-443.79414	-441.10984	1
93	H	80.75853	73.71802	74.52275	2404.15973	-568.14894	1149.30085	1
94	C	82.74791	74.56186	74.75272	-544.54484	466.16019	331.29119	1
95	H	83.26780	74.57196	75.73775	-1409.80988	-170.17955	2325.32679	1
96	C	83.22539	73.41530	73.76870	-184.48284	116.78282	-758.89137	1
97	H	82.93156	72.41792	74.16768	1893.78641	1861.14652	611.04528	1
98	H	82.71548	73.51069	72.78365	-2170.79665	-974.19311	1327.50117	1
99	C	84.77351	73.50868	73.59500	389.51668	672.81878	-138.49152	1
100	H	85.05838	74.52198	73.22657	510.64577	1933.03327	1851.02484	1
101	H	85.27753	73.43257	74.58387	-2302.30869	-1105.72939	-948.89774	1
102	C	85.35032	72.40824	72.62587	-559.93427	-126.34590	542.30857	1
103	O	86.53399	72.37135	72.40804	-670.36003	-111.83166	76.36448	1
104	N	84.41853	71.57469	72.11468	-216.06729	-537.07037	446.51379	1
105	H	83.40435	71.54852	72.27126	-1251.96487	1074.12894	-2168.52500	1
106	H	84.63175	70.80150	71.47489	-2451.83023	-720.73851	944.84612	1
107	C	82.89088	76.01953	74.03750	546.24052	-563.88337	-85.11809	1
108	O	84.02370	76.42590	73.95218	71.70702	-307.40463	606.69673	1
109	N	81.77596	76.60583	73.56928	479.90863	-504.50129	222.86849	1
110	C	81.80437	77.94129	73.06412	75.51268	-600.91904	506.73700	1
111	H	82.84400	78.12634	72.70512	-2033.61562	1795.30103	254.89480	1
112	C	80.66210	77.90772	71.95708	523.79067	517.99274	284.45581	1
113	H	80.30376	78.92455	71.67972	1599.61665	-1127.00911	1895.98173	1
114	H	81.00717	77.41567	71.02053	-1881.83093	1275.82488	-1501.55016	1
115	C	79.58891	77.05200	72.69701	-600.05639	-404.05026	316.64485	1
116	H	79.05774	77.65546	73.46812	-2597.05260	496.36221	657.73249	1
117	H	78.80086	76.63008	72.03001	-1666.24518	1294.38985	-1723.90591	1
118	C	80.49617	75.93673	73.37498	493.57570	-129.95376	-602.56394	1
119	H	80.14565	75.61095	74.38186	-1469.08415	-637.84797	2204.22581	1
120	H	80.70401	75.04110	72.74320	-1038.97840	1068.88701	-2280.71789	1
121	C	81.30911	79.01563	74.20533	188.88100	241.05089	-727.87821	1
122	O	80.83056	80.06569	73.83653	531.88613	-49.19943	427.07960	1
123	N	81.61085	78.62348	75.43803	708.14833	26.93417	-179.73509	1
124	H	81.98022	77.67330	75.45891	-2232.69501	-1179.09831	1023.94816	1
125	C	81.10893	79.26921	76.65109	-738.32412	259.92548	104.42456	1
126	H	81.75994	78.84480	77.45221	2028.89123	1260.02983	1311.33324	1
127	C	81.30663	80.76250	76.46395	-258.65678	-345.52513	661.28459	1
128	H	80.71202	81.07124	75.55997	-1826.06090	-1801.46097	-918.64554	1
129	C	80.85221	81.63227	77.62058	-541.23400	531.92970	-218.41428	1
130	H	81.17636	82.70100	77.48234	1311.73218	-2219.18200	882.19023	1
131	H	79.73024	81.64627	77.71983	-1048.71298	1223.58118	-2196.97971	1
132	H	81.27953	81.28225	78.60106	419.06414	1903.92898	1903.44670	1
133	C	82.76501	81.07387	76.16731	-423.86431	152.66566	-648.55262	1
134	H	82.91993	82.16046	75.92414	105.68386	-2342.50080	1387.51238	1
135	H	83.42791	80.82784	77.04121	-1695.63603	-1484.73621	-1531.02793	1

136	H	83.13771	80.47762	75.28946	-1853.57121	-487.39031	1936.59343	1
137	C	79.55979	78.71309	76.82434	539.71428	-510.58232	267.58633	1
138	O	79.10924	77.81371	76.11910	-15.93758	-278.34085	-624.49402	1
139	N	78.98754	79.31020	77.84050	-676.81886	12.05292	276.17960	1
140	H	79.57302	79.99564	78.30806	-1694.44250	-373.84189	-2100.66098	1
141	C	77.57924	79.28029	78.09080	412.33078	-664.70360	108.35451	1
142	H	77.33122	78.19643	78.04189	1765.77476	1294.44366	1621.76594	1
143	C	77.39739	79.96543	79.50023	-179.66635	-721.95667	-264.73915	1
144	H	78.12370	79.55696	80.23835	-607.34922	2587.87032	-598.10018	1
145	H	77.63701	81.04986	79.41679	-359.69332	-1479.13954	-2259.74260	1
146	C	75.92735	79.78663	80.00759	-240.01076	616.02425	431.85322	1
147	H	75.20266	80.06751	79.20734	-1359.17131	782.54425	2227.99181	1
148	H	75.71398	78.72628	80.27060	-820.36667	85.81767	-2596.78715	1
149	C	75.77528	80.73789	81.26294	-513.07015	236.18570	-551.87280	1
150	H	76.53950	80.49633	82.03708	1816.11944	-1183.11722	-1650.94321	1
151	H	75.96680	81.79647	80.97206	-1800.04429	-1361.53473	1526.34643	1
152	C	74.35058	80.59160	81.84391	726.08972	-253.19732	-179.64713	1
153	H	73.53617	80.86090	81.14232	1224.27271	-456.51798	-2390.90304	1
154	H	74.13942	79.60963	82.31219	1206.40339	-1150.93514	-2154.90344	1
155	N	74.21606	81.62879	83.01168	329.70796	-633.68968	-155.67358	1
156	H	73.27785	81.64683	83.50607	1348.31305	1938.76845	1359.00643	1
157	H	74.88189	81.52667	83.83191	2096.92035	1446.54551	-966.48890	1
158	H	74.33608	82.65268	82.75891	-1197.07217	-2303.53719	827.28733	1
159	C	76.76258	80.13083	76.95982	-378.01186	-556.17301	-413.96481	1
160	O	75.97698	80.99209	77.26513	-409.44433	-307.55053	-453.30833	1
161	N	77.13741	79.72060	75.74775	-429.02477	524.70884	274.08502	1
162	H	77.77713	78.89932	75.68512	1706.34263	-1425.96036	1574.38926	1
163	C	76.23554	79.92840	74.65391	-45.25864	-626.22952	478.93267	1
164	H	75.53548	80.69919	75.05348	1988.63164	570.90773	1772.87287	1
165	C	77.14629	80.43490	73.46471	551.77128	-20.49526	-564.54996	1
166	H	77.95079	81.09499	73.86139	1434.61535	-1753.10253	1513.99471	1
167	H	77.68291	79.58241	72.99100	-714.67738	1819.09770	1898.36494	1
168	C	76.28277	81.20836	72.41330	446.99263	-555.77305	338.97221	1
169	H	75.46685	80.57238	72.00381	1953.68466	1892.25957	-161.67766	1
170	H	75.77997	82.09048	72.86941	-403.03785	2688.07032	-188.43591	1
171	C	77.29004	81.64656	71.27507	567.86262	335.74681	434.04421	1
172	H	77.98031	82.43981	71.64409	-1080.02275	1568.26081	-1948.78900	1
173	H	77.94430	80.79396	70.98116	-919.54108	2111.34692	1456.13463	1
174	C	76.47857	82.14174	70.05590	195.81897	173.33862	-745.11536	1
175	H	75.85280	81.36465	69.57326	1405.67949	-2301.21089	-390.08113	1
176	H	75.87684	83.05546	70.23432	-940.37328	-1118.32446	2299.72133	1
177	N	77.51709	82.55187	68.95680	319.26422	656.36007	-42.02424	1
178	H	77.10889	82.85841	68.02713	1961.03633	619.91968	1787.09422	1
179	H	78.15773	83.36774	69.18162	854.14343	-2156.80752	1429.08711	1
180	H	78.21034	81.81048	68.64602	1237.02905	-1378.50857	-1998.28500	1
181	C	75.54002	78.46909	74.43817	532.53319	-268.57236	517.55729	1
182	O	75.16907	77.85043	75.43818	266.16714	-290.73804	-558.88002	1
183	N	75.41906	78.15509	73.17201	-226.25352	640.49678	-270.32839	1
184	H	75.78739	78.84394	72.51905	2007.69063	-1035.27229	1523.50231	1
185	C	74.95021	76.91989	72.66294	-540.76542	-573.33303	49.50000	1
186	H	75.19866	76.98251	71.58060	-2374.20950	-1036.76023	843.75774	1
187	C	75.70344	75.72048	73.40699	-77.09082	666.87422	-415.84136	1
188	H	75.54504	75.82405	74.51774	-985.81834	617.19825	2463.91927	1
189	O	77.13133	75.63250	73.22863	293.29899	-391.65602	-477.80926	1
190	H	77.44086	75.79355	74.14297	2528.72714	-681.76262	-751.27122	1
191	C	74.86256	74.50759	72.86692	252.47363	-605.14473	440.05134	1
192	H	75.11466	73.56087	73.40025	-2052.65063	1456.49051	-1043.51830	1
193	H	73.76500	74.68078	72.99903	-2152.98800	-1661.97574	-161.70652	1
194	H	75.04165	74.33972	71.77894	-473.12726	-1584.27339	2165.61725	1
195	C	73.32741	76.74978	72.88730	360.36307	488.46713	505.10056	1
196	O	72.65330	76.38318	71.95636	-200.08817	-528.03552	-385.82850	1
197	N	72.98025	76.94678	74.14803	-597.54095	-226.44775	355.20479	1

198	H	73.69426	77.22388	74.86788	2179.23655	-1300.70981	-991.33835	1
199	C	71.59030	76.89621	74.47814	-687.68921	297.39807	-249.45179	1
200	H	71.22949	75.90452	74.12845	-349.16256	-2467.37713	-1101.72831	1
201	C	71.46551	77.15395	76.04413	672.47345	361.54328	-201.62880	1
202	H	71.77890	78.20050	76.26516	1541.41502	582.18425	2169.97026	1
203	H	70.39369	77.07043	76.33869	-2534.67717	60.25153	997.72295	1
204	C	72.32180	76.18152	76.87174	574.26774	-389.43119	-377.02542	1
205	C	71.90262	74.83155	77.06536	688.82679	-287.33580	-257.96133	1
206	H	70.97382	74.45760	76.59703	331.14182	1470.38163	2269.80013	1
207	C	73.52799	76.65209	77.47367	-383.52382	-675.04808	144.24917	1
208	H	73.87059	77.69183	77.31027	4.09847	1517.59662	2262.86397	1
209	C	72.68210	73.99842	77.87059	-134.76730	428.45285	-649.50303	1
210	H	72.35306	72.95604	78.02647	-903.23433	1600.49020	2011.53387	1
211	C	74.27234	75.78332	78.27518	-335.53281	-615.00040	-364.39058	1
212	H	75.19876	76.16496	78.73950	1596.45398	-1369.33862	1732.02659	1
213	C	73.87878	74.43361	78.51091	585.48547	-340.24194	-406.23938	1
214	O	74.62824	73.55057	79.33396	-419.15649	-173.04408	-511.94141	1
215	H	75.31108	74.17790	79.67053	-1071.84350	1559.71507	-1960.13012	1
216	C	70.81854	78.13378	73.74901	291.41878	-183.13091	710.72246	1
217	O	71.24041	79.26710	73.72757	379.87695	523.47396	-222.23622	1
218	N	69.61107	77.69512	73.38597	564.30591	373.09380	277.24371	1
219	H	69.39239	76.70495	73.49357	-120.59931	-2436.07824	-1214.35098	1
220	C	68.87940	78.48734	72.45326	404.07514	-299.37480	608.84009	1
221	H	69.33917	79.49904	72.55232	-1071.07882	-841.69025	2359.66467	1
222	C	69.06482	77.83661	71.02024	-683.12807	68.71770	-390.13096	1
223	H	70.14364	77.69876	70.77858	2068.88918	1596.58590	770.89603	1
224	H	68.61382	76.81881	70.99193	1379.86429	2342.49779	-179.85638	1
225	C	68.36242	78.78795	70.00292	-176.39967	537.49466	550.97268	1
226	H	67.30349	78.96013	70.30739	-396.28051	1942.22168	1869.33314	1
227	H	68.84479	79.79086	69.99786	-94.44700	586.00678	-2659.20016	1
228	C	68.42849	78.10940	68.55885	-291.69381	-718.18079	-150.72929	1
229	H	69.45619	77.93978	68.14759	-2303.38776	1089.76242	964.62032	1
230	H	67.84974	77.15761	68.44308	884.16729	2568.80533	-207.74283	1
231	N	67.80611	79.09303	67.77391	-594.49522	-252.81478	342.29276	1
232	H	67.49639	79.92627	68.24986	-1735.17426	2084.05705	-263.71605	1
233	C	67.61026	79.00645	66.52094	595.23177	-271.52487	442.22352	1
234	N	68.04353	77.84534	65.87200	585.53813	-424.79750	-105.81303	1
235	H	68.50921	77.02456	66.25710	959.88797	1327.56823	-2177.11905	1
236	H	67.94191	77.66186	64.87327	1578.48647	16.27378	-2220.76233	1
237	N	66.96920	80.15418	66.03310	-452.17763	-390.33541	-421.51853	1
238	H	66.65496	80.99884	66.50846	470.26107	1974.25629	-1817.92087	1
239	H	66.72394	80.28131	65.05056	1856.67307	-1573.97321	-1224.35416	1
240	C	67.29009	78.40443	72.85614	-531.47271	-581.45780	-55.06206	1
241	O	66.47185	77.84775	72.12189	-243.00837	192.73507	609.52485	1
242	N	67.09348	79.00338	74.00792	343.49288	-644.25607	38.09164	1
243	H	67.98692	79.30792	74.39404	-1691.16043	-1535.97525	-1484.73099	1
244	C	65.82578	79.45870	74.53761	542.66492	350.14337	454.42563	1
245	H	66.11065	80.16375	75.35574	1209.57979	-2396.95920	463.86744	1
246	C	65.02251	80.10919	73.41530	-737.14309	145.93010	242.71942	1
247	H	65.02362	79.40558	72.54832	-1050.18303	159.36419	-2509.06125	1
248	C	63.58222	80.34423	73.82679	-706.77696	-252.88343	-245.16230	1
249	H	62.97537	80.78872	72.99024	-1624.64039	-1665.49085	1417.86935	1
250	H	63.07855	79.38466	74.13302	2566.10521	598.51109	693.22305	1
251	H	63.51166	81.04708	74.70254	-1972.69758	107.10018	-1876.34312	1
252	C	65.65932	81.40576	72.95329	412.85148	672.58832	-27.69222	1
253	H	65.09995	81.86041	72.08958	1447.02277	1762.76533	-1490.78944	1
254	H	65.68021	82.17199	73.77690	1320.77379	-145.20455	2378.68491	1
255	H	66.72215	81.24599	72.61995	-1512.10848	1470.52031	1724.75147	1
256	C	64.94412	78.16742	75.12700	-607.11113	499.56689	73.73769	1
257	O	64.41098	78.27265	76.20003	357.97126	460.81534	356.68785	1
258	N	64.84647	77.20130	74.23269	536.55407	-368.62270	332.76306	1
259	H	65.36826	77.26010	73.32436	524.38866	2297.69985	1367.20941	1

260	C	64.18698	76.01985	74.65565	46.50277	-774.29190	-147.97904	1
261	H	63.53084	76.34174	75.49675	1676.51875	1883.29066	1032.55549	1
262	C	63.41743	75.38175	73.38858	-559.41456	-34.19198	-556.30433	1
263	H	64.16000	75.14567	72.58885	-64.66664	395.18769	2695.05373	1
264	H	62.94747	74.40887	73.66938	-2703.44278	-60.40056	333.79418	1
265	C	62.38451	76.34960	72.87459	-519.76435	377.31045	459.42366	1
266	H	62.88378	77.32666	72.68413	-1746.74323	1667.50644	-1261.73691	1
267	C	61.79128	75.84582	71.56463	570.95554	16.46261	-545.27700	1
268	H	61.02012	76.55131	71.16044	2391.58273	28.05277	-1305.07271	1
269	H	62.57647	75.72359	70.77443	175.75588	917.63458	2559.43867	1
270	H	61.29325	74.85033	71.69376	-1063.97851	-2155.34650	1283.00462	1
271	C	61.26911	76.56438	73.88858	193.76014	2.62946	-765.53141	1
272	H	60.46640	77.23391	73.48452	507.39394	-846.55087	2539.60089	1
273	H	60.78064	75.59726	74.17496	1337.57841	1818.19054	1526.01994	1
274	H	61.65037	77.03702	74.83039	1100.88635	-1172.91350	-2199.08909	1
275	C	65.32006	74.95921	75.12243	-549.21115	475.64486	-309.38218	1
276	O	66.38356	74.83210	74.57611	556.06106	-390.37755	-78.24250	1
277	O	64.91344	74.05190	76.12794	-572.27940	-310.19032	-209.75862	1
278	H	64.02696	74.45248	76.34955	-1380.08193	2212.14486	790.85944	1

Listing 94: C00094.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.4465	0.0000	300.0000
3	H	72.88353	83.36807	69.46098	-2043.14101	-1757.64893	399.89339		1
4	N	72.89145	84.34422	69.74821	426.75047	490.45733	-334.42467		1
5	H	71.98457	84.66884	69.41908	442.25559	-1110.30854	-2448.52907		1
6	C	73.99588	85.08932	69.28646	415.32972	-666.39213	83.73172		1
7	H	74.85081	84.39249	69.41256	879.32219	2491.00447	667.35213		1
8	C	73.77508	85.49183	67.74295	31.35357	477.41777	628.23362		1
9	H	72.81078	86.04272	67.62427	1168.38489	2240.25337	-1019.71136		1
10	H	74.57460	86.20453	67.42706	-360.43770	2534.90498	931.67112		1
11	C	73.79201	84.25888	66.87644	463.18208	512.70242	-382.34388		1
12	H	72.98880	83.56965	67.22035	1725.29117	1863.52247	-987.07854		1
13	C	73.52025	84.62424	65.42235	710.42801	-144.27427	-313.15367		1
14	H	73.51880	83.71840	64.76237	364.20195	-1033.13725	2494.72524		1
15	H	72.52692	85.12763	65.29813	2567.61904	335.80679	847.48802		1
16	H	74.29886	85.32334	65.02134	-2587.99029	680.92867	-512.16411		1
17	C	75.12799	83.53367	66.96824	268.17616	741.64379	-40.42634		1
18	H	75.17943	82.66995	66.25630	1283.54314	-1945.37420	-1411.27812		1
19	H	75.98355	84.21556	66.72534	-1258.57796	1317.15249	-2026.02085		1
20	H	75.31271	83.12342	67.99417	-2502.84526	909.80597	575.92391		1
21	C	74.17925	86.44321	70.16097	619.36578	-458.64843	-172.09273		1
22	O	74.84223	87.36265	69.72884	-81.40433	433.87611	522.34594		1
23	N	73.61462	86.34455	71.36571	175.23996	-622.20190	341.55523		1
24	H	73.05297	85.51170	71.53366	-876.57256	-303.22879	-2561.90213		1
25	C	73.68330	87.46763	72.24343	-571.88214	-534.10783	-106.15033		1
26	H	73.78558	88.32172	71.53298	-2713.20841	-16.25800	-248.80809		1
27	C	72.32681	87.46349	73.09448	166.60354	288.16399	-716.09568		1
28	H	72.25902	86.49949	73.66995	-2097.85574	1636.78449	-586.18044		1
29	O	71.11845	87.53373	72.31510	-317.80580	-363.38227	484.43082		1
30	H	70.69124	86.68720	72.55315	1863.74748	-1451.84923	1357.29467		1
31	C	72.55869	88.64123	74.10884	503.80731	517.99032	318.51606		1
32	H	71.71737	88.72491	74.83557	640.61020	-2157.10410	-1536.29104		1
33	H	73.49639	88.50410	74.69946	1687.88455	465.60692	2087.56452		1
34	H	72.64074	89.62010	73.58144	-1293.07895	-1899.88581	-1463.57452		1
35	C	74.99702	87.38342	73.20721	-153.07550	-733.68902	248.70981		1
36	O	75.45737	88.45165	73.52501	186.15459	-480.78787	-449.34387		1
37	N	75.36297	86.16954	73.64924	-487.53139	543.18517	42.03850		1
38	C	76.54222	86.03904	74.44941	-699.35871	69.34393	360.10701		1
39	H	76.75729	87.05295	74.86445	2.81126	-221.99807	-2715.58072		1

40	C	76.08375	84.93341	75.50225	-507.46439	-592.59194	122.07761	1
41	H	76.94623	84.44171	76.01873	-1975.08116	525.87560	-1801.71556	1
42	H	75.43617	85.36824	76.29607	1588.27743	-1913.22100	1113.83566	1
43	C	75.27973	83.96620	74.58128	-613.62442	-457.55993	-194.14490	1
44	H	75.96499	83.30306	74.00665	1707.54637	-721.27992	1996.92523	1
45	H	74.59026	83.29520	75.14116	758.23357	2100.81767	1560.55011	1
46	C	74.52056	84.98110	73.62215	-352.41524	704.96076	49.21465	1
47	H	74.45022	84.64619	72.56143	1714.76886	-2070.42778	443.35792	1
48	H	73.51449	85.30202	73.97777	1224.15040	1801.50881	1636.97633	1
49	C	77.78393	85.41339	73.59380	566.85117	537.05831	117.62814	1
50	O	78.76891	84.99468	74.21530	-550.26779	-406.08867	4.21666	1
51	N	77.57499	85.44289	72.30388	566.34832	-425.77725	180.18749	1
52	H	76.67665	85.85408	72.05352	644.44502	2646.80550	-52.73430	1
53	C	78.54433	85.09084	71.33156	612.34801	-281.48662	411.56221	1
54	H	78.06293	85.35837	70.36566	1667.23498	-1490.75142	1556.16753	1
55	C	79.84765	85.96986	71.63180	-714.45746	-175.43074	286.98927	1
56	H	80.12007	85.87124	72.72126	-787.09484	1763.03619	-1922.46060	1
57	O	79.67998	87.38370	71.40881	-429.46514	516.51932	-128.40526	1
58	H	79.73919	87.72835	72.32148	1981.82785	436.16847	-1818.18182	1
59	C	80.95662	85.26717	70.76946	630.79189	-468.94448	76.03230	1
60	H	81.94007	85.78095	70.88058	-1775.71861	2062.30353	131.89849	1
61	H	81.11012	84.20258	71.07555	-1855.14608	88.94118	1993.53760	1
62	H	80.69941	85.27488	69.68462	-1504.82350	-780.94249	-2132.90992	1
63	C	78.83821	83.48124	71.43597	288.57638	618.62814	-397.00270	1
64	O	78.50655	82.76382	70.52405	321.70495	-185.26452	574.37218	1
65	N	79.44342	83.15983	72.57227	-447.05792	-446.53431	367.76425	1
66	H	79.68985	83.88747	73.28931	350.31316	1975.63644	-1843.31522	1
67	C	79.94249	81.82645	72.68945	-511.23061	374.03917	-471.51480	1
68	H	79.17454	81.21393	72.16022	2234.79579	-898.70890	-1273.45190	1
69	C	81.33773	81.78739	71.88287	529.53781	-159.34528	563.72604	1
70	H	81.69807	80.72650	71.91868	654.59388	2347.94251	1217.51488	1
71	H	81.09126	82.01196	70.80853	-1526.55661	2103.42026	817.87394	1
72	O	82.34809	82.73527	72.29893	-554.84278	14.12789	399.58769	1
73	H	82.78193	82.20964	73.00060	1297.06236	2061.84854	1220.68812	1
74	C	80.16132	81.44770	74.23786	-662.15484	-412.13544	123.62687	1
75	O	80.89797	80.51958	74.53836	-540.01537	-317.05804	274.91456	1
76	N	79.46035	82.21684	75.05827	-202.76299	-690.00100	-131.49145	1
77	H	78.87691	82.94529	74.63770	-702.62132	-2617.37191	281.70413	1
78	C	79.48694	82.00914	76.50528	-491.73914	576.34187	222.73509	1
79	H	80.56225	81.76816	76.67959	1977.17978	-1823.58850	-434.68928	1
80	C	79.00431	83.27801	77.18204	-649.50797	-328.66843	306.11224	1
81	H	77.99712	83.53028	76.76268	2075.07803	1452.16490	-1004.45904	1
82	C	78.85880	83.10064	78.68196	-615.18735	-489.99689	-70.96352	1
83	H	78.49771	84.04360	79.17846	-1226.32661	-1724.38906	-1716.47170	1
84	H	78.11928	82.28660	78.92818	2381.64273	-969.84735	900.46860	1
85	H	79.83654	82.82298	79.16428	2122.74991	1702.23946	-141.36228	1
86	C	79.93137	84.44398	76.89302	-501.86074	-479.61276	-376.42482	1
87	H	79.55985	85.39870	77.35703	993.79261	-2246.95401	-1177.81305	1
88	H	80.96858	84.26001	77.28817	42.71279	-626.15391	-2651.37258	1
89	H	80.01832	84.62349	75.77579	-2026.39012	-1590.33709	-887.82922	1
90	C	78.52576	80.67945	76.81273	-672.89153	382.57394	-156.34072	1
91	O	77.44925	80.78913	77.33673	410.04627	221.86223	500.35950	1
92	N	79.21579	79.61104	76.47670	-378.11782	-443.79414	-441.10984	1
93	H	80.12066	79.75501	75.97924	2404.15973	-568.14894	1149.30085	1
94	C	78.62917	78.30372	76.41676	-544.54484	466.16019	331.29119	1
95	H	79.41395	77.66631	76.88765	-1409.80988	-170.17955	2325.32679	1
96	C	77.23797	78.23347	77.15325	-184.48284	116.78282	-758.89137	1
97	H	77.30358	78.66915	78.17864	1893.78641	1861.14652	611.04528	1
98	H	76.47801	78.84943	76.61451	-2170.79665	-974.19311	1327.50117	1
99	C	76.86392	76.71298	77.17927	389.51668	672.81878	-138.49152	1
100	H	76.83304	76.31562	76.13960	510.64577	1933.03327	1851.02484	1
101	H	77.68294	76.13140	77.65664	-2302.30869	-1105.72939	-948.89774	1

102	C	75.51463	76.37352	77.90457	-559.93427	-126.34590	542.30857	1
103	O	75.17360	75.21802	78.01759	-670.36003	-111.83166	76.36448	1
104	N	74.85592	77.45823	78.35411	-216.06729	-537.07037	446.51379	1
105	H	75.10792	78.45148	78.27721	-1251.96487	1074.12894	-2168.52500	1
106	H	73.96089	77.42469	78.85427	-2451.83023	-720.73851	944.84612	1
107	C	78.44231	77.95124	74.82860	546.24052	-563.88337	-85.11809	1
108	O	77.49122	78.36686	74.22119	71.70702	-307.40463	606.69673	1
109	N	79.46440	77.19723	74.39725	479.90863	-504.50129	222.86849	1
110	C	79.40629	76.50857	73.14471	75.51268	-600.91904	506.73700	1
111	H	78.86136	77.16837	72.43077	-2033.61562	1795.30103	254.89480	1
112	C	80.94546	76.26641	72.82740	523.79067	517.99274	284.45581	1
113	H	81.11431	75.43411	72.10799	1599.61665	-1127.00911	1895.98173	1
114	H	81.42215	77.17205	72.39039	-1881.83093	1275.82488	-1501.55016	1
115	C	81.49945	75.96731	74.25373	-600.05639	-404.05026	316.64485	1
116	H	81.22326	74.93895	74.57997	-2597.05260	496.36221	657.73249	1
117	H	82.60747	76.04273	74.33238	-1666.24518	1294.38985	-1723.90591	1
118	C	80.73182	77.06932	75.10367	493.57570	-129.95376	-602.56394	1
119	H	80.53340	76.78530	76.16838	-1469.08415	-637.84797	2204.22581	1
120	H	81.18774	78.08844	75.07057	-1038.97840	1068.88701	-2280.71789	1
121	C	78.65834	75.07430	73.37916	188.88100	241.05089	-727.87821	1
122	O	78.36880	74.64253	74.46668	531.88613	-49.19943	427.07960	1
123	N	78.57347	74.40392	72.17925	708.14833	26.93417	-179.73509	1
124	H	78.76867	75.16248	71.51600	-2232.69501	-1179.09831	1023.94816	1
125	C	77.42174	73.49329	71.98122	-738.32412	259.92548	104.42456	1
126	H	76.52786	74.09136	72.26933	2028.89123	1260.02983	1311.33324	1
127	C	77.43288	73.06894	70.53618	-258.65678	-345.52513	661.28459	1
128	H	78.48965	72.86192	70.25224	-1826.06090	-1801.46097	-918.64554	1
129	C	76.62858	71.79961	70.30989	-541.23400	531.92970	-218.41428	1
130	H	76.58864	71.51875	69.22183	1311.73218	-2219.18200	882.19023	1
131	H	77.07331	70.92615	70.86136	-1048.71298	1223.58118	-2196.97971	1
132	H	75.56753	71.91009	70.66573	419.06414	1903.92898	1903.44670	1
133	C	76.90815	74.16177	69.61968	-423.86431	152.66566	-648.55262	1
134	H	76.95694	73.85594	68.53866	105.68386	-2342.50080	1387.51238	1
135	H	75.83481	74.40929	69.84607	-1695.63603	-1484.73621	-1531.02793	1
136	H	77.49730	75.11330	69.72493	-1853.57121	-487.39031	1936.59343	1
137	C	77.66924	72.19166	72.96829	539.71428	-510.58232	267.58633	1
138	O	78.64198	71.47986	72.85167	-15.93758	-278.34085	-624.49402	1
139	N	76.58600	71.99553	73.71595	-676.81886	12.05292	276.17960	1
140	H	75.87792	72.72267	73.63426	-1694.44250	-373.84189	-2100.66098	1
141	C	76.71960	71.25468	74.93916	412.33078	-664.70360	108.35451	1
142	H	77.76413	71.47344	75.25428	1765.77476	1294.44366	1621.76594	1
143	C	75.62528	71.85864	75.89193	-179.66635	-721.95667	-264.73915	1
144	H	75.64727	72.97144	75.84149	-607.34922	2587.87032	-598.10018	1
145	H	74.60591	71.56325	75.55554	-359.69332	-1479.13954	-2259.74260	1
146	C	75.87590	71.38216	77.36946	-240.01076	616.02425	431.85322	1
147	H	75.74486	70.27636	77.44779	-1359.17131	782.54425	2227.99181	1
148	H	76.92090	71.60011	77.68797	-820.36667	85.81767	-2596.78715	1
149	C	74.84949	72.15330	78.26076	-513.07015	236.18570	-551.87280	1
150	H	74.95923	73.27679	78.14877	1816.11944	-1183.11722	-1650.94321	1
151	H	73.80306	71.91425	77.95766	-1800.04429	-1361.53473	1526.34643	1
152	C	75.10067	71.72001	79.77833	726.08972	-253.19732	-179.64713	1
153	H	74.98049	70.62171	79.94805	1224.27271	-456.51798	-2390.90304	1
154	H	76.08552	72.05279	80.19068	1206.40339	-1150.93514	-2154.90344	1
155	N	74.08889	72.37555	80.55791	329.70796	-633.68968	-155.67358	1
156	H	74.10304	70.19372	82.05419	1348.31305	1938.76845	1359.00643	1
157	H	74.24086	72.35775	81.56211	2096.92035	1446.54551	-966.48890	1
158	H	73.16657	71.95603	80.48864	-1197.07217	-2303.53719	827.28733	1
159	C	76.51732	69.64846	74.67528	-378.01186	-556.17301	-413.96481	1
160	O	76.24063	68.90714	75.58739	-409.44433	-307.55053	-453.30833	1
161	N	76.76410	69.36803	73.40284	-429.02477	524.70884	274.08502	1
162	H	77.05083	70.16915	72.82952	1706.34263	-1425.96036	1574.38926	1
163	C	76.78393	68.06586	72.84602	-45.25864	-626.22952	478.93267	1

164	H	77.06976	68.26267	71.78868	1988.63164	570.90773	1772.87287	1
165	C	77.87866	67.23042	73.62319	551.77128	-20.49526	-564.54996	1
166	H	78.86983	67.73309	73.55296	1434.61535	-1753.10253	1513.99471	1
167	H	77.65323	67.18212	74.71298	-714.67738	1819.09770	1898.36494	1
168	C	77.91871	65.80959	72.96860	446.99263	-555.77305	338.97221	1
169	H	76.96742	65.25805	73.16024	1953.68466	1892.25957	-161.67766	1
170	H	78.00615	65.89433	71.86205	-403.03785	2688.07032	-188.43591	1
171	C	79.15352	65.01323	73.55269	567.86262	335.74681	434.04421	1
172	H	80.10641	65.56187	73.37096	-1080.02275	1568.26081	-1948.78900	1
173	H	79.07156	64.90312	74.65826	-919.54108	2111.34692	1456.13463	1
174	C	79.17081	63.63193	72.85653	195.81897	173.33862	-745.11536	1
175	H	78.29815	62.98930	73.08927	1405.67949	-2301.21089	-390.08113	1
176	H	79.33003	63.66979	71.76023	-940.37328	-1118.32446	2299.72133	1
177	N	80.40437	62.83647	73.40084	319.26422	656.36007	-42.02424	1
178	H	80.52309	61.85771	73.00928	1961.03633	619.91968	1787.09422	1
179	H	81.36624	63.24925	73.22330	854.14343	-2156.80752	1429.08711	1
180	H	80.43470	62.64671	74.44463	1237.02905	-1378.50857	-1998.28500	1
181	C	75.26911	67.41778	72.94018	532.53319	-268.57236	517.55729	1
182	O	74.48005	67.63652	72.05170	266.16714	-290.73804	-558.88002	1
183	N	75.09326	66.71327	74.04783	-226.25352	640.49678	-270.32839	1
184	H	75.86344	66.67685	74.71227	2007.69063	-1035.27229	1523.50231	1
185	C	73.95362	65.83615	74.12718	-540.76542	-573.33303	49.50000	1
186	H	73.74121	65.54513	73.07143	-2374.20950	-1036.76023	843.75774	1
187	C	74.45079	64.60066	75.03573	-77.09082	666.87422	-415.84136	1
188	H	74.75871	64.99772	76.04097	-985.81834	617.19825	2463.91927	1
189	O	75.59656	63.91031	74.50870	293.29899	-391.65602	-477.80926	1
190	H	76.23615	64.03186	75.23976	2528.72714	-681.76262	-751.27122	1
191	C	73.15308	63.73650	75.21524	252.47363	-605.14473	440.05134	1
192	H	73.34812	62.83419	75.84088	-2052.65063	1456.49051	-1043.51830	1
193	H	72.33295	64.31004	75.71217	-2152.98800	-1661.97574	-161.70652	1
194	H	72.76073	63.37997	74.23426	-473.12726	-1584.27339	2165.61725	1
195	C	72.71938	66.63884	74.72613	360.36307	488.46713	505.10056	1
196	O	71.49574	66.08771	74.60198	-200.08817	-528.03552	-385.82850	1
197	N	73.01986	67.70219	75.36084	-597.54095	-226.44775	355.20479	1
198	H	74.03831	67.84221	75.26848	2179.23655	-1300.70981	-991.33835	1
199	C	72.16898	68.75131	75.80939	-687.68921	297.39807	-249.45179	1
200	H	72.57840	69.64161	75.28766	-349.16256	-2467.37713	-1101.72831	1
201	C	70.61024	68.48615	75.53245	672.47345	361.54328	-201.62880	1
202	H	70.30748	67.49266	75.95587	1541.41502	582.18425	2169.97026	1
203	H	69.98901	69.27195	76.02797	-2534.67717	60.25153	997.72295	1
204	C	70.41479	68.50480	74.02832	574.26774	-389.43119	-377.02542	1
205	C	70.21239	69.66991	73.26034	688.82679	-287.33580	-257.96133	1
206	H	70.11322	70.66060	73.74626	331.14182	1470.38163	2269.80013	1
207	C	70.50390	67.15054	73.41792	-383.52382	-675.04808	144.24917	1
208	H	69.80383	66.35276	73.85730	4.09847	1517.59662	2262.86397	1
209	C	70.18591	69.54224	71.85914	-134.76730	428.45285	-649.50303	1
210	H	70.03854	70.44712	71.24775	-903.23433	1600.49020	2011.53387	1
211	C	70.56626	67.14567	71.94664	-335.53281	-615.00040	-364.39058	1
212	H	70.70963	66.18752	71.42751	1596.45398	-1369.33862	1732.02659	1
213	C	70.37374	68.29734	71.18637	585.48547	-340.24194	-406.23938	1
214	O	70.35662	68.29345	69.72794	-419.15649	-173.04408	-511.94141	1
215	H	70.59153	67.36682	69.56569	-1071.84350	1559.71507	-1960.13012	1
216	C	72.29817	68.91992	77.42405	291.41878	-183.13091	710.72246	1
217	O	72.51564	70.02669	77.90382	379.87695	523.47396	-222.23622	1
218	N	72.02083	67.78782	78.04610	564.30591	373.09380	277.24371	1
219	H	71.83393	66.99133	77.43636	-120.59931	-2436.07824	-1214.35098	1
220	C	72.09585	67.62183	79.45464	404.07514	-299.37480	608.84009	1
221	H	72.19384	66.52213	79.60223	-1071.07882	-841.69025	2359.66467	1
222	C	73.32010	68.47571	79.99146	-683.12807	68.71770	-390.13096	1
223	H	74.24325	68.27586	79.40287	2068.88918	1596.58590	770.89603	1
224	H	73.11272	69.56846	79.86520	1379.86429	2342.49779	-179.85638	1
225	C	73.50427	68.11194	81.50454	-176.39967	537.49466	550.97268	1

226	H	72.52142	68.14243	82.03531	-396.28051	1942.22168	1869.33314	1
227	H	73.88652	67.07232	81.62149	-94.44700	586.00678	-2659.20016	1
228	C	74.50425	69.15550	82.11677	-291.69381	-718.18079	-150.72929	1
229	H	75.48563	69.14393	81.58768	-2303.38776	1089.76242	964.62032	1
230	H	74.70884	68.94448	83.19629	884.16729	2568.80533	-207.74283	1
231	N	75.71331	68.74671	84.77664	-594.49522	-252.81478	342.29276	2
232	H	75.72420	68.06537	85.52604	-1735.17426	2084.05705	-263.71605	2
233	C	76.54388	69.69533	84.98847	595.23177	-271.52487	442.22352	2
234	N	76.72039	70.80573	84.05041	585.53813	-424.79750	-105.81303	2
235	H	76.44469	70.64373	83.08912	959.88797	1327.56823	-2177.11905	2
236	H	77.68259	71.11681	83.96527	1578.48647	16.27378	-2220.76233	2
237	N	77.36598	69.70619	86.19905	-452.17763	-390.33541	-421.51853	2
238	H	76.98872	69.29075	87.04371	470.26107	1974.25629	-1817.92087	2
239	H	77.60651	70.64979	86.48496	1856.67307	-1573.97321	-1224.35416	2
240	C	70.78027	68.22750	80.21510	-531.47271	-581.45780	-55.06206	1
241	O	70.41281	67.73736	81.25113	-243.00837	192.73507	609.52485	1
242	N	70.33913	69.33979	79.62271	343.49288	-644.25607	38.09164	1
243	H	70.84644	69.65946	78.78214	-1691.16043	-1535.97525	-1484.73099	1
244	C	69.02738	69.88772	79.99980	542.66492	350.14337	454.42563	1
245	H	68.74543	69.25711	80.87985	1209.57979	-2396.95920	463.86744	1
246	C	69.19446	71.35886	80.35732	-737.14309	145.93010	242.71942	1
247	H	69.46299	71.90663	79.42684	-1050.18303	159.36419	-2509.06125	1
248	C	67.90974	71.95165	80.90288	-706.77696	-252.88343	-245.16230	1
249	H	68.01541	73.04945	81.12423	-1624.64039	-1665.49085	1417.86935	1
250	H	67.05675	71.83483	80.16841	2566.10521	598.51109	693.22305	1
251	H	67.59484	71.44863	81.85874	-1972.69758	107.10018	-1876.34312	1
252	C	70.32083	71.56287	81.35405	412.85148	672.58832	-27.69222	1
253	H	70.51302	72.65293	81.55397	1447.02277	1762.76533	-1490.78944	1
254	H	70.08907	71.07606	82.34130	1320.77379	-145.20455	2378.68491	1
255	H	71.28095	71.11032	80.98289	-1512.10848	1470.52031	1724.75147	1
256	C	68.00552	69.69326	78.72827	-607.11113	499.56689	73.73769	1
257	O	67.02008	70.39346	78.63778	357.97126	460.81534	356.68785	1
258	N	68.39623	68.71626	77.90867	536.55407	-368.62270	332.76306	1
259	H	69.27428	68.25845	78.18541	524.38866	2297.69985	1367.20941	1
260	C	67.35483	67.77383	77.55512	46.50277	-774.29190	-147.97904	1
261	H	66.61471	67.82423	78.38345	1676.51875	1883.29066	1032.55549	1
262	C	66.69798	68.16856	76.13855	-559.41456	-34.19198	-556.30433	1
263	H	67.48738	68.59646	75.47509	-64.66664	395.18769	2695.05373	1
264	H	66.31247	67.25978	75.61609	-2703.44278	-60.40056	333.79418	1
265	C	65.58007	69.15462	76.35077	-519.76435	377.31045	459.42366	1
266	H	65.93860	69.94502	77.07363	-1746.74323	1667.50644	-1261.73691	1
267	C	65.20349	69.81886	75.03318	570.95554	16.46261	-545.27700	1
268	H	64.39951	70.58727	75.17224	2391.58273	28.05277	-1305.07271	1
269	H	66.07993	70.33567	74.56353	175.75588	917.63458	2559.43867	1
270	H	64.82174	69.07157	74.29023	-1063.97851	-2155.34650	1283.00462	1
271	C	64.34959	68.48655	76.94814	193.76014	2.62946	-765.53141	1
272	H	63.51308	69.21908	77.09015	507.39394	-846.55087	2539.60089	1
273	H	63.96263	67.66592	76.29060	1337.57841	1818.19054	1526.01994	1
274	H	64.56468	68.03548	77.95083	1100.88635	-1172.91350	-2199.08909	1
275	C	68.09667	66.37057	77.42577	-549.21115	475.64486	-309.38218	1
276	O	69.28802	66.24741	77.58025	556.06106	-390.37755	-78.24250	1
277	O	67.29731	65.25079	77.08762	-572.27940	-310.19032	-209.75862	1
278	H	66.40256	65.68846	77.10308	-1380.08193	2212.14486	790.85944	1

Listing 95: C00095.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	1.4615	5846
		0.2500	300.00	0.00	0.00	0.00	-1293.4429	0.0000	300.0000
3	H	68.73413	74.71237	66.33684	-2043.14101	-1757.64893	399.89339		1
4	N	69.31873	75.26091	66.96709	426.75047	490.45733	-334.42467		1
5	H	69.67105	74.56061	67.63452	442.25559	-1110.30854	-2448.52907		1

6	C	70.38829	75.92082	66.32218	415.32972	-666.39213	83.73172	1
7	H	70.14154	75.98903	65.24009	879.32219	2491.00447	667.35213	1
8	C	70.56939	77.37015	67.00735	31.35357	477.41777	628.23362	1
9	H	70.76082	77.24016	68.09920	1168.38489	2240.25337	-1019.71136	1
10	H	71.46414	77.89572	66.59505	-360.43770	2534.90498	931.67112	1
11	C	69.31416	78.17119	66.78271	463.18208	512.70242	-382.34388	1
12	H	68.44356	77.52160	67.02923	1725.29117	1863.52247	-987.07854	1
13	C	69.28146	79.38784	67.69938	710.42801	-144.27427	-313.15367	1
14	H	68.33869	79.97923	67.56767	364.20195	-1033.13725	2494.72524	1
15	H	69.34194	79.09507	68.77936	2567.61904	335.80679	847.48802	1
16	H	70.13800	80.08069	67.49487	-2587.99029	680.92867	-512.16411	1
17	C	69.19041	78.62597	65.33475	268.17616	741.64379	-40.42634	1
18	H	68.25641	79.22258	65.16841	1283.54314	-1945.37420	-1411.27812	1
19	H	70.05394	79.27205	65.03069	-1258.57796	1317.15249	-2026.02085	1
20	H	69.15880	77.75862	64.62669	-2502.84526	909.80597	575.92391	1
21	C	71.65086	74.95599	66.65975	619.36578	-458.64843	-172.09273	1
22	O	71.58551	74.09070	67.51601	-81.40433	433.87611	522.34594	1
23	N	72.68356	75.28283	65.89199	175.23996	-622.20190	341.55523	1
24	H	72.60380	76.07385	65.25445	-876.57256	-303.22879	-2561.90213	1
25	C	73.87378	74.51415	66.01707	-571.88214	-534.10783	-106.15033	1
26	H	73.53478	73.54625	66.45220	-2713.20841	-16.25800	-248.80809	1
27	C	74.52476	74.41620	64.55698	166.60354	288.16399	-716.09568	1
28	H	74.74403	75.46013	64.20306	-2097.85574	1636.78449	-586.18044	1
29	O	73.68027	73.82166	63.55343	-317.80580	-363.38227	484.43082	1
30	H	73.57959	74.56540	62.92813	1863.74748	-1451.84923	1357.29467	1
31	C	75.88383	73.66827	64.81064	503.80731	517.99032	318.51606	1
32	H	76.50408	73.63634	63.88458	640.61020	-2157.10410	-1536.29104	1
33	H	76.51289	74.15520	65.61391	1687.88455	465.60692	2087.56452	1
34	H	75.71282	72.61109	65.11971	-1293.07895	-1899.88581	-1463.57452	1
35	C	74.88307	75.35568	66.99289	-153.07550	-733.68902	248.70981	1
36	O	75.01358	76.54030	66.84491	186.15459	-480.78787	-449.34387	1
37	N	75.52513	74.51965	67.81883	-487.53139	543.18517	42.03850	1
38	C	76.58274	74.97193	68.67357	-699.35871	69.34393	360.10701	1
39	H	76.25656	75.95435	69.08490	2.81126	-221.99807	-2715.58072	1
40	C	76.69564	73.79929	69.73471	-507.46439	-592.59194	122.07761	1
41	H	77.73558	73.70703	70.16679	-1975.08116	525.87560	-1801.71556	1
42	H	75.99904	73.95255	70.58998	1588.27743	-1913.22100	1113.83566	1
43	C	76.29973	72.54661	68.89361	-613.62442	-457.55993	-194.14490	1
44	H	77.14676	72.21621	68.25114	1707.54637	-721.27992	1996.92523	1
45	H	76.00222	71.66803	69.50963	758.23357	2100.81767	1560.55011	1
46	C	75.10929	73.13860	68.02370	-352.41524	704.96076	49.21465	1
47	H	74.96112	72.64852	67.03347	1714.76886	-2070.42778	443.35792	1
48	H	74.12818	73.19684	68.55393	1224.15040	1801.50881	1636.97633	1
49	C	77.97674	75.11100	67.82701	566.85117	537.05831	117.62814	1
50	O	78.13113	74.62024	66.73044	-550.26779	-406.08867	4.21666	1
51	N	78.85557	75.74523	68.59478	566.34832	-425.77725	180.18749	1
52	H	78.50875	76.07024	69.49578	644.44502	2646.80550	-52.73430	1
53	C	80.03419	76.29589	68.00521	612.34801	-281.48662	411.56221	1
54	H	79.80478	76.41128	66.92110	1667.23498	-1490.75142	1556.16753	1
55	C	80.32968	77.65342	68.80258	-714.45746	-175.43074	286.98927	1
56	H	80.45491	77.39841	69.89151	-787.09484	1763.03619	-1922.46060	1
57	O	79.28395	78.63972	68.75188	-429.46514	516.51932	-128.40526	1
58	H	79.04293	78.71185	69.69724	1981.82785	436.16847	-1818.18182	1
59	C	81.72180	78.10162	68.22572	630.79189	-468.94448	76.03230	1
60	H	82.11206	79.00142	68.75547	-1775.71861	2062.30353	131.89849	1
61	H	82.49357	77.30053	68.32538	-1855.14608	88.94118	1993.53760	1
62	H	81.64935	78.35907	67.14355	-1504.82350	-780.94249	-2132.90992	1
63	C	81.28474	75.29505	68.27060	288.57638	618.62814	-397.00270	1
64	O	82.18116	75.20265	67.47434	321.70495	-185.26452	574.37218	1
65	N	81.24732	74.84451	69.54618	-447.05792	-446.53431	367.76425	1
66	H	80.32056	74.88049	70.02067	350.31316	1975.63644	-1843.31522	1
67	C	81.92530	73.57954	69.72546	-511.23061	374.03917	-471.51480	1

68	H	82.33587	73.29668	68.72779	2234.79579	-898.70890	-1273.45190	1
69	C	83.06510	73.74920	70.83968	529.53781	-159.34528	563.72604	1
70	H	83.55369	72.74151	70.94376	654.59388	2347.94251	1217.51488	1
71	H	83.84337	74.43893	70.42072	-1526.55661	2103.42026	817.87394	1
72	O	82.62844	74.16324	72.15852	-554.84278	14.12789	399.58769	1
73	H	82.83653	75.11562	72.10350	1297.06236	2061.84854	1220.68812	1
74	C	80.69959	72.68064	70.24384	-662.15484	-412.13544	123.62687	1
75	O	79.59263	73.20135	70.38559	-540.01537	-317.05804	274.91456	1
76	N	81.06398	71.42868	70.48196	-202.76299	-690.00100	-131.49145	1
77	H	82.04415	71.22064	70.28596	-702.62132	-2617.37191	281.70413	1
78	C	80.07324	70.35987	70.61707	-491.73914	576.34187	222.73509	1
79	H	79.22784	70.67607	69.96021	1977.17978	-1823.58850	-434.68928	1
80	C	80.73708	69.06509	70.18053	-649.50797	-328.66843	306.11224	1
81	H	81.68673	68.96136	70.75145	2075.07803	1452.16490	-1004.45904	1
82	C	79.87153	67.85622	70.48137	-615.18735	-489.99689	-70.96352	1
83	H	80.38921	66.89419	70.21218	-1226.32661	-1724.38906	-1716.47170	1
84	H	79.60281	67.80361	71.57572	2381.64273	-969.84735	900.46860	1
85	H	78.90432	67.88781	69.90766	2122.74991	1702.23946	-141.36228	1
86	C	81.08691	69.09433	68.70321	-501.86074	-479.61276	-376.42482	1
87	H	81.66601	68.18222	68.39161	993.79261	-2246.95401	-1177.81305	1
88	H	80.16309	69.13660	68.06307	42.71279	-626.15391	-2651.37258	1
89	H	81.70871	69.99404	68.44081	-2026.39012	-1590.33709	-887.82922	1
90	C	79.58380	70.30618	72.20249	-672.89153	382.57394	-156.34072	1
91	O	78.61359	69.64729	72.49422	410.04627	221.86223	500.35950	1
92	N	80.37453	70.98935	73.01276	-378.11782	-443.79414	-441.10984	1
93	H	81.15599	71.48805	72.59093	2404.15973	-568.14894	1149.30085	1
94	C	79.92700	71.17765	74.36075	-544.54484	466.16019	331.29119	1
95	H	78.82052	71.08060	74.26503	-1409.80988	-170.17955	2325.32679	1
96	C	80.55503	69.99747	75.21554	-184.48284	116.78282	-758.89137	1
97	H	80.32270	69.01564	74.74378	1893.78641	1861.14652	611.04528	1
98	H	81.66579	70.07387	75.24034	-2170.79665	-974.19311	1327.50117	1
99	C	79.95437	70.09130	76.65179	389.51668	672.81878	-138.49152	1
100	H	80.25760	71.05540	77.12289	510.64577	1933.03327	1851.02484	1
101	H	78.84463	70.14847	76.60208	-2302.30869	-1105.72939	-948.89774	1
102	C	80.37184	68.89088	77.58296	-559.93427	-126.34590	542.30857	1
103	O	79.94747	68.84895	78.70876	-670.36003	-111.83166	76.36448	1
104	N	81.18914	67.98882	76.99891	-216.06729	-537.07037	446.51379	1
105	H	81.59090	67.98155	76.05395	-1251.96487	1074.12894	-2168.52500	1
106	H	81.55515	67.15649	77.47364	-2451.83023	-720.73851	944.84612	1
107	C	80.45864	72.61995	74.90376	546.24052	-563.88337	-85.11809	1
108	O	81.25474	72.63317	75.80503	71.70702	-307.40463	606.69673	1
109	N	79.87990	73.64818	74.26510	479.90863	-504.50129	222.86849	1
110	C	80.25153	75.00234	74.53141	75.51268	-600.91904	506.73700	1
111	H	81.31964	75.00274	74.85109	-2033.61562	1795.30103	254.89480	1
112	C	79.94769	75.67200	73.11727	523.79067	517.99274	284.45581	1
113	H	79.87511	76.78128	73.16634	1599.61665	-1127.00911	1895.98173	1
114	H	80.74565	75.42775	72.37787	-1881.83093	1275.82488	-1501.55016	1
115	C	78.60590	74.97975	72.73320	-600.05639	-404.05026	316.64485	1
116	H	77.74713	75.43110	73.27780	-2597.05260	496.36221	657.73249	1
117	H	78.36831	75.05139	71.64859	-1666.24518	1294.38985	-1723.90591	1
118	C	78.88644	73.48937	73.21173	493.57570	-129.95376	-602.56394	1
119	H	78.00643	72.95545	73.64080	-1469.08415	-637.84797	2204.22581	1
120	H	79.37425	72.83785	72.44230	-1038.97840	1068.88701	-2280.71789	1
121	C	79.23552	75.59994	75.66106	188.88100	241.05089	-727.87821	1
122	O	78.23016	75.02777	76.00672	531.88613	-49.19943	427.07960	1
123	N	79.64139	76.83831	75.98359	708.14833	26.93417	-179.73509	1
124	H	80.55933	77.05468	75.59648	-2232.69501	-1179.09831	1023.94816	1
125	C	79.11468	77.50179	77.18761	-738.32412	259.92548	104.42456	1
126	H	79.32914	76.80207	78.02711	2028.89123	1260.02983	1311.33324	1
127	C	79.80427	78.83951	77.30737	-258.65678	-345.52513	661.28459	1
128	H	79.80476	79.31487	76.30033	-1826.06090	-1801.46097	-918.64554	1
129	C	79.06738	79.76653	78.25895	-541.23400	531.92970	-218.41428	1

130	H	79.55211	80.77989	78.31242	1311.73218	-2219.18200	882.19023	1
131	H	77.99970	79.92149	77.93854	-1048.71298	1223.58118	-2196.97971	1
132	H	79.04206	79.35182	79.30372	419.06414	1903.92898	1903.44670	1
133	C	81.25248	78.70619	77.74604	-423.86431	152.66566	-648.55262	1
134	H	81.77616	79.70149	77.75505	105.68386	-2342.50080	1387.51238	1
135	H	81.33181	78.28012	78.78344	-1695.63603	-1484.73621	-1531.02793	1
136	H	81.83461	78.02809	77.06403	-1853.57121	-487.39031	1936.59343	1
137	C	77.48194	77.68114	76.94029	539.71428	-510.58232	267.58633	1
138	O	76.70375	77.41602	77.85573	-15.93758	-278.34085	-624.49402	1
139	N	77.23790	78.23088	75.76947	-676.81886	12.05292	276.17960	1
140	H	78.14368	78.31874	75.30392	-1694.44250	-373.84189	-2100.66098	1
141	C	76.01944	78.17288	75.04620	412.33078	-664.70360	108.35451	1
142	H	76.31326	78.52819	74.03290	1765.77476	1294.44366	1621.76594	1
143	C	75.51882	76.66978	75.05805	-179.66635	-721.95667	-264.73915	1
144	H	76.31389	75.96556	74.72300	-607.34922	2587.87032	-598.10018	1
145	H	75.25370	76.34678	76.08986	-359.69332	-1479.13954	-2259.74260	1
146	C	74.27384	76.66107	74.11045	-240.01076	616.02425	431.85322	1
147	H	73.54615	77.44196	74.43156	-1359.17131	782.54425	2227.99181	1
148	H	74.56248	76.92506	73.06827	-820.36667	85.81767	-2596.78715	1
149	C	73.59597	75.23516	74.16435	-513.07015	236.18570	-551.87280	1
150	H	74.27419	74.44684	73.76377	1816.11944	-1183.11722	-1650.94321	1
151	H	73.36984	74.94094	75.21506	-1800.04429	-1361.53473	1526.34643	1
152	C	72.29900	75.34808	73.32646	726.08972	-253.19732	-179.64713	1
153	H	71.62106	76.17313	73.63376	1224.27271	-456.51798	-2390.90304	1
154	H	72.45255	75.38088	72.22881	1206.40339	-1150.93514	-2154.90344	1
155	N	71.46767	74.05070	73.58853	329.70796	-633.68968	-155.67358	1
156	H	70.50485	74.03965	73.14302	1348.31305	1938.76845	1359.00643	1
157	H	71.87991	73.15040	73.20824	2096.92035	1446.54551	-966.48890	1
158	H	71.24012	73.77946	74.58975	-1197.07217	-2303.53719	827.28733	1
159	C	74.82131	79.08746	75.70232	-378.01186	-556.17301	-413.96481	1
160	O	74.24279	79.84584	74.96474	-409.44433	-307.55053	-453.30833	1
161	N	74.57622	78.78121	76.96521	-429.02477	524.70884	274.08502	1
162	H	75.21033	78.10192	77.46894	1706.34263	-1425.96036	1574.38926	1
163	C	73.75702	79.64955	77.74710	-45.25864	-626.22952	478.93267	1
164	H	74.16052	79.48150	78.77137	1988.63164	570.90773	1772.87287	1
165	C	73.93959	81.13825	77.23491	551.77128	-20.49526	-564.54996	1
166	H	75.00857	81.35588	77.01077	1434.61535	-1753.10253	1513.99471	1
167	H	73.38656	81.29790	76.27466	-714.67738	1819.09770	1898.36494	1
168	C	73.38471	82.07549	78.35922	446.99263	-555.77305	338.97221	1
169	H	72.31210	81.83278	78.55747	1953.68466	1892.25957	-161.67766	1
170	H	73.92295	81.90845	79.31896	-403.03785	2688.07032	-188.43591	1
171	C	73.53429	83.57724	77.88752	567.86262	335.74681	434.04421	1
172	H	74.60633	83.86706	77.79402	-1080.02275	1568.26081	-1948.78900	1
173	H	73.08899	83.72539	76.87675	-919.54108	2111.34692	1456.13463	1
174	C	72.80543	84.44102	78.94344	195.81897	173.33862	-745.11536	1
175	H	71.71562	84.25220	79.01652	1405.67949	-2301.21089	-390.08113	1
176	H	73.26025	84.41792	79.95392	-940.37328	-1118.32446	2299.72133	1
177	N	72.91230	85.93576	78.49266	319.26422	656.36007	-42.02424	1
178	H	72.42000	86.63556	79.11972	1961.03633	619.91968	1787.09422	1
179	H	73.88478	86.35704	78.43346	854.14343	-2156.80752	1429.08711	1
180	H	72.50589	86.18386	77.54390	1237.02905	-1378.50857	-1998.28500	1
181	C	72.18431	79.22305	77.64667	532.53319	-268.57236	517.55729	1
182	O	71.32066	80.05942	77.79954	266.16714	-290.73804	-558.88002	1
183	N	72.01985	77.91036	77.46675	-226.25352	640.49678	-270.32839	1
184	H	72.87632	77.35738	77.43282	2007.69063	-1035.27229	1523.50231	1
185	C	70.76357	77.37074	77.88415	-540.76542	-573.33303	49.50000	1
186	H	70.02686	78.20311	77.79187	-2374.20950	-1036.76023	843.75774	1
187	C	70.45219	76.08627	76.98029	-77.09082	666.87422	-415.84136	1
188	H	71.25548	75.31924	77.15530	-985.81834	617.19825	2463.91927	1
189	O	70.40113	76.30441	75.55979	293.29899	-391.65602	-477.80926	1
190	H	71.03128	75.62788	75.23929	2528.72714	-681.76262	-751.27122	1
191	C	69.10819	75.58182	77.62254	252.47363	-605.14473	440.05134	1

192	H	68.75823	74.63626	77.14816	-2052.65063	1456.49051	-1043.51830	1
193	H	69.21752	75.38531	78.71462	-2152.98800	-1661.97574	-161.70652	1
194	H	68.29314	76.33201	77.50118	-473.12726	-1584.27339	2165.61725	1
195	C	70.95503	76.81547	79.40480	360.36307	488.46713	505.10056	1
196	O	71.93911	76.14907	79.70870	-200.08817	-528.03552	-385.82850	1
197	N	69.90103	77.10046	80.14282	-597.54095	-226.44775	355.20479	1
198	H	69.12980	77.61770	79.72552	2179.23655	-1300.70981	-991.33835	1
199	C	69.81076	76.46231	81.41525	-687.68921	297.39807	-249.45179	1
200	H	70.85153	76.53823	81.80439	-349.16256	-2467.37713	-1101.72831	1
201	C	68.66110	77.10636	82.31192	672.47345	361.54328	-201.62880	1
202	H	67.67671	76.97056	81.80756	1541.41502	582.18425	2169.97026	1
203	H	68.60293	76.55288	83.27810	-2534.67717	60.25153	997.72295	1
204	C	68.92433	78.59754	82.57251	574.26774	-389.43119	-377.02542	1
205	C	69.87077	78.99072	83.56546	688.82679	-287.33580	-257.96133	1
206	H	70.43796	78.23380	84.13754	331.14182	1470.38163	2269.80013	1
207	C	68.19951	79.57867	81.83178	-383.52382	-675.04808	144.24917	1
208	H	67.46922	79.27510	81.05998	4.09847	1517.59662	2262.86397	1
209	C	70.06031	80.35235	83.80142	-134.76730	428.45285	-649.50303	1
210	H	70.78868	80.65831	84.57256	-903.23433	1600.49020	2011.53387	1
211	C	68.42417	80.92994	82.10637	-335.53281	-615.00040	-364.39058	1
212	H	67.85393	81.68077	81.53205	1596.45398	-1369.33862	1732.02659	1
213	C	69.35414	81.36798	83.09373	585.48547	-340.24194	-406.23938	1
214	O	69.58865	82.73877	83.37822	-419.15649	-173.04408	-511.94141	1
215	H	68.94557	83.15026	82.75363	-1071.84350	1559.71507	-1960.13012	1
216	C	69.35171	74.91105	81.17529	291.41878	-183.13091	710.72246	1
217	O	68.22215	74.53884	81.38447	379.87695	523.47396	-222.23622	1
218	N	70.39262	74.21633	80.72421	564.30591	373.09380	277.24371	1
219	H	71.29897	74.68391	80.49696	-120.59931	-2436.07824	-1214.35098	1
220	C	70.16380	72.81698	80.51065	404.07514	-299.37480	608.84009	1
221	H	69.63407	72.48330	81.42967	-1071.07882	-841.69025	2359.66467	1
222	C	69.21574	72.73332	79.24897	-683.12807	68.71770	-390.13096	1
223	H	68.38750	73.47268	79.36855	2068.88918	1596.58590	770.89603	1
224	H	69.76813	73.03307	78.33009	1379.86429	2342.49779	-179.85638	1
225	C	68.63089	71.29435	79.09851	-176.39967	537.49466	550.97268	1
226	H	69.44002	70.54183	78.97108	-396.28051	1942.22168	1869.33314	1
227	H	68.07562	70.99068	80.01384	-94.44700	586.00678	-2659.20016	1
228	C	67.66244	71.32757	77.82684	-291.69381	-718.18079	-150.72929	1
229	H	66.77814	72.00888	77.91747	-2303.38776	1089.76242	964.62032	1
230	H	68.15853	71.55000	76.84807	884.16729	2568.80533	-207.74283	1
231	N	67.17128	70.01529	77.76411	-594.49522	-252.81478	342.29276	1
232	H	67.47016	69.38480	78.49144	-1735.17426	2084.05705	-263.71605	1
233	C	66.38323	69.57652	76.86950	595.23177	-271.52487	442.22352	1
234	N	65.97086	70.46049	75.86581	585.53813	-424.79750	-105.81303	1
235	H	66.19790	71.44534	75.73513	959.88797	1327.56823	-2177.11905	1
236	H	65.33463	70.22004	75.10483	1578.48647	16.27378	-2220.76233	1
237	N	66.07186	68.22530	77.08093	-452.17763	-390.33541	-421.51853	1
238	H	66.36435	67.57525	77.80881	470.26107	1974.25629	-1817.92087	1
239	H	65.45138	67.69544	76.46750	1856.67307	-1573.97321	-1224.35416	1
240	C	71.64832	72.16421	80.27671	-531.47271	-581.45780	-55.06206	1
241	O	72.29687	72.37808	79.27038	-243.00837	192.73507	609.52485	1
242	N	71.97233	71.44135	81.33603	343.49288	-644.25607	38.09164	1
243	H	71.26335	71.43964	82.06945	-1691.16043	-1535.97525	-1484.73099	1
244	C	73.17143	70.63675	81.47206	542.66492	350.14337	454.42563	1
245	H	72.92937	69.95463	82.32169	1209.57979	-2396.95920	463.86744	1
246	C	73.45490	69.91084	80.16302	-737.14309	145.93010	242.71942	1
247	H	73.43511	70.67867	79.34487	-1050.18303	159.36419	-2509.06125	1
248	C	74.82666	69.26524	80.17972	-706.77696	-252.88343	-245.16230	1
249	H	75.09127	68.81250	79.18449	-1624.64039	-1665.49085	1417.86935	1
250	H	75.63124	70.01309	80.43756	2566.10521	598.51109	693.22305	1
251	H	74.88792	68.44578	80.94820	-1972.69758	107.10018	-1876.34312	1
252	C	72.38788	68.87928	79.85122	412.85148	672.58832	-27.69222	1
253	H	72.56385	68.38486	78.85622	1447.02277	1762.76533	-1490.78944	1

254	H	72.35971	68.06578	80.62785	1320.77379	-145.20455	2378.68491	1
255	H	71.36435	69.34545	79.81943	-1512.10848	1470.52031	1724.75147	1
256	C	74.51985	71.56218	81.81525	-607.11113	499.56689	73.73769	1
257	O	75.40041	71.04850	82.46356	357.97126	460.81534	356.68785	1
258	N	74.52426	72.73519	81.20801	536.55407	-368.62270	332.76306	1
259	H	73.69157	72.99772	80.67115	524.38866	2297.69985	1367.20941	1
260	C	75.60736	73.60206	81.50574	46.50277	-774.29190	-147.97904	1
261	H	76.31516	72.96525	82.08861	1676.51875	1883.29066	1032.55549	1
262	C	76.23586	74.17686	80.13089	-559.41456	-34.19198	-556.30433	1
263	H	75.44232	74.70093	79.54567	-64.66664	395.18769	2695.05373	1
264	H	77.00818	74.95078	80.35526	-2703.44278	-60.40056	333.79418	1
265	C	76.83050	73.05592	79.32646	-519.76435	377.31045	459.42366	1
266	H	76.01740	72.33204	79.09183	-1746.74323	1667.50644	-1261.73691	1
267	C	77.41751	73.57508	78.01569	570.95554	16.46261	-545.27700	1
268	H	77.84212	72.74503	77.39314	2391.58273	28.05277	-1305.07271	1
269	H	76.65524	74.10470	77.38378	175.75588	917.63458	2559.43867	1
270	H	78.24858	74.31191	78.18097	-1063.97851	-2155.34650	1283.00462	1
271	C	77.91768	72.31809	80.09654	193.76014	2.62946	-765.53141	1
272	H	78.41841	71.53838	79.46522	507.39394	-846.55087	2539.60089	1
273	H	78.71731	73.01657	80.45509	1337.57841	1818.19054	1526.01994	1
274	H	77.50532	71.79217	80.99674	1100.88635	-1172.91350	-2199.08909	1
275	C	75.05457	74.85174	82.36383	-549.21115	475.64486	-309.38218	1
276	O	73.89052	75.11527	82.50938	556.06106	-390.37755	-78.24250	1
277	O	76.05575	75.68924	82.91587	-572.27940	-310.19032	-209.75862	1
278	H	76.85908	75.16749	82.64042	-1380.08193	2212.14486	790.85944	1

Listing 96: C00096.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.8450	3380
		0.2500	300.00	0.00	0.00	0.00	-1293.4425	0.0000	300.0000
3	H	67.04811	73.55345	87.78173	-2043.14101	-1757.64893	399.89339		1
4	N	68.03048	73.32915	87.63426	426.75047	490.45733	-334.42467		1
5	H	67.99948	72.77435	86.78050	442.25559	-1110.30854	-2448.52907		1
6	C	68.88762	74.44488	87.53209	415.32972	-666.39213	83.73172		1
7	H	68.50938	75.21053	88.24264	879.32219	2491.00447	667.35213		1
8	C	70.38275	73.93569	87.84799	31.35357	477.41777	628.23362		1
9	H	70.65995	73.15346	87.10073	1168.38489	2240.25337	-1019.71136		1
10	H	71.12049	74.76430	87.71855	-360.43770	2534.90498	931.67112		1
11	C	70.43830	73.37047	89.24573	463.18208	512.70242	-382.34388		1
12	H	69.51727	72.76643	89.41025	1725.29117	1863.52247	-987.07854		1
13	C	71.64476	72.45482	89.40653	710.42801	-144.27427	-313.15367		1
14	H	71.69541	72.01381	90.43567	364.20195	-1033.13725	2494.72524		1
15	H	71.61608	71.60105	88.68088	2567.61904	335.80679	847.48802		1
16	H	72.60592	73.00462	89.23428	-2587.99029	680.92867	-512.16411		1
17	C	70.49310	74.47760	90.28882	268.17616	741.64379	-40.42634		1
18	H	70.51879	74.06332	91.33010	1283.54314	-1945.37420	-1411.27812		1
19	H	71.40623	75.11556	90.16437	-1258.57796	1317.15249	-2026.02085		1
20	H	69.60328	75.15528	90.22220	-2502.84526	909.80597	575.92391		1
21	C	68.85512	74.90384	85.96213	619.36578	-458.64843	-172.09273		1
22	O	69.16409	74.15033	85.06535	-81.40433	433.87611	522.34594		1
23	N	68.49981	76.18462	85.88710	175.23996	-622.20190	341.55523		1
24	H	68.31192	76.69640	86.74877	-876.57256	-303.22879	-2561.90213		1
25	C	68.73289	76.87047	84.66342	-571.88214	-534.10783	-106.15033		1
26	H	68.98416	76.07836	83.92110	-2713.20841	-16.25800	-248.80809		1
27	C	67.38983	77.67594	84.32459	166.60354	288.16399	-716.09568		1
28	H	67.06540	78.21719	85.25358	-2097.85574	1636.78449	-586.18044		1
29	O	66.28295	76.84421	83.92175	-317.80580	-363.38227	484.43082		1
30	H	65.66064	76.99495	84.65950	1863.74748	-1451.84923	1357.29467		1
31	C	67.84447	78.73116	83.25369	503.80731	517.99032	318.51606		1
32	H	66.99760	79.39086	82.95234	640.61020	-2157.10410	-1536.29104		1
33	H	68.65944	79.39294	83.63253	1687.88455	465.60692	2087.56452		1

34	H	68.21906	78.23473	82.32838	-1293.07895	-1899.88581	-1463.57452	1
35	C	69.96378	77.90241	84.97370	-153.07550	-733.68902	248.70981	1
36	O	69.75476	78.91846	85.58146	186.15459	-480.78787	-449.34387	1
37	N	71.12959	77.40574	84.51651	-487.53139	543.18517	42.03850	1
38	C	72.28425	78.22889	84.41287	-699.35871	69.34393	360.10701	1
39	H	72.05102	79.17129	84.96121	2.81126	-221.99807	-2715.58072	1
40	C	73.39413	77.27906	85.03465	-507.46439	-592.59194	122.07761	1
41	H	74.42911	77.59467	84.77418	-1975.08116	525.87560	-1801.71556	1
42	H	73.33351	77.24600	86.14556	1588.27743	-1913.22100	1113.83566	1
43	C	72.98846	75.91241	84.39746	-613.62442	-457.55993	-194.14490	1
44	H	73.34269	75.85487	83.34172	1707.54637	-721.27992	1996.92523	1
45	H	73.41534	75.02922	84.92445	758.23357	2100.81767	1560.55011	1
46	C	71.40471	75.97235	84.46521	-352.41524	704.96076	49.21465	1
47	H	70.88706	75.55185	83.57159	1714.76886	-2070.42778	443.35792	1
48	H	70.95236	75.53780	85.38877	1224.15040	1801.50881	1636.97633	1
49	C	72.65154	78.43449	82.80902	566.85117	537.05831	117.62814	1
50	O	73.63777	77.90009	82.36223	-550.26779	-406.08867	4.21666	1
51	N	71.77047	79.22963	82.22874	566.34832	-425.77725	180.18749	1
52	H	71.02903	79.57375	82.83892	644.44502	2646.80550	-52.73430	1
53	C	71.74288	79.47712	80.83254	612.34801	-281.48662	411.56221	1
54	H	70.97146	80.27543	80.75310	1667.23498	-1490.75142	1556.16753	1
55	C	73.18798	79.93197	80.33265	-714.45746	-175.43074	286.98927	1
56	H	73.88085	79.04971	80.43143	-787.09484	1763.03619	-1922.46060	1
57	O	73.79057	81.01944	81.06096	-429.46514	516.51932	-128.40526	1
58	H	74.51985	80.55290	81.51655	1981.82785	436.16847	-1818.18182	1
59	C	72.91379	80.22565	78.81119	630.79189	-468.94448	76.03230	1
60	H	73.85784	80.45139	78.26292	-1775.71861	2062.30353	131.89849	1
61	H	72.43439	79.35859	78.29822	-1855.14608	88.94118	1993.53760	1
62	H	72.23701	81.10177	78.68160	-1504.82350	-780.94249	-2132.90992	1
63	C	71.27800	78.08590	80.09343	288.57638	618.62814	-397.00270	1
64	O	71.98429	77.44836	79.34590	321.70495	-185.26452	574.37218	1
65	N	70.03431	77.81391	80.49690	-447.05792	-446.53431	367.76425	1
66	H	69.59663	78.53284	81.07088	350.31316	1975.63644	-1843.31522	1
67	C	69.26388	76.95668	79.64510	-511.23061	374.03917	-471.51480	1
68	H	70.04048	76.21791	79.33484	2234.79579	-898.70890	-1273.45190	1
69	C	68.07963	76.34062	80.52268	529.53781	-159.34528	563.72604	1
70	H	67.69912	75.42016	80.00284	654.59388	2347.94251	1217.51488	1
71	H	68.50580	75.97178	81.49164	-1526.55661	2103.42026	817.87394	1
72	O	66.92329	77.20185	80.76900	-554.84278	14.12789	399.58769	1
73	H	66.74209	76.98759	81.70471	1297.06236	2061.84854	1220.68812	1
74	C	68.73658	77.82011	78.38008	-662.15484	-412.13544	123.62687	1
75	O	69.08092	78.96944	78.12774	-540.01537	-317.05804	274.91456	1
76	N	67.94877	77.03612	77.66894	-202.76299	-690.00100	-131.49145	1
77	H	67.80535	76.11135	78.06609	-702.62132	-2617.37191	281.70413	1
78	C	67.29274	77.45038	76.41980	-491.73914	576.34187	222.73509	1
79	H	66.58884	76.61261	76.19170	1977.17978	-1823.58850	-434.68928	1
80	C	66.58856	78.78462	76.67970	-649.50797	-328.66843	306.11224	1
81	H	67.35434	79.50515	77.06039	2075.07803	1452.16490	-1004.45904	1
82	C	65.99452	79.35285	75.40676	-615.18735	-489.99689	-70.96352	1
83	H	65.52518	80.36071	75.58009	-1226.32661	-1724.38906	-1716.47170	1
84	H	66.77560	79.48182	74.60765	2381.64273	-969.84735	900.46860	1
85	H	65.19726	78.68125	74.98420	2122.74991	1702.23946	-141.36228	1
86	C	65.53336	78.64962	77.75947	-501.86074	-479.61276	-376.42482	1
87	H	65.06464	79.64120	78.01094	993.79261	-2246.95401	-1177.81305	1
88	H	64.70358	77.95831	77.44493	42.71279	-626.15391	-2651.37258	1
89	H	65.97340	78.23304	78.71102	-2026.39012	-1590.33709	-887.82922	1
90	C	68.47389	77.57091	75.31425	-672.89153	382.57394	-156.34072	1
91	O	68.58384	76.72157	74.37943	410.04627	221.86223	500.35950	1
92	N	69.24121	78.59581	75.48310	-378.11782	-443.79414	-441.10984	1
93	H	69.15745	79.20431	76.32432	2404.15973	-568.14894	1149.30085	1
94	C	70.37239	78.60637	74.61004	-544.54484	466.16019	331.29119	1
95	H	70.49227	79.65891	74.28079	-1409.80988	-170.17955	2325.32679	1

96	C	71.55879	78.15619	75.52492	-184.48284	116.78282	-758.89137	1
97	H	71.56665	78.73846	76.47472	1893.78641	1861.14652	611.04528	1
98	H	71.45451	77.08698	75.82193	-2170.79665	-974.19311	1327.50117	1
99	C	72.86508	78.39462	74.69718	389.51668	672.81878	-138.49152	1
100	H	72.86645	77.73500	73.79784	510.64577	1933.03327	1851.02484	1
101	H	72.87596	79.42390	74.27550	-2302.30869	-1105.72939	-948.89774	1
102	C	74.16927	78.16626	75.54461	-559.93427	-126.34590	542.30857	1
103	O	75.23880	78.37466	75.03162	-670.36003	-111.83166	76.36448	1
104	N	73.96411	77.75562	76.81665	-216.06729	-537.07037	446.51379	1
105	H	73.11065	77.54767	77.35523	-1251.96487	1074.12894	-2168.52500	1
106	H	74.73655	77.59404	77.47199	-2451.83023	-720.73851	944.84612	1
107	C	70.10311	77.48003	73.36523	546.24052	-563.88337	-85.11809	1
108	O	70.97425	76.62208	73.15860	71.70702	-307.40463	606.69673	1
109	N	69.40305	78.09670	72.34885	479.90863	-504.50129	222.86849	1
110	C	68.75049	77.32190	71.36290	75.51268	-600.91904	506.73700	1
111	H	68.69750	76.28511	71.77361	-2033.61562	1795.30103	254.89480	1
112	C	67.35350	78.08215	71.19590	523.79067	517.99274	284.45581	1
113	H	66.84901	77.84885	70.23172	1599.61665	-1127.00911	1895.98173	1
114	H	66.64346	77.81020	72.00852	-1881.83093	1275.82488	-1501.55016	1
115	C	67.80889	79.56448	71.31239	-600.05639	-404.05026	316.64485	1
116	H	68.25399	79.92349	70.35775	-2597.05260	496.36221	657.73249	1
117	H	66.98196	80.26575	71.56237	-1666.24518	1294.38985	-1723.90591	1
118	C	68.90801	79.45126	72.46804	493.57570	-129.95376	-602.56394	1
119	H	69.77136	80.15132	72.36344	-1469.08415	-637.84797	2204.22581	1
120	H	68.50075	79.53193	73.50393	-1038.97840	1068.88701	-2280.71789	1
121	C	69.55405	77.38983	69.92390	188.88100	241.05089	-727.87821	1
122	O	68.95054	77.42156	68.88146	531.88613	-49.19943	427.07960	1
123	N	70.87512	77.27549	70.10980	708.14833	26.93417	-179.73509	1
124	H	71.12886	77.28213	71.10012	-2232.69501	-1179.09831	1023.94816	1
125	C	71.80138	77.72086	69.06948	-738.32412	259.92548	104.42456	1
126	H	71.14875	78.24078	68.32775	2028.89123	1260.02983	1311.33324	1
127	C	72.83919	78.61551	69.72056	-258.65678	-345.52513	661.28459	1
128	H	73.34558	78.02606	70.51820	-1826.06090	-1801.46097	-918.64554	1
129	C	73.89885	79.07684	68.73762	-541.23400	531.92970	-218.41428	1
130	H	74.63614	79.77784	69.21731	1311.73218	-2219.18200	882.19023	1
131	H	74.48848	78.21011	68.32171	-1048.71298	1223.58118	-2196.97971	1
132	H	73.44401	79.61670	67.86163	419.06414	1903.92898	1903.44670	1
133	C	72.19367	79.81908	70.38506	-423.86431	152.66566	-648.55262	1
134	H	72.94885	80.45310	70.92528	105.68386	-2342.50080	1387.51238	1
135	H	71.67997	80.47838	69.63259	-1695.63603	-1484.73621	-1531.02793	1
136	H	71.41667	79.50632	71.13521	-1853.57121	-487.39031	1936.59343	1
137	C	72.53936	76.38081	68.40760	539.71428	-510.58232	267.58633	1
138	O	73.25372	76.54238	67.44238	-15.93758	-278.34085	-624.49402	1
139	N	72.25932	75.26619	69.05227	-676.81886	12.05292	276.17960	1
140	H	71.57616	75.39527	69.79439	-1694.44250	-373.84189	-2100.66098	1
141	C	72.82770	74.00050	68.71244	412.33078	-664.70360	108.35451	1
142	H	72.01363	73.28537	68.97066	1765.77476	1294.44366	1621.76594	1
143	C	73.23593	73.99239	67.18318	-179.66635	-721.95667	-264.73915	1
144	H	72.46345	74.51012	66.56868	-607.34922	2587.87032	-598.10018	1
145	H	74.17025	74.58958	67.04162	-359.69332	-1479.13954	-2259.74260	1
146	C	73.46416	72.51881	66.70922	-240.01076	616.02425	431.85322	1
147	H	74.20883	72.01346	67.37163	-1359.17131	782.54425	2227.99181	1
148	H	72.52819	71.92019	66.77683	-820.36667	85.81767	-2596.78715	1
149	C	73.99782	72.58176	65.22155	-513.07015	236.18570	-551.87280	1
150	H	73.21575	72.97625	64.53275	1816.11944	-1183.11722	-1650.94321	1
151	H	74.85691	73.28687	65.13899	-1800.04429	-1361.53473	1526.34643	1
152	C	74.42955	71.15281	64.81847	726.08972	-253.19732	-179.64713	1
153	H	75.27691	70.74573	65.40569	1224.27271	-456.51798	-2390.90304	1
154	H	73.60507	70.41332	64.78194	1206.40339	-1150.93514	-2154.90344	1
155	N	74.96905	71.22233	63.34990	329.70796	-633.68968	-155.67358	1
156	H	75.31608	70.30524	62.94530	1348.31305	1938.76845	1359.00643	1
157	H	74.28808	71.53719	62.59912	2096.92035	1446.54551	-966.48890	1

158	H	75.80113	71.85685	63.17148	-1197.07217	-2303.53719	827.28733	1
159	C	74.16942	73.72093	69.58669	-378.01186	-556.17301	-413.96481	1
160	O	75.02695	72.95467	69.13943	-409.44433	-307.55053	-453.30833	1
161	N	74.12140	74.32275	70.75176	-429.02477	524.70884	274.08502	1
162	H	73.30551	74.91891	70.88503	1706.34263	-1425.96036	1574.38926	1
163	C	75.06281	74.12889	71.79469	-45.25864	-626.22952	478.93267	1
164	H	74.58252	74.61259	72.67447	1988.63164	570.90773	1772.87287	1
165	C	75.30599	72.57490	71.97940	551.77128	-20.49526	-564.54996	1
166	H	74.36622	72.06661	72.29207	1434.61535	-1753.10253	1513.99471	1
167	H	75.58835	72.10413	71.00541	-714.67738	1819.09770	1898.36494	1
168	C	76.43948	72.35934	73.03556	446.99263	-555.77305	338.97221	1
169	H	77.40454	72.82669	72.67903	1953.68466	1892.25957	-161.67766	1
170	H	76.18847	72.85262	74.00172	-403.03785	2688.07032	-188.43591	1
171	C	76.62153	70.79974	73.22376	567.86262	335.74681	434.04421	1
172	H	75.68252	70.33296	73.60066	-1080.02275	1568.26081	-1948.78900	1
173	H	76.83249	70.30761	72.24631	-919.54108	2111.34692	1456.13463	1
174	C	77.78988	70.56330	74.20885	195.81897	173.33862	-745.11536	1
175	H	78.78769	70.84914	73.81904	1405.67949	-2301.21089	-390.08113	1
176	H	77.63751	70.99413	75.21854	-940.37328	-1118.32446	2299.72133	1
177	N	77.89070	69.01895	74.45155	319.26422	656.36007	-42.02424	1
178	H	78.63783	68.69408	75.13236	1961.03633	619.91968	1787.09422	1
179	H	77.02962	68.53033	74.83515	854.14343	-2156.80752	1429.08711	1
180	H	78.11532	68.42820	73.60013	1237.02905	-1378.50857	-1998.28500	1
181	C	76.49712	74.85532	71.43030	532.53319	-268.57236	517.55729	1
182	O	76.90320	75.66649	72.22540	266.16714	-290.73804	-558.88002	1
183	N	77.01422	74.40473	70.30496	-226.25352	640.49678	-270.32839	1
184	H	76.46908	73.70097	69.74858	2007.69063	-1035.27229	1523.50231	1
185	C	78.31420	74.76845	69.86816	-540.76542	-573.33303	49.50000	1
186	H	78.34301	74.43030	68.80849	-2374.20950	-1036.76023	843.75774	1
187	C	78.43494	76.35986	69.99100	-77.09082	666.87422	-415.84136	1
188	H	78.29863	76.64235	71.07931	-985.81834	617.19825	2463.91927	1
189	O	77.43446	77.08692	69.24621	293.29899	-391.65602	-477.80926	1
190	H	76.87195	77.41088	69.97801	2528.72714	-681.76262	-751.27122	1
191	C	79.91618	76.68956	69.58626	252.47363	-605.14473	440.05134	1
192	H	80.12038	77.78259	69.66450	-2052.65063	1456.49051	-1043.51830	1
193	H	80.65275	76.17083	70.24312	-2152.98800	-1661.97574	-161.70652	1
194	H	80.13024	76.39006	68.53391	-473.12726	-1584.27339	2165.61725	1
195	C	79.37767	73.93725	70.77815	360.36307	488.46713	505.10056	1
196	O	79.08926	73.42317	71.84231	-200.08817	-528.03552	-385.82850	1
197	N	80.64338	73.99905	70.23875	-597.54095	-226.44775	355.20479	1
198	H	80.42355	74.34550	69.29575	2179.23655	-1300.70981	-991.33835	1
199	C	81.34890	72.73714	70.35574	-687.68921	297.39807	-249.45179	1
200	H	80.71495	71.98479	69.84042	-349.16256	-2467.37713	-1101.72831	1
201	C	82.77730	72.92806	69.69250	672.47345	361.54328	-201.62880	1
202	H	83.33012	73.72861	70.23600	1541.41502	582.18425	2169.97026	1
203	H	83.36164	71.98587	69.82156	-2534.67717	60.25153	997.72295	1
204	C	82.69569	73.29177	68.19988	574.26774	-389.43119	-377.02542	1
205	C	82.79614	72.26111	67.21846	688.82679	-287.33580	-257.96133	1
206	H	82.88766	71.19680	67.52002	331.14182	1470.38163	2269.80013	1
207	C	82.57445	74.65786	67.80502	-383.52382	-675.04808	144.24917	1
208	H	82.48968	75.45647	68.56418	4.09847	1517.59662	2262.86397	1
209	C	82.80026	72.62196	65.87076	-134.76730	428.45285	-649.50303	1
210	H	82.89460	71.82510	65.11218	-903.23433	1600.49020	2011.53387	1
211	C	82.58147	74.96856	66.44221	-335.53281	-615.00040	-364.39058	1
212	H	82.49807	76.02924	66.14769	1596.45398	-1369.33862	1732.02659	1
213	C	82.69937	73.97305	65.42881	585.48547	-340.24194	-406.23938	1
214	O	82.71239	74.27819	64.04207	-419.15649	-173.04408	-511.94141	1
215	H	82.67735	75.26252	64.08785	-1071.84350	1559.71507	-1960.13012	1
216	C	81.59762	72.39696	71.91883	291.41878	-183.13091	710.72246	1
217	O	81.48618	71.24231	72.32622	379.87695	523.47396	-222.23622	1
218	N	82.16228	73.43855	72.52639	564.30591	373.09380	277.24371	1
219	H	82.12800	74.25901	71.91811	-120.59931	-2436.07824	-1214.35098	1

220	C	82.16592	73.63407	73.93986	404.07514	-299.37480	608.84009	1
221	H	82.57220	74.66414	74.05534	-1071.07882	-841.69025	2359.66467	1
222	C	80.65032	73.56714	74.41058	-683.12807	68.71770	-390.13096	1
223	H	80.01469	74.19638	73.74424	2068.88918	1596.58590	770.89603	1
224	H	80.24928	72.53400	74.30800	1379.86429	2342.49779	-179.85638	1
225	C	80.57315	74.06811	75.88391	-176.39967	537.49466	550.97268	1
226	H	81.10234	73.36788	76.57102	-396.28051	1942.22168	1869.33314	1
227	H	81.08928	75.04693	76.00148	-94.44700	586.00678	-2659.20016	1
228	C	79.02208	74.20092	76.24971	-291.69381	-718.18079	-150.72929	1
229	H	78.43037	74.93517	75.64612	-2303.38776	1089.76242	964.62032	1
230	H	78.46857	73.22746	76.27151	884.16729	2568.80533	-207.74283	1
231	N	79.12135	74.68206	77.56384	-594.49522	-252.81478	342.29276	1
232	H	79.99552	74.51549	78.03937	-1735.17426	2084.05705	-263.71605	1
233	C	78.19717	75.28219	78.19941	595.23177	-271.52487	442.22352	1
234	N	76.97690	75.49549	77.55108	585.53813	-424.79750	-105.81303	1
235	H	76.69501	75.26874	76.59825	959.88797	1327.56823	-2177.11905	1
236	H	76.17378	75.97165	77.96259	1578.48647	16.27378	-2220.76233	1
237	N	78.62110	75.61313	79.49405	-452.17763	-390.33541	-421.51853	1
238	H	79.51318	75.46709	79.96436	470.26107	1974.25629	-1817.92087	1
239	H	78.02909	76.10420	80.16502	1856.67307	-1573.97321	-1224.35416	1
240	C	83.06221	72.52808	74.71536	-531.47271	-581.45780	-55.06206	1
241	O	83.12435	72.52447	75.92069	-243.00837	192.73507	609.52485	1
242	N	83.74169	71.73850	73.85420	343.49288	-644.25607	38.09164	1
243	H	83.45515	71.95235	72.89117	-1691.16043	-1535.97525	-1484.73099	1
244	C	83.95047	70.31246	74.18721	542.66492	350.14337	454.42563	1
245	H	84.62469	70.34288	75.07371	1209.57979	-2396.95920	463.86744	1
246	C	82.63241	69.63201	74.47017	-737.14309	145.93010	242.71942	1
247	H	81.92435	69.87376	73.62320	-1050.18303	159.36419	-2509.06125	1
248	C	82.79709	68.12402	74.53785	-706.77696	-252.88343	-245.16230	1
249	H	81.81781	67.60660	74.73296	-1624.64039	-1665.49085	1417.86935	1
250	H	83.20478	67.71028	73.57480	2566.10521	598.51109	693.22305	1
251	H	83.50501	67.82104	75.35758	-1972.69758	107.10018	-1876.34312	1
252	C	81.96729	70.12956	75.74233	412.85148	672.58832	-27.69222	1
253	H	81.24145	69.37910	76.16117	1447.02277	1762.76533	-1490.78944	1
254	H	82.72566	70.36112	76.54334	1320.77379	-145.20455	2378.68491	1
255	H	81.39083	71.07959	75.56002	-1512.10848	1470.52031	1724.75147	1
256	C	84.67533	69.71956	72.82660	-607.11113	499.56689	73.73769	1
257	O	85.84059	69.40866	72.87573	357.97126	460.81534	356.68785	1
258	N	83.85061	69.66312	71.78955	536.55407	-368.62270	332.76306	1
259	H	82.87200	69.98136	71.86175	524.38866	2297.69985	1367.20941	1
260	C	84.37454	69.05369	70.61381	46.50277	-774.29190	-147.97904	1
261	H	85.45252	69.33188	70.62422	1676.51875	1883.29066	1032.55549	1
262	C	84.17831	67.44943	70.68626	-559.41456	-34.19198	-556.30433	1
263	H	83.13777	67.21761	71.01553	-64.66664	395.18769	2695.05373	1
264	H	84.28051	67.01305	69.66402	-2703.44278	-60.40056	333.79418	1
265	C	85.18073	66.82200	71.61393	-519.76435	377.31045	459.42366	1
266	H	85.06421	67.27378	72.62657	-1746.74323	1667.50644	-1261.73691	1
267	C	84.93889	65.32027	71.71361	570.95554	16.46261	-545.27700	1
268	H	85.66206	64.83120	72.41589	2391.58273	28.05277	-1305.07271	1
269	H	83.90709	65.08903	72.08350	175.75588	917.63458	2559.43867	1
270	H	85.05456	64.81888	70.71829	-1063.97851	-2155.34650	1283.00462	1
271	C	86.61068	67.07168	71.15282	193.76014	2.62946	-765.53141	1
272	H	87.34524	66.46016	71.73749	507.39394	-846.55087	2539.60089	1
273	H	86.75077	66.81706	70.07057	1337.57841	1818.19054	1526.01994	1
274	H	86.90054	68.14771	71.29068	1100.88635	-1172.91350	-2199.08909	1
275	C	83.54855	69.55955	69.33028	-549.21115	475.64486	-309.38218	1
276	O	82.41140	69.95317	69.37744	556.06106	-390.37755	-78.24250	1
277	O	84.20098	69.41473	68.07926	-572.27940	-310.19032	-209.75862	1
278	H	85.05678	69.01783	68.40171	-1380.08193	2212.14486	790.85944	1

Listing 97: C00097.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.4419	0.0000	300.0000
3	H	78.63710	61.70117	66.93972	-2043.14101	-1757.64893	399.89339		1
4	N	79.00914	62.41968	67.55825	426.75047	490.45733	-334.42467		1
5	H	78.16977	62.94462	67.79671	442.25559	-1110.30854	-2448.52907		1
6	C	80.05901	63.18055	67.00922	415.32972	-666.39213	83.73172		1
7	H	80.59767	62.46120	66.35713	879.32219	2491.00447	667.35213		1
8	C	79.46116	64.42625	66.18697	31.35357	477.41777	628.23362		1
9	H	78.84102	65.05587	66.86953	1168.38489	2240.25337	-1019.71136		1
10	H	80.29841	65.08213	65.84560	-360.43770	2534.90498	931.67112		1
11	C	78.63951	63.96013	65.01038	463.18208	512.70242	-382.34388		1
12	H	77.88350	63.22697	65.36962	1725.29117	1863.52247	-987.07854		1
13	C	77.90510	65.13899	64.38398	710.42801	-144.27427	-313.15367		1
14	H	77.27972	64.82075	63.51014	364.20195	-1033.13725	2494.72524		1
15	H	77.22169	65.63971	65.11751	2567.61904	335.80679	847.48802		1
16	H	78.62013	65.91804	64.01270	-2587.99029	680.92867	-512.16411		1
17	C	79.50747	63.28759	63.95605	268.17616	741.64379	-40.42634		1
18	H	78.90744	62.98478	63.05904	1283.54314	-1945.37420	-1411.27812		1
19	H	80.31969	63.97059	63.59541	-1258.57796	1317.15249	-2026.02085		1
20	H	80.00225	62.36288	64.35008	-2502.84526	909.80597	575.92391		1
21	C	81.00504	63.78495	68.18974	619.36578	-458.64843	-172.09273		1
22	O	81.70812	64.74467	67.95323	-81.40433	433.87611	522.34594		1
23	N	80.92048	63.07084	69.30744	175.23996	-622.20190	341.55523		1
24	H	80.30977	62.25689	69.24409	-876.57256	-303.22879	-2561.90213		1
25	C	81.66098	63.36111	70.48856	-571.88214	-534.10783	-106.15033		1
26	H	81.40518	62.49535	71.14121	-2713.20841	-16.25800	-248.80809		1
27	C	83.20985	63.37766	70.06815	166.60354	288.16399	-716.09568		1
28	H	83.37445	64.30520	69.45099	-2097.85574	1636.78449	-586.18044		1
29	O	83.64943	62.26080	69.27591	-317.80580	-363.38227	484.43082		1
30	H	83.80295	62.69899	68.41379	1863.74748	-1451.84923	1357.29467		1
31	C	83.93767	63.51302	71.45495	503.80731	517.99032	318.51606		1
32	H	85.04012	63.61514	71.32563	640.61020	-2157.10410	-1536.29104		1
33	H	83.58637	64.40434	72.03172	1687.88455	465.60692	2087.56452		1
34	H	83.76410	62.61470	72.09225	-1293.07895	-1899.88581	-1463.57452		1
35	C	81.16699	64.77083	71.10374	-153.07550	-733.68902	248.70981		1
36	O	81.99268	65.65158	71.30777	186.15459	-480.78787	-449.34387		1
37	N	79.86754	64.77672	71.39213	-487.53139	543.18517	42.03850		1
38	C	79.23924	65.92835	71.97188	-699.35871	69.34393	360.10701		1
39	H	79.68095	66.83125	71.49344	2.81126	-221.99807	-2715.58072		1
40	C	77.70868	65.65040	71.66516	-507.46439	-592.59194	122.07761		1
41	H	77.02337	66.22593	72.32713	-1975.08116	525.87560	-1801.71556		1
42	H	77.44123	65.91402	70.61739	1588.27743	-1913.22100	1113.83566		1
43	C	77.64205	64.10943	71.90043	-613.62442	-457.55993	-194.14490		1
44	H	77.69313	63.87253	72.98931	1707.54637	-721.27992	1996.92523		1
45	H	76.71957	63.62889	71.50292	758.23357	2100.81767	1560.55011		1
46	C	78.96579	63.65297	71.15292	-352.41524	704.96076	49.21465		1
47	H	79.43898	62.72373	71.54597	1714.76886	-2070.42778	443.35792		1
48	H	78.86845	63.57992	70.04406	1224.15040	1801.50881	1636.97633		1
49	C	79.46987	65.88115	73.59854	566.85117	537.05831	117.62814		1
50	O	79.36154	64.84532	74.21325	-550.26779	-406.08867	4.21666		1
51	N	79.57540	67.12732	74.03553	566.34832	-425.77725	180.18749		1
52	H	79.56594	67.84810	73.31392	644.44502	2646.80550	-52.73430		1
53	C	80.15328	67.46456	75.29490	612.34801	-281.48662	411.56221		1
54	H	79.78809	68.50330	75.45277	1667.23498	-1490.75142	1556.16753		1
55	C	79.70771	66.43222	76.42205	-714.45746	-175.43074	286.98927		1
56	H	80.11144	65.41433	76.14610	-787.09484	1763.03619	-1922.46060		1
57	O	78.27989	66.28242	76.58062	-429.46514	516.51932	-128.40526		1
58	H	78.13213	65.48567	76.02406	1981.82785	436.16847	-1818.18182		1
59	C	80.49725	66.97782	77.66843	630.79189	-468.94448	76.03230		1
60	H	80.35661	66.32140	78.55840	-1775.71861	2062.30353	131.89849		1

61	H	81.59500	67.03277	77.46335	-1855.14608	88.94118	1993.53760	1
62	H	80.15649	68.00020	77.95395	-1504.82350	-780.94249	-2132.90992	1
63	C	81.78165	67.42408	75.09399	288.57638	618.62814	-397.00270	1
64	O	82.45883	66.48130	75.42024	321.70495	-185.26452	574.37218	1
65	N	82.14790	68.58057	74.57098	-447.05792	-446.53431	367.76425	1
66	H	81.51524	69.36255	74.32176	350.31316	1975.63644	-1843.31522	1
67	C	83.52816	68.78651	74.22720	-511.23061	374.03917	-471.51480	1
68	H	84.10184	68.58163	75.15963	2234.79579	-898.70890	-1273.45190	1
69	C	83.91694	67.72911	73.09629	529.53781	-159.34528	563.72604	1
70	H	85.03821	67.76569	73.02208	654.59388	2347.94251	1217.51488	1
71	H	83.65760	66.70761	73.48995	-1526.55661	2103.42026	817.87394	1
72	O	83.36882	67.91554	71.78169	-554.84278	14.12789	399.58769	1
73	H	82.81714	67.05958	71.68470	1297.06236	2061.84854	1220.68812	1
74	C	83.46418	70.34019	73.79263	-662.15484	-412.13544	123.62687	1
75	O	82.39143	70.93580	73.85935	-540.01537	-317.05804	274.91456	1
76	N	84.65504	70.81199	73.45402	-202.76299	-690.00100	-131.49145	1
77	H	85.40085	70.11452	73.48325	-702.62132	-2617.37191	281.70413	1
78	C	84.83475	72.04515	72.69637	-491.73914	576.34187	222.73509	1
79	H	85.91689	72.00264	72.43011	1977.17978	-1823.58850	-434.68928	1
80	C	83.92380	71.99855	71.48272	-649.50797	-328.66843	306.11224	1
81	H	82.87441	71.90900	71.85046	2075.07803	1452.16490	-1004.45904	1
82	C	84.05218	73.25496	70.64029	-615.18735	-489.99689	-70.96352	1
83	H	83.32157	73.25788	69.78581	-1226.32661	-1724.38906	-1716.47170	1
84	H	83.86638	74.18671	71.24172	2381.64273	-969.84735	900.46860	1
85	H	85.08134	73.35028	70.19792	2122.74991	1702.23946	-141.36228	1
86	C	84.19099	70.78001	70.61763	-501.86074	-479.61276	-376.42482	1
87	H	83.52259	70.75706	69.71365	993.79261	-2246.95401	-1177.81305	1
88	H	85.25260	70.75891	70.24754	42.71279	-626.15391	-2651.37258	1
89	H	84.01306	69.81741	71.18746	-2026.39012	-1590.33709	-887.82922	1
90	C	84.52976	73.29488	73.76017	-672.89153	382.57394	-156.34072	1
91	O	85.35720	73.54780	74.60168	410.04627	221.86223	500.35950	1
92	N	83.37348	73.89192	73.54622	-378.11782	-443.79414	-441.10984	1
93	H	82.76363	73.53770	72.81494	2404.15973	-568.14894	1149.30085	1
94	C	82.99579	74.99538	74.37045	-544.54484	466.16019	331.29119	1
95	H	83.62602	74.87353	75.28458	-1409.80988	-170.17955	2325.32679	1
96	C	83.34097	76.32288	73.56296	-184.48284	116.78282	-758.89137	1
97	H	84.43628	76.39767	73.37921	1893.78641	1861.14652	611.04528	1
98	H	82.85920	76.31554	72.55958	-2170.79665	-974.19311	1327.50117	1
99	C	82.81974	77.51223	74.42689	389.51668	672.81878	-138.49152	1
100	H	81.71948	77.40538	74.56295	510.64577	1933.03327	1851.02484	1
101	H	83.23456	77.43834	75.45678	-2302.30869	-1105.72939	-948.89774	1
102	C	83.11941	78.94240	73.85173	-559.93427	-126.34590	542.30857	1
103	O	82.64140	79.90725	74.40263	-670.36003	-111.83166	76.36448	1
104	N	83.91929	78.94440	72.77055	-216.06729	-537.07037	446.51379	1
105	H	84.35029	78.15217	72.27873	-1251.96487	1074.12894	-2168.52500	1
106	H	84.22464	79.79266	72.27885	-2451.83023	-720.73851	944.84612	1
107	C	81.39194	74.88992	74.61650	546.24052	-563.88337	-85.11809	1
108	O	80.61939	75.51481	73.90619	71.70702	-307.40463	606.69673	1
109	N	81.12287	74.05251	75.61279	479.90863	-504.50129	222.86849	1
110	C	79.76996	73.83106	76.06258	75.51268	-600.91904	506.73700	1
111	H	79.20634	73.69991	75.11087	-2033.61562	1795.30103	254.89480	1
112	C	79.89346	72.53312	76.96195	523.79067	517.99274	284.45581	1
113	H	79.15659	72.52151	77.79683	1599.61665	-1127.00911	1895.98173	1
114	H	79.71222	71.60945	76.36765	-1881.83093	1275.82488	-1501.55016	1
115	C	81.37312	72.59889	77.45614	-600.05639	-404.05026	316.64485	1
116	H	81.48207	73.32954	78.28933	-2597.05260	496.36221	657.73249	1
117	H	81.76611	71.62594	77.82790	-1666.24518	1294.38985	-1723.90591	1
118	C	82.09817	73.10695	76.13675	493.57570	-129.95376	-602.56394	1
119	H	83.07333	73.62908	76.29311	-1469.08415	-637.84797	2204.22581	1
120	H	82.21536	72.32832	75.32621	-1038.97840	1068.88701	-2280.71789	1
121	C	79.25377	75.13674	76.87993	188.88100	241.05089	-727.87821	1
122	O	79.04003	75.09682	78.06159	531.88613	-49.19943	427.07960	1

123	N	79.11609	76.17716	76.04614	708.14833	26.93417	-179.73509	1
124	H	79.36891	76.07100	75.03568	-2232.69501	-1179.09831	1023.94816	1
125	C	78.55119	77.41737	76.57573	-738.32412	259.92548	104.42456	1
126	H	78.69680	77.32495	77.67947	2028.89123	1260.02983	1311.33324	1
127	C	79.28027	78.57647	75.91915	-258.65678	-345.52513	661.28459	1
128	H	79.32731	78.36739	74.82634	-1826.06090	-1801.46097	-918.64554	1
129	C	78.54996	79.89141	76.11791	-541.23400	531.92970	-218.41428	1
130	H	79.09369	80.74559	75.62655	1311.73218	-2219.18200	882.19023	1
131	H	77.51357	79.85704	75.67894	-1048.71298	1223.58118	-2196.97971	1
132	H	78.44047	80.14627	77.20856	419.06414	1903.92898	1903.44670	1
133	C	80.70115	78.68965	76.43371	-423.86431	152.66566	-648.55262	1
134	H	81.36130	79.31080	75.72897	105.68386	-2342.50080	1387.51238	1
135	H	80.73872	79.17385	77.44839	-1695.63603	-1484.73621	-1531.02793	1
136	H	81.17748	77.67514	76.53588	-1853.57121	-487.39031	1936.59343	1
137	C	76.94113	77.44940	76.13801	539.71428	-510.58232	267.58633	1
138	O	76.59177	77.52414	74.98632	-15.93758	-278.34085	-624.49402	1
139	N	76.20144	77.47793	77.23406	-676.81886	12.05292	276.17960	1
140	H	76.67014	77.37795	78.13225	-1694.44250	-373.84189	-2100.66098	1
141	C	74.78548	77.48052	77.11205	412.33078	-664.70360	108.35451	1
142	H	74.60845	77.85374	76.07595	1765.77476	1294.44366	1621.76594	1
143	C	74.27821	75.99871	77.35057	-179.66635	-721.95667	-264.73915	1
144	H	74.83547	75.27923	76.70939	-607.34922	2587.87032	-598.10018	1
145	H	74.48125	75.68828	78.40026	-359.69332	-1479.13954	-2259.74260	1
146	C	72.74424	75.95813	77.04818	-240.01076	616.02425	431.85322	1
147	H	72.21930	76.76785	77.60789	-1359.17131	782.54425	2227.99181	1
148	H	72.54312	76.14309	75.96897	-820.36667	85.81767	-2596.78715	1
149	C	72.20053	74.54166	77.49596	-513.07015	236.18570	-551.87280	1
150	H	72.74409	73.71994	76.97537	1816.11944	-1183.11722	-1650.94321	1
151	H	72.37245	74.37965	78.58506	-1800.04429	-1361.53473	1526.34643	1
152	C	70.69045	74.50147	77.16672	726.08972	-253.19732	-179.64713	1
153	H	70.08986	75.29034	77.66275	1224.27271	-456.51798	-2390.90304	1
154	H	70.45865	74.46949	76.08381	1206.40339	-1150.93514	-2154.90344	1
155	N	70.11044	73.16490	77.74090	329.70796	-633.68968	-155.67358	1
156	H	69.07007	73.01716	77.59590	1348.31305	1938.76845	1359.00643	1
157	H	70.50731	72.25615	77.36233	2096.92035	1446.54551	-966.48890	1
158	H	70.19325	73.02238	78.78947	-1197.07217	-2303.53719	827.28733	1
159	C	74.18949	78.40907	78.33146	-378.01186	-556.17301	-413.96481	1
160	O	73.43858	77.93286	79.15219	-409.44433	-307.55053	-453.30833	1
161	N	74.64105	79.65317	78.24839	-429.02477	524.70884	274.08502	1
162	H	75.25683	79.89049	77.47181	1706.34263	-1425.96036	1574.38926	1
163	C	74.25530	80.57511	79.26541	-45.25864	-626.22952	478.93267	1
164	H	73.88657	79.94414	80.10958	1988.63164	570.90773	1772.87287	1
165	C	75.51740	81.48546	79.57484	551.77128	-20.49526	-564.54996	1
166	H	76.37736	80.87587	79.93143	1434.61535	-1753.10253	1513.99471	1
167	H	75.86690	81.98636	78.64448	-714.67738	1819.09770	1898.36494	1
168	C	75.08555	82.54134	80.64374	446.99263	-555.77305	338.97221	1
169	H	74.15264	83.05655	80.32068	1953.68466	1892.25957	-161.67766	1
170	H	74.84869	82.05633	81.61713	-403.03785	2688.07032	-188.43591	1
171	C	76.26354	83.58632	80.79509	567.86262	335.74681	434.04421	1
172	H	77.18198	83.09956	81.19637	-1080.02275	1568.26081	-1948.78900	1
173	H	76.54969	84.00412	79.80253	-919.54108	2111.34692	1456.13463	1
174	C	75.77225	84.71198	81.73483	195.81897	173.33862	-745.11536	1
175	H	74.89088	85.27099	81.36148	1405.67949	-2301.21089	-390.08113	1
176	H	75.60478	84.39860	82.78460	-940.37328	-1118.32446	2299.72133	1
177	N	76.90863	85.78530	81.81161	319.26422	656.36007	-42.02424	1
178	H	76.70647	86.62929	82.42166	1961.03633	619.91968	1787.09422	1
179	H	77.84952	85.47242	82.19053	854.14343	-2156.80752	1429.08711	1
180	H	77.18197	86.24946	80.89781	1237.02905	-1378.50857	-1998.28500	1
181	C	73.10956	81.56870	78.64866	532.53319	-268.57236	517.55729	1
182	O	73.38287	82.42665	77.81703	266.16714	-290.73804	-558.88002	1
183	N	71.97110	81.26354	79.18880	-226.25352	640.49678	-270.32839	1
184	H	71.84588	80.45873	79.83589	2007.69063	-1035.27229	1523.50231	1

185	C	70.78591	82.05407	79.00403	-540.76542	-573.33303	49.50000	1
186	H	70.95141	82.99398	79.57582	-2374.20950	-1036.76023	843.75774	1
187	C	70.73419	82.39938	77.44033	-77.09082	666.87422	-415.84136	1
188	H	71.42396	81.65534	76.94430	-985.81834	617.19825	2463.91927	1
189	O	71.28605	83.67771	77.12210	293.29899	-391.65602	-477.80926	1
190	H	72.29248	83.44048	77.15882	2528.72714	-681.76262	-751.27122	1
191	C	69.26590	82.12581	76.96221	252.47363	-605.14473	440.05134	1
192	H	69.18542	82.14103	75.84495	-2052.65063	1456.49051	-1043.51830	1
193	H	68.90772	81.12384	77.31259	-2152.98800	-1661.97574	-161.70652	1
194	H	68.55802	82.89614	77.34909	-473.12726	-1584.27339	2165.61725	1
195	C	69.70738	81.08885	79.71654	360.36307	488.46713	505.10056	1
196	O	70.11171	80.06990	80.27156	-200.08817	-528.03552	-385.82850	1
197	N	68.46433	81.55238	79.67865	-597.54095	-226.44775	355.20479	1
198	H	68.27050	82.44384	79.22509	2179.23655	-1300.70981	-991.33835	1
199	C	67.45452	80.76878	80.29306	-687.68921	297.39807	-249.45179	1
200	H	67.99514	80.16480	81.05792	-349.16256	-2467.37713	-1101.72831	1
201	C	66.30779	81.72822	80.86099	672.47345	361.54328	-201.62880	1
202	H	65.80396	82.25691	80.02002	1541.41502	582.18425	2169.97026	1
203	H	65.53050	81.11210	81.36913	-2534.67717	60.25153	997.72295	1
204	C	66.91876	82.74257	81.83768	574.26774	-389.43119	-377.02542	1
205	C	67.20120	82.35505	83.18198	688.82679	-287.33580	-257.96133	1
206	H	66.98620	81.32863	83.53086	331.14182	1470.38163	2269.80013	1
207	C	67.20946	84.06662	81.38973	-383.52382	-675.04808	144.24917	1
208	H	67.00042	84.36631	80.34694	4.09847	1517.59662	2262.86397	1
209	C	67.75318	83.30056	84.04588	-134.76730	428.45285	-649.50303	1
210	H	67.96786	83.00346	85.08726	-903.23433	1600.49020	2011.53387	1
211	C	67.76076	84.97749	82.29384	-335.53281	-615.00040	-364.39058	1
212	H	67.97620	86.00024	81.93827	1596.45398	-1369.33862	1732.02659	1
213	C	68.05119	84.63597	83.64706	585.48547	-340.24194	-406.23938	1
214	O	68.61369	85.55428	84.57153	-419.15649	-173.04408	-511.94141	1
215	H	68.65780	86.35817	84.00175	-1071.84350	1559.71507	-1960.13012	1
216	C	66.70300	79.81794	79.19023	291.41878	-183.13091	710.72246	1
217	O	66.20868	78.77229	79.54839	379.87695	523.47396	-222.23622	1
218	N	66.61585	80.39723	77.99704	564.30591	373.09380	277.24371	1
219	H	67.06044	81.30372	77.87091	-120.59931	-2436.07824	-1214.35098	1
220	C	66.06729	79.64423	76.92570	404.07514	-299.37480	608.84009	1
221	H	65.72775	78.68029	77.37673	-1071.07882	-841.69025	2359.66467	1
222	C	64.90028	80.52034	76.29143	-683.12807	68.71770	-390.13096	1
223	H	64.41320	81.15381	77.06590	2068.88918	1596.58590	770.89603	1
224	H	65.30256	81.22572	75.52776	1379.86429	2342.49779	-179.85638	1
225	C	63.87863	79.53188	75.65327	-176.39967	537.49466	550.97268	1
226	H	64.38168	78.81484	74.96807	-396.28051	1942.22168	1869.33314	1
227	H	63.38926	78.90795	76.43429	-94.44700	586.00678	-2659.20016	1
228	C	62.80781	80.40741	74.85439	-291.69381	-718.18079	-150.72929	1
229	H	62.22798	81.14893	75.46073	-2303.38776	1089.76242	964.62032	1
230	H	63.20053	80.93463	73.94796	884.16729	2568.80533	-207.74283	1
231	N	61.92191	79.40142	74.43783	-594.49522	-252.81478	342.29276	1
232	H	62.19209	78.44814	74.62543	-1735.17426	2084.05705	-263.71605	1
233	C	60.80956	79.61124	73.85787	595.23177	-271.52487	442.22352	1
234	N	60.45896	80.93941	73.59463	585.53813	-424.79750	-105.81303	1
235	H	60.97876	81.79463	73.78784	959.88797	1327.56823	-2177.11905	1
236	H	59.59808	81.23845	73.13595	1578.48647	16.27378	-2220.76233	1
237	N	60.14621	78.40370	73.59461	-452.17763	-390.33541	-421.51853	1
238	H	60.38910	77.44309	73.83208	470.26107	1974.25629	-1817.92087	1
239	H	59.21959	78.35783	73.16994	1856.67307	-1573.97321	-1224.35416	1
240	C	67.18044	79.50229	75.73074	-531.47271	-581.45780	-55.06206	1
241	O	68.04234	80.32031	75.49320	-243.00837	192.73507	609.52485	1
242	N	66.88357	78.40884	75.03911	343.49288	-644.25607	38.09164	1
243	H	66.10556	77.85484	75.39187	-1691.16043	-1535.97525	-1484.73099	1
244	C	67.69336	77.99786	73.90059	542.66492	350.14337	454.42563	1
245	H	68.59759	78.64935	73.99988	1209.57979	-2396.95920	463.86744	1
246	C	67.97308	76.50686	74.03630	-737.14309	145.93010	242.71942	1

247	H	67.01127	75.97041	73.87374	-1050.18303	159.36419	-2509.06125	1
248	C	68.96251	76.02740	72.99201	-706.77696	-252.88343	-245.16230	1
249	H	69.10023	74.91154	73.02731	-1624.64039	-1665.49085	1417.86935	1
250	H	68.61673	76.29624	71.94874	2566.10521	598.51109	693.22305	1
251	H	69.97649	76.49255	73.13723	-1972.69758	107.10018	-1876.34312	1
252	C	68.46556	76.14870	75.42655	412.85148	672.58832	-27.69222	1
253	H	68.54059	75.03611	75.56838	1447.02277	1762.76533	-1490.78944	1
254	H	69.48200	76.58565	75.62863	1320.77379	-145.20455	2378.68491	1
255	H	67.77698	76.54157	76.22423	-1512.10848	1470.52031	1724.75147	1
256	C	66.84214	78.30656	72.50805	-607.11113	499.56689	73.73769	1
257	O	67.16503	77.76784	71.46697	357.97126	460.81534	356.68785	1
258	N	65.85507	79.16388	72.71023	536.55407	-368.62270	332.76306	1
259	H	65.78409	79.53210	73.65698	524.38866	2297.69985	1367.20941	1
260	C	65.30142	79.84200	71.59376	46.50277	-774.29190	-147.97904	1
261	H	65.95427	79.56383	70.73572	1676.51875	1883.29066	1032.55549	1
262	C	63.76292	79.39666	71.38228	-559.41456	-34.19198	-556.30433	1
263	H	63.14426	79.76638	72.23440	-64.66664	395.18769	2695.05373	1
264	H	63.34724	79.88991	70.47126	-2703.44278	-60.40056	333.79418	1
265	C	63.64716	77.89902	71.28139	-519.76435	377.31045	459.42366	1
266	H	64.04501	77.45705	72.22340	-1746.74323	1667.50644	-1261.73691	1
267	C	62.18309	77.50306	71.13388	570.95554	16.46261	-545.27700	1
268	H	62.05055	76.39053	71.12936	2391.58273	28.05277	-1305.07271	1
269	H	61.56251	77.91055	71.97254	175.75588	917.63458	2559.43867	1
270	H	61.74378	77.89364	70.18012	-1063.97851	-2155.34650	1283.00462	1
271	C	64.45424	77.34634	70.11737	193.76014	2.62946	-765.53141	1
272	H	64.25792	76.25428	69.95846	507.39394	-846.55087	2539.60089	1
273	H	64.21296	77.86964	69.15594	1337.57841	1818.19054	1526.01994	1
274	H	65.56823	77.46246	70.30764	1100.88635	-1172.91350	-2199.08909	1
275	C	65.26344	81.41073	71.96968	-549.21115	475.64486	-309.38218	1
276	O	65.13384	81.81459	73.09424	556.06106	-390.37755	-78.24250	1
277	O	65.21445	82.30090	70.87139	-572.27940	-310.19032	-209.75862	1
278	H	65.33972	81.64363	70.13140	-1380.08193	2212.14486	790.85944	1

Listing 98: C00098.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.4398	0.0000	300.0000
3	H	79.28104	64.21731	80.25313	-2043.14101	-1757.64893	399.89339		1
4	N	79.05101	64.98594	79.62374	426.75047	490.45733	-334.42467		1
5	H	78.38976	65.54825	80.17676	442.25559	-1110.30854	-2448.52907		1
6	C	80.16943	65.75835	79.23345	415.32972	-666.39213	83.73172		1
7	H	81.05531	65.24291	79.66299	879.32219	2491.00447	667.35213		1
8	C	80.23521	65.83825	77.62351	31.35357	477.41777	628.23362		1
9	H	79.26570	66.23339	77.23804	1168.38489	2240.25337	-1019.71136		1
10	H	81.01617	66.56519	77.29599	-360.43770	2534.90498	931.67112		1
11	C	80.51610	64.47231	77.05752	463.18208	512.70242	-382.34388		1
12	H	79.73398	63.77248	77.42945	1725.29117	1863.52247	-987.07854		1
13	C	80.45700	64.50995	75.53484	710.42801	-144.27427	-313.15367		1
14	H	80.70251	63.51267	75.08718	364.20195	-1033.13725	2494.72524		1
15	H	79.43933	64.79709	75.16608	2567.61904	335.80679	847.48802		1
16	H	81.18449	65.25045	75.11280	-2587.99029	680.92867	-512.16411		1
17	C	81.87886	63.94867	77.49149	268.17616	741.64379	-40.42634		1
18	H	82.11155	62.96138	77.01529	1283.54314	-1945.37420	-1411.27812		1
19	H	82.70184	64.65459	77.20952	-1258.57796	1317.15249	-2026.02085		1
20	H	81.93485	63.79839	78.59996	-2502.84526	909.80597	575.92391		1
21	C	79.87378	67.20589	79.90020	619.36578	-458.64843	-172.09273		1
22	O	78.95404	67.38288	80.67813	-81.40433	433.87611	522.34594		1
23	N	80.81699	68.06420	79.52126	175.23996	-622.20190	341.55523		1
24	H	81.50189	67.75737	78.83233	-876.57256	-303.22879	-2561.90213		1
25	C	80.63387	69.44803	79.81971	-571.88214	-534.10783	-106.15033		1
26	H	80.20402	69.45960	80.84522	-2713.20841	-16.25800	-248.80809		1

27	C	82.07346	70.12476	79.66255	166.60354	288.16399	-716.09568	1
28	H	82.39388	70.00246	78.59159	-2097.85574	1636.78449	-586.18044	1
29	O	83.12437	69.54162	80.45795	-317.80580	-363.38227	484.43082	1
30	H	83.72941	69.21882	79.76206	1863.74748	-1451.84923	1357.29467	1
31	C	81.79598	71.64797	79.93736	503.80731	517.99032	318.51606	1
32	H	82.69086	72.27014	79.70297	640.61020	-2157.10410	-1536.29104	1
33	H	80.94488	72.04951	79.32388	1687.88455	465.60692	2087.56452	1
34	H	81.54857	71.82911	81.00887	-1293.07895	-1899.88581	-1463.57452	1
35	C	79.63025	70.05781	78.68696	-153.07550	-733.68902	248.70981	1
36	O	79.75561	69.72316	77.53976	186.15459	-480.78787	-449.34387	1
37	N	78.82231	70.98521	79.22132	-487.53139	543.18517	42.03850	1
38	C	77.99638	71.82036	78.40761	-699.35871	69.34393	360.10701	1
39	H	77.65117	71.22958	77.52750	2.81126	-221.99807	-2715.58072	1
40	C	76.88724	72.29349	79.44340	-507.46439	-592.59194	122.07761	1
41	H	76.35673	73.21372	79.11159	-1975.08116	525.87560	-1801.71556	1
42	H	76.10821	71.51686	79.61543	1588.27743	-1913.22100	1113.83566	1
43	C	77.77729	72.50758	80.70462	-613.62442	-457.55993	-194.14490	1
44	H	78.42620	73.40748	80.58377	1707.54637	-721.27992	1996.92523	1
45	H	77.21041	72.63607	81.65340	758.23357	2100.81767	1560.55011	1
46	C	78.63623	71.17073	80.65559	-352.41524	704.96076	49.21465	1
47	H	79.62872	71.23237	81.15718	1714.76886	-2070.42778	443.35792	1
48	H	78.09859	70.25860	81.01023	1224.15040	1801.50881	1636.97633	1
49	C	78.80193	73.20060	78.01003	566.85117	537.05831	117.62814	1
50	O	79.69734	73.63633	78.69772	-550.26779	-406.08867	4.21666	1
51	N	78.13323	73.75911	77.01460	566.34832	-425.77725	180.18749	1
52	H	77.36639	73.19652	76.64570	644.44502	2646.80550	-52.73430	1
53	C	78.67335	74.76762	76.16402	612.34801	-281.48662	411.56221	1
54	H	77.77301	75.14426	75.61454	1667.23498	-1490.75142	1556.16753	1
55	C	79.35313	75.91248	77.04170	-714.45746	-175.43074	286.98927	1
56	H	80.19060	75.45835	77.64429	-787.09484	1763.03619	-1922.46060	1
57	O	78.45999	76.57165	77.96573	-429.46514	516.51932	-128.40526	1
58	H	78.82093	76.25417	78.81719	1981.82785	436.16847	-1818.18182	1
59	C	79.95227	76.83510	75.91878	630.79189	-468.94448	76.03230	1
60	H	80.52314	77.68813	76.35452	-1775.71861	2062.30353	131.89849	1
61	H	80.64617	76.27547	75.24840	-1855.14608	88.94118	1993.53760	1
62	H	79.14692	77.26917	75.28057	-1504.82350	-780.94249	-2132.90992	1
63	C	79.68988	73.97457	75.15501	288.57638	618.62814	-397.00270	1
64	O	80.80696	73.60508	75.51005	321.70495	-185.26452	574.37218	1
65	N	79.11261	73.91244	73.97979	-447.05792	-446.53431	367.76425	1
66	H	78.19005	74.34915	73.92574	350.31316	1975.63644	-1843.31522	1
67	C	79.39482	72.89137	73.02506	-511.23061	374.03917	-471.51480	1
68	H	78.94809	73.31570	72.09835	2234.79579	-898.70890	-1273.45190	1
69	C	80.97257	72.69767	72.91780	529.53781	-159.34528	563.72604	1
70	H	81.21121	72.31109	71.88911	654.59388	2347.94251	1217.51488	1
71	H	81.41989	73.72442	72.99761	-1526.55661	2103.42026	817.87394	1
72	O	81.59611	71.80411	73.85857	-554.84278	14.12789	399.58769	1
73	H	81.52812	72.40455	74.69632	1297.06236	2061.84854	1220.68812	1
74	C	78.60935	71.53171	73.46240	-662.15484	-412.13544	123.62687	1
75	O	77.89822	71.46046	74.43663	-540.01537	-317.05804	274.91456	1
76	N	78.78130	70.62311	72.48952	-202.76299	-690.00100	-131.49145	1
77	H	79.46067	70.94606	71.79976	-702.62132	-2617.37191	281.70413	1
78	C	78.48834	69.20209	72.62781	-491.73914	576.34187	222.73509	1
79	H	79.07350	68.77034	71.78255	1977.17978	-1823.58850	-434.68928	1
80	C	78.93477	68.70537	73.98556	-649.50797	-328.66843	306.11224	1
81	H	78.43670	69.33825	74.76070	2075.07803	1452.16490	-1004.45904	1
82	C	78.53006	67.25790	74.20787	-615.18735	-489.99689	-70.96352	1
83	H	78.85364	66.88993	75.21854	-1226.32661	-1724.38906	-1716.47170	1
84	H	77.41338	67.12585	74.14818	2381.64273	-969.84735	900.46860	1
85	H	78.98753	66.57518	73.44035	2122.74991	1702.23946	-141.36228	1
86	C	80.43526	68.83519	74.17556	-501.86074	-479.61276	-376.42482	1
87	H	80.75058	68.50170	75.20269	993.79261	-2246.95401	-1177.81305	1
88	H	81.00158	68.20856	73.43272	42.71279	-626.15391	-2651.37258	1

89	H	80.78537	69.90690	74.04709	-2026.39012	-1590.33709	-887.82922	1
90	C	76.84267	68.97958	72.41510	-672.89153	382.57394	-156.34072	1
91	O	76.10561	68.80407	73.35520	410.04627	221.86223	500.35950	1
92	N	76.55761	68.99055	71.12453	-378.11782	-443.79414	-441.10984	1
93	H	77.35334	69.12678	70.50380	2404.15973	-568.14894	1149.30085	1
94	C	75.23032	68.84507	70.63630	-544.54484	466.16019	331.29119	1
95	H	75.35943	68.91913	69.53256	-1409.80988	-170.17955	2325.32679	1
96	C	74.76708	67.39764	71.10858	-184.48284	116.78282	-758.89137	1
97	H	75.58608	66.66135	70.94694	1893.78641	1861.14652	611.04528	1
98	H	74.56993	67.39673	72.20628	-2170.79665	-974.19311	1327.50117	1
99	C	73.49512	67.00333	70.29953	389.51668	672.81878	-138.49152	1
100	H	72.65786	67.69922	70.54926	510.64577	1933.03327	1851.02484	1
101	H	73.67079	67.16861	69.21342	-2302.30869	-1105.72939	-948.89774	1
102	C	73.02864	65.51457	70.51865	-559.93427	-126.34590	542.30857	1
103	O	72.04050	65.12124	69.95465	-670.36003	-111.83166	76.36448	1
104	N	73.82625	64.79096	71.33303	-216.06729	-537.07037	446.51379	1
105	H	74.66399	65.07419	71.85447	-1251.96487	1074.12894	-2168.52500	1
106	H	73.65614	63.80778	71.57295	-2451.83023	-720.73851	944.84612	1
107	C	74.21331	69.96948	71.23133	546.24052	-563.88337	-85.11809	1
108	O	73.06486	69.64293	71.42401	71.70702	-307.40463	606.69673	1
109	N	74.74353	71.19525	71.30438	479.90863	-504.50129	222.86849	1
110	C	74.09954	72.23141	72.05711	75.51268	-600.91904	506.73700	1
111	H	73.71265	71.76008	72.98859	-2033.61562	1795.30103	254.89480	1
112	C	75.29344	73.25975	72.24453	523.79067	517.99274	284.45581	1
113	H	74.94669	74.28618	72.49641	1599.61665	-1127.00911	1895.98173	1
114	H	75.97959	72.94293	73.06265	-1881.83093	1275.82488	-1501.55016	1
115	C	75.99788	73.16894	70.85579	-600.05639	-404.05026	316.64485	1
116	H	75.40581	73.68432	70.06452	-2597.05260	496.36221	657.73249	1
117	H	77.01928	73.61104	70.83698	-1666.24518	1294.38985	-1723.90591	1
118	C	75.98561	71.59272	70.65360	493.57570	-129.95376	-602.56394	1
119	H	75.96071	71.23686	69.59652	-1469.08415	-637.84797	2204.22581	1
120	H	76.79536	71.06235	71.20745	-1038.97840	1068.88701	-2280.71789	1
121	C	72.91668	72.85853	71.11997	188.88100	241.05089	-727.87821	1
122	O	73.15077	73.46162	70.09649	531.88613	-49.19943	427.07960	1
123	N	71.69197	72.74080	71.72881	708.14833	26.93417	-179.73509	1
124	H	71.88243	72.02952	72.44429	-2232.69501	-1179.09831	1023.94816	1
125	C	70.52047	72.60127	70.82686	-738.32412	259.92548	104.42456	1
126	H	70.93563	72.19752	69.87523	2028.89123	1260.02983	1311.33324	1
127	C	69.52117	71.68375	71.48880	-258.65678	-345.52513	661.28459	1
128	H	69.43648	71.99166	72.55533	-1826.06090	-1801.46097	-918.64554	1
129	C	68.14814	71.80514	70.85040	-541.23400	531.92970	-218.41428	1
130	H	67.36730	71.22634	71.41590	1311.73218	-2219.18200	882.19023	1
131	H	67.80867	72.87954	70.80645	-1048.71298	1223.58118	-2196.97971	1
132	H	68.14856	71.42276	69.79280	419.06414	1903.92898	1903.44670	1
133	C	69.97675	70.23647	71.44876	-423.86431	152.66566	-648.55262	1
134	H	69.35555	69.58700	72.12529	105.68386	-2342.50080	1387.51238	1
135	H	69.88938	69.80976	70.41199	-1695.63603	-1484.73621	-1531.02793	1
136	H	71.06520	70.11868	71.75511	-1853.57121	-487.39031	1936.59343	1
137	C	69.88046	74.10531	70.63311	539.71428	-510.58232	267.58633	1
138	O	69.17086	74.33122	69.68121	-15.93758	-278.34085	-624.49402	1
139	N	70.12414	74.89776	71.67797	-676.81886	12.05292	276.17960	1
140	H	70.74161	74.49751	72.38297	-1694.44250	-373.84189	-2100.66098	1
141	C	70.04474	76.31027	71.45873	412.33078	-664.70360	108.35451	1
142	H	69.41071	76.40338	70.54458	1765.77476	1294.44366	1621.76594	1
143	C	69.39849	76.95701	72.75111	-179.66635	-721.95667	-264.73915	1
144	H	68.51890	76.36806	73.09571	-607.34922	2587.87032	-598.10018	1
145	H	70.12135	76.95219	73.60478	-359.69332	-1479.13954	-2259.74260	1
146	C	68.98763	78.41419	72.35323	-240.01076	616.02425	431.85322	1
147	H	69.89356	78.98206	72.01736	-1359.17131	782.54425	2227.99181	1
148	H	68.28763	78.40987	71.48719	-820.36667	85.81767	-2596.78715	1
149	C	68.32395	79.11594	73.60253	-513.07015	236.18570	-551.87280	1
150	H	67.32423	78.67480	73.82485	1816.11944	-1183.11722	-1650.94321	1

151	H	68.95848	78.94220	74.53588	-1800.04429	-1361.53473	1526.34643	1
152	C	68.21315	80.62743	73.29469	726.08972	-253.19732	-179.64713	1
153	H	69.18363	81.13303	73.11778	1224.27271	-456.51798	-2390.90304	1
154	H	67.49661	80.88847	72.49000	1206.40339	-1150.93514	-2154.90344	1
155	N	67.64981	81.31307	74.58307	329.70796	-633.68968	-155.67358	1
156	H	67.54404	82.36803	74.54428	1348.31305	1938.76845	1359.00643	1
157	H	66.68400	81.01427	74.90681	2096.92035	1446.54551	-966.48890	1
158	H	68.22378	81.18807	75.46564	-1197.07217	-2303.53719	827.28733	1
159	C	71.53549	76.95065	71.27841	-378.01186	-556.17301	-413.96481	1
160	O	71.67696	78.15502	71.32530	-409.44433	-307.55053	-453.30833	1
161	N	72.44815	76.02302	71.06197	-429.02477	524.70884	274.08502	1
162	H	72.15698	75.04370	70.96965	1706.34263	-1425.96036	1574.38926	1
163	C	73.82327	76.36002	70.87081	-45.25864	-626.22952	478.93267	1
164	H	74.22307	75.46642	70.33638	1988.63164	570.90773	1772.87287	1
165	C	73.90260	77.68974	69.99842	551.77128	-20.49526	-564.54996	1
166	H	73.17797	77.64811	69.15457	1434.61535	-1753.10253	1513.99471	1
167	H	73.60606	78.57875	70.61034	-714.67738	1819.09770	1898.36494	1
168	C	75.37073	77.83972	69.48139	446.99263	-555.77305	338.97221	1
169	H	76.08650	77.81360	70.34039	1953.68466	1892.25957	-161.67766	1
170	H	75.65244	76.99080	68.81877	-403.03785	2688.07032	-188.43591	1
171	C	75.47632	79.21925	68.71389	567.86262	335.74681	434.04421	1
172	H	74.90312	79.18981	67.75892	-1080.02275	1568.26081	-1948.78900	1
173	H	75.02688	80.04384	69.31338	-919.54108	2111.34692	1456.13463	1
174	C	76.97762	79.48913	68.46085	195.81897	173.33862	-745.11536	1
175	H	77.57541	79.65789	69.37893	1405.67949	-2301.21089	-390.08113	1
176	H	77.48000	78.74212	67.81444	-940.37328	-1118.32446	2299.72133	1
177	N	77.08186	80.83604	67.66989	319.26422	656.36007	-42.02424	1
178	H	78.06609	81.16569	67.45131	1961.03633	619.91968	1787.09422	1
179	H	76.63413	80.86442	66.70789	854.14343	-2156.80752	1429.08711	1
180	H	76.66921	81.69941	68.12921	1237.02905	-1378.50857	-1998.28500	1
181	C	74.56268	76.58744	72.29336	532.53319	-268.57236	517.55729	1
182	O	75.70067	77.05966	72.27390	266.16714	-290.73804	-558.88002	1
183	N	73.84584	76.20282	73.30297	-226.25352	640.49678	-270.32839	1
184	H	72.87613	75.86185	73.15729	2007.69063	-1035.27229	1523.50231	1
185	C	74.26237	76.17067	74.67725	-540.76542	-573.33303	49.50000	1
186	H	74.49433	75.09443	74.83318	-2374.20950	-1036.76023	843.75774	1
187	C	75.58718	77.00614	74.92725	-77.09082	666.87422	-415.84136	1
188	H	75.49141	77.96874	74.35407	-985.81834	617.19825	2463.91927	1
189	O	76.76041	76.34256	74.39165	293.29899	-391.65602	-477.80926	1
190	H	76.76715	76.76812	73.46344	2528.72714	-681.76262	-751.27122	1
191	C	75.73137	77.31882	76.45538	252.47363	-605.14473	440.05134	1
192	H	76.79942	77.52811	76.72183	-2052.65063	1456.49051	-1043.51830	1
193	H	75.14780	78.22315	76.76007	-2152.98800	-1661.97574	-161.70652	1
194	H	75.41165	76.45849	77.09078	-473.12726	-1584.27339	2165.61725	1
195	C	72.79638	76.42232	75.33448	360.36307	488.46713	505.10056	1
196	O	71.84187	75.95239	74.72861	-200.08817	-528.03552	-385.82850	1
197	N	72.80617	77.04539	76.49948	-597.54095	-226.44775	355.20479	1
198	H	73.67631	77.40198	76.89061	2179.23655	-1300.70981	-991.33835	1
199	C	71.61948	77.12159	77.27508	-687.68921	297.39807	-249.45179	1
200	H	71.03585	76.23683	76.93530	-349.16256	-2467.37713	-1101.72831	1
201	C	72.04491	77.14412	78.81644	672.47345	361.54328	-201.62880	1
202	H	72.78154	77.96322	78.99410	1541.41502	582.18425	2169.97026	1
203	H	71.14138	77.37329	79.42814	-2534.67717	60.25153	997.72295	1
204	C	72.66284	75.82659	79.30418	574.26774	-389.43119	-377.02542	1
205	C	71.83782	74.68397	79.53226	688.82679	-287.33580	-257.96133	1
206	H	70.76260	74.70149	79.27751	331.14182	1470.38163	2269.80013	1
207	C	74.05408	75.79951	79.62949	-383.52382	-675.04808	144.24917	1
208	H	74.69468	76.68094	79.44411	4.09847	1517.59662	2262.86397	1
209	C	72.41596	73.55748	80.11708	-134.76730	428.45285	-649.50303	1
210	H	71.77851	72.67799	80.31383	-903.23433	1600.49020	2011.53387	1
211	C	74.58101	74.65137	80.22517	-335.53281	-615.00040	-364.39058	1
212	H	75.64971	74.65245	80.50313	1596.45398	-1369.33862	1732.02659	1

213	C	73.78876	73.49674	80.49459	585.48547	-340.24194	-406.23938	1
214	O	74.31292	72.32376	81.09966	-419.15649	-173.04408	-511.94141	1
215	H	75.21132	72.65023	81.34076	-1071.84350	1559.71507	-1960.13012	1
216	C	70.83004	78.51386	76.93952	291.41878	-183.13091	710.72246	1
217	O	70.08113	78.57492	75.98334	379.87695	523.47396	-222.23622	1
218	N	71.06299	79.43655	77.86008	564.30591	373.09380	277.24371	1
219	H	71.77646	79.25259	78.56517	-120.59931	-2436.07824	-1214.35098	1
220	C	70.71678	80.79049	77.56213	404.07514	-299.37480	608.84009	1
221	H	69.78858	80.73704	76.94752	-1071.07882	-841.69025	2359.66467	1
222	C	70.55659	81.49288	78.97538	-683.12807	68.71770	-390.13096	1
223	H	69.96563	80.83979	79.65589	2068.88918	1596.58590	770.89603	1
224	H	71.55214	81.60230	79.46114	1379.86429	2342.49779	-179.85638	1
225	C	69.86776	82.88447	78.83585	-176.39967	537.49466	550.97268	1
226	H	70.47127	83.57569	78.20592	-396.28051	1942.22168	1869.33314	1
227	H	68.87806	82.79777	78.33462	-94.44700	586.00678	-2659.20016	1
228	C	69.72224	83.44810	80.32497	-291.69381	-718.18079	-150.72929	1
229	H	69.12530	82.80575	81.02150	-2303.38776	1089.76242	964.62032	1
230	H	70.68310	83.70210	80.84063	884.16729	2568.80533	-207.74283	1
231	N	69.00721	84.64034	80.14534	-594.49522	-252.81478	342.29276	1
232	H	68.70359	84.84960	79.20730	-1735.17426	2084.05705	-263.71605	1
233	C	68.71725	85.45525	81.07677	595.23177	-271.52487	442.22352	1
234	N	69.14664	85.14480	82.37223	585.53813	-424.79750	-105.81303	1
235	H	69.67525	84.33944	82.70450	959.88797	1327.56823	-2177.11905	1
236	H	68.97360	85.72000	83.19703	1578.48647	16.27378	-2220.76233	1
237	N	67.98893	86.54796	80.58468	-452.17763	-390.33541	-421.51853	1
238	H	67.67273	86.77380	79.64298	470.26107	1974.25629	-1817.92087	1
239	H	67.65892	87.30886	81.17956	1856.67307	-1573.97321	-1224.35416	1
240	C	71.98234	81.43300	76.75958	-531.47271	-581.45780	-55.06206	1
241	O	73.10039	80.95890	76.75979	-243.00837	192.73507	609.52485	1
242	N	71.62661	82.65733	76.26416	343.49288	-644.25607	38.09164	1
243	H	70.60619	82.62828	76.40310	-1691.16043	-1535.97525	-1484.73099	1
244	C	72.15778	83.06807	74.94393	542.66492	350.14337	454.42563	1
245	H	71.86422	82.23473	74.26674	1209.57979	-2396.95920	463.86744	1
246	C	71.49683	84.38098	74.62649	-737.14309	145.93010	242.71942	1
247	H	71.55726	85.01430	75.54160	-1050.18303	159.36419	-2509.06125	1
248	C	72.21132	85.11502	73.50422	-706.77696	-252.88343	-245.16230	1
249	H	71.73180	86.10809	73.28474	-1624.64039	-1665.49085	1417.86935	1
250	H	73.28849	85.31379	73.77115	2566.10521	598.51109	693.22305	1
251	H	72.20646	84.52202	72.54923	-1972.69758	107.10018	-1876.34312	1
252	C	70.02759	84.21504	74.27486	412.85148	672.58832	-27.69222	1
253	H	69.53532	85.20476	74.07096	1447.02277	1762.76533	-1490.78944	1
254	H	69.89121	83.58029	73.35730	1320.77379	-145.20455	2378.68491	1
255	H	69.45259	83.72239	75.10531	-1512.10848	1470.52031	1724.75147	1
256	C	73.80331	83.24574	75.06325	-607.11113	499.56689	73.73769	1
257	O	74.27778	84.25142	75.53773	357.97126	460.81534	356.68785	1
258	N	74.40812	82.20163	74.52360	536.55407	-368.62270	332.76306	1
259	H	73.78853	81.46796	74.18304	524.38866	2297.69985	1367.20941	1
260	C	75.81064	82.10896	74.34406	46.50277	-774.29190	-147.97904	1
261	H	75.91033	81.25077	73.64238	1676.51875	1883.29066	1032.55549	1
262	C	76.42356	83.49142	73.76632	-559.41456	-34.19198	-556.30433	1
263	H	76.12730	84.33161	74.44685	-64.66664	395.18769	2695.05373	1
264	H	77.53886	83.44721	73.79872	-2703.44278	-60.40056	333.79418	1
265	C	75.94369	83.75315	72.36779	-519.76435	377.31045	459.42366	1
266	H	74.83024	83.76478	72.37231	-1746.74323	1667.50644	-1261.73691	1
267	C	76.44568	85.11214	71.89162	570.95554	16.46261	-545.27700	1
268	H	76.09827	85.34222	70.85185	2391.58273	28.05277	-1305.07271	1
269	H	76.08745	85.94175	72.55395	175.75588	917.63458	2559.43867	1
270	H	77.56523	85.15645	71.88311	-1063.97851	-2155.34650	1283.00462	1
271	C	76.41852	82.67586	71.40081	193.76014	2.62946	-765.53141	1
272	H	76.14608	82.92042	70.34216	507.39394	-846.55087	2539.60089	1
273	H	77.53152	82.55294	71.43611	1337.57841	1818.19054	1526.01994	1
274	H	75.96746	81.67760	71.63396	1100.88635	-1172.91350	-2199.08909	1

275	C	76.54536	81.81816	75.73821	-549.21115	475.64486	-309.38218	1
276	O	77.70916	82.09894	75.86443	556.06106	-390.37755	-78.24250	1
277	O	75.86576	81.06054	76.70040	-572.27940	-310.19032	-209.75862	1
278	H	74.91019	81.18298	76.38268	-1380.08193	2212.14486	790.85944	1

Listing 99: C00099.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	1.3310	5324
		0.2500	300.00	0.00	0.00	0.00	-1293.4318	0.0000	300.0000
3	H	64.41057	73.24798	72.34644	-2043.14101	-1757.64893	399.89339		1
4	N	65.14137	72.75704	71.83185	426.75047	490.45733	-334.42467		1
5	H	64.61975	72.26968	71.09166	442.25559	-1110.30854	-2448.52907		1
6	C	66.14976	73.60045	71.30588	415.32972	-666.39213	83.73172		1
7	H	65.97987	74.60398	71.75745	879.32219	2491.00447	667.35213		1
8	C	67.60181	73.00154	71.69033	31.35357	477.41777	628.23362		1
9	H	67.77067	72.05742	71.12002	1168.38489	2240.25337	-1019.71136		1
10	H	68.41019	73.70031	71.36768	-360.43770	2534.90498	931.67112		1
11	C	67.67650	72.73533	73.16770	463.18208	512.70242	-382.34388		1
12	H	66.80863	72.09642	73.44978	1725.29117	1863.52247	-987.07854		1
13	C	68.96410	71.99147	73.50364	710.42801	-144.27427	-313.15367		1
14	H	69.05869	71.79326	74.60292	364.20195	-1033.13725	2494.72524		1
15	H	69.02401	71.00374	72.97746	2567.61904	335.80679	847.48802		1
16	H	69.86595	72.58002	73.19898	-2587.99029	680.92867	-512.16411		1
17	C	67.61284	74.02419	73.97673	268.17616	741.64379	-40.42634		1
18	H	67.70135	73.82592	75.07628	1283.54314	-1945.37420	-1411.27812		1
19	H	68.44142	74.72616	73.70043	-1258.57796	1317.15249	-2026.02085		1
20	H	66.64668	74.56796	73.81506	-2502.84526	909.80597	575.92391		1
21	C	65.88669	73.53281	69.72377	619.36578	-458.64843	-172.09273		1
22	O	64.92304	72.88960	69.27462	-81.40433	433.87611	522.34594		1
23	N	66.76948	74.24381	69.04570	175.23996	-622.20190	341.55523		1
24	H	67.50518	74.69370	69.59097	-876.57256	-303.22879	-2561.90213		1
25	C	67.05499	73.80813	67.70188	-571.88214	-534.10783	-106.15033		1
26	H	66.86433	72.71168	67.73909	-2713.20841	-16.25800	-248.80809		1
27	C	65.98881	74.50551	66.75055	166.60354	288.16399	-716.09568		1
28	H	65.91279	75.61389	66.98208	-2097.85574	1636.78449	-586.18044		1
29	O	64.59885	74.15610	66.94045	-317.80580	-363.38227	484.43082		1
30	H	64.66565	73.63296	67.81335	1863.74748	-1451.84923	1357.29467		1
31	C	66.58932	74.28721	65.32125	503.80731	517.99032	318.51606		1
32	H	66.01009	74.84451	64.54780	640.61020	-2157.10410	-1536.29104		1
33	H	67.64982	74.62971	65.25578	1687.88455	465.60692	2087.56452		1
34	H	66.57494	73.20934	65.03525	-1293.07895	-1899.88581	-1463.57452		1
35	C	68.61601	74.14568	67.37616	-153.07550	-733.68902	248.70981		1
36	O	69.26586	73.20204	67.00440	186.15459	-480.78787	-449.34387		1
37	N	69.00085	75.43093	67.46729	-487.53139	543.18517	42.03850		1
38	C	70.38049	75.75201	67.28906	-699.35871	69.34393	360.10701		1
39	H	70.87254	74.82762	66.89951	2.81126	-221.99807	-2715.58072		1
40	C	70.25296	76.97838	66.27861	-507.46439	-592.59194	122.07761		1
41	H	71.18760	77.57459	66.18795	-1975.08116	525.87560	-1801.71556		1
42	H	69.98551	76.63793	65.25382	1588.27743	-1913.22100	1113.83566		1
43	C	69.08316	77.76104	66.94724	-613.62442	-457.55993	-194.14490		1
44	H	69.43273	78.30509	67.85360	1707.54637	-721.27992	1996.92523		1
45	H	68.61782	78.51973	66.27911	758.23357	2100.81767	1560.55011		1
46	C	68.10055	76.56964	67.32153	-352.41524	704.96076	49.21465		1
47	H	67.55512	76.69250	68.28652	1714.76886	-2070.42778	443.35792		1
48	H	67.38171	76.30433	66.51336	1224.15040	1801.50881	1636.97633		1
49	C	71.02562	76.32710	68.68743	566.85117	537.05831	117.62814		1
50	O	70.43593	76.33667	69.73997	-550.26779	-406.08867	4.21666		1
51	N	72.24680	76.76702	68.40918	566.34832	-425.77725	180.18749		1
52	H	72.59451	76.68872	67.45494	644.44502	2646.80550	-52.73430		1
53	C	73.04541	77.30389	69.44437	612.34801	-281.48662	411.56221		1
54	H	72.44348	77.22408	70.38084	1667.23498	-1490.75142	1556.16753		1

55	C	74.41162	76.46194	69.42606	-714.45746	-175.43074	286.98927	1
56	H	75.01711	76.79766	68.53917	-787.09484	1763.03619	-1922.46060	1
57	O	74.29735	75.03421	69.30250	-429.46514	516.51932	-128.40526	1
58	H	74.69312	74.88724	68.41952	1981.82785	436.16847	-1818.18182	1
59	C	75.07908	76.97145	70.75428	630.79189	-468.94448	76.03230	1
60	H	76.11312	76.56486	70.86499	-1775.71861	2062.30353	131.89849	1
61	H	75.14985	78.08304	70.79026	-1855.14608	88.94118	1993.53760	1
62	H	74.50235	76.63919	71.65282	-1504.82350	-780.94249	-2132.90992	1
63	C	73.45533	78.82619	68.97227	288.57638	618.62814	-397.00270	1
64	O	73.84738	79.04627	67.85231	321.70495	-185.26452	574.37218	1
65	N	73.42002	79.64813	70.01833	-447.05792	-446.53431	367.76425	1
66	H	73.06426	79.30592	70.91114	350.31316	1975.63644	-1843.31522	1
67	C	73.39677	81.04724	69.76547	-511.23061	374.03917	-471.51480	1
68	H	73.48341	81.13523	68.65738	2234.79579	-898.70890	-1273.45190	1
69	C	72.00845	81.58329	70.36048	529.53781	-159.34528	563.72604	1
70	H	71.94516	82.67957	70.13548	654.59388	2347.94251	1217.51488	1
71	H	71.19809	81.08193	69.76272	-1526.55661	2103.42026	817.87394	1
72	O	71.74049	81.29670	71.75814	-554.84278	14.12789	399.58769	1
73	H	71.87406	82.18287	72.14056	1297.06236	2061.84854	1220.68812	1
74	C	74.63879	81.75218	70.55419	-662.15484	-412.13544	123.62687	1
75	O	74.59658	82.91292	70.88938	-540.01537	-317.05804	274.91456	1
76	N	75.67621	80.90932	70.62420	-202.76299	-690.00100	-131.49145	1
77	H	75.50398	79.97400	70.25768	-702.62132	-2617.37191	281.70413	1
78	C	76.63289	81.11667	71.66342	-491.73914	576.34187	222.73509	1
79	H	76.70315	82.21870	71.80930	1977.17978	-1823.58850	-434.68928	1
80	C	76.06793	80.35392	72.94161	-649.50797	-328.66843	306.11224	1
81	H	75.74833	79.32561	72.66742	2075.07803	1452.16490	-1004.45904	1
82	C	77.17939	80.31126	74.04399	-615.18735	-489.99689	-70.96352	1
83	H	76.80403	79.85337	74.98917	-1226.32661	-1724.38906	-1716.47170	1
84	H	78.05503	79.70738	73.70959	2381.64273	-969.84735	900.46860	1
85	H	77.55230	81.33278	74.29231	2122.74991	1702.23946	-141.36228	1
86	C	74.85965	81.15945	73.52923	-501.86074	-479.61276	-376.42482	1
87	H	74.44338	80.67198	74.44217	993.79261	-2246.95401	-1177.81305	1
88	H	75.15698	82.19755	73.80958	42.71279	-626.15391	-2651.37258	1
89	H	74.02718	81.24354	72.78951	-2026.39012	-1590.33709	-887.82922	1
90	C	78.00470	80.36950	71.20246	-672.89153	382.57394	-156.34072	1
91	O	78.00792	79.21982	70.81727	410.04627	221.86223	500.35950	1
92	N	79.06060	81.14992	71.49673	-378.11782	-443.79414	-441.10984	1
93	H	78.77698	82.10062	71.74085	2404.15973	-568.14894	1149.30085	1
94	C	80.22302	80.96587	70.64634	-544.54484	466.16019	331.29119	1
95	H	79.78896	80.92753	69.62317	-1409.80988	-170.17955	2325.32679	1
96	C	81.16139	82.21344	70.87115	-184.48284	116.78282	-758.89137	1
97	H	80.62867	83.16501	70.64487	1893.78641	1861.14652	611.04528	1
98	H	81.47615	82.28930	71.93611	-2170.79665	-974.19311	1327.50117	1
99	C	82.39928	82.01628	69.93752	389.51668	672.81878	-138.49152	1
100	H	82.85766	81.01554	70.12083	510.64577	1933.03327	1851.02484	1
101	H	82.07364	81.96329	68.87527	-2302.30869	-1105.72939	-948.89774	1
102	C	83.48916	83.14112	70.09868	-559.93427	-126.34590	542.30857	1
103	O	84.52358	83.05759	69.48780	-670.36003	-111.83166	76.36448	1
104	N	83.13309	84.14461	70.93010	-216.06729	-537.07037	446.51379	1
105	H	82.26489	84.28061	71.46060	-1251.96487	1074.12894	-2168.52500	1
106	H	83.72097	84.96309	71.12294	-2451.83023	-720.73851	944.84612	1
107	C	81.02763	79.59672	70.98232	546.24052	-563.88337	-85.11809	1
108	O	81.59253	79.11329	70.03475	71.70702	-307.40463	606.69673	1
109	N	81.08339	79.21964	72.26451	479.90863	-504.50129	222.86849	1
110	C	81.65209	77.95465	72.64410	75.51268	-600.91904	506.73700	1
111	H	82.57813	77.81781	72.03926	-2033.61562	1795.30103	254.89480	1
112	C	81.87493	78.12343	74.21001	523.79067	517.99274	284.45581	1
113	H	81.86222	77.15098	74.75154	1599.61665	-1127.00911	1895.98173	1
114	H	82.85584	78.59818	74.43469	-1881.83093	1275.82488	-1501.55016	1
115	C	80.69165	79.06114	74.59875	-600.05639	-404.05026	316.64485	1
116	H	79.72818	78.50399	74.62427	-2597.05260	496.36221	657.73249	1

117	H	80.80967	79.54708	75.59302	-1666.24518	1294.38985	-1723.90591	1
118	C	80.74819	80.08781	73.38366	493.57570	-129.95376	-602.56394	1
119	H	79.79511	80.61568	73.14513	-1469.08415	-637.84797	2204.22581	1
120	H	81.57500	80.83381	73.44998	-1038.97840	1068.88701	-2280.71789	1
121	C	80.58547	76.75260	72.40762	188.88100	241.05089	-727.87821	1
122	O	80.94764	75.61098	72.52921	531.88613	-49.19943	427.07960	1
123	N	79.33210	77.21784	72.26723	708.14833	26.93417	-179.73509	1
124	H	79.25900	78.23368	72.11316	-2232.69501	-1179.09831	1023.94816	1
125	C	78.25818	76.37552	71.71611	-738.32412	259.92548	104.42456	1
126	H	77.45018	77.13449	71.55916	2028.89123	1260.02983	1311.33324	1
127	C	78.75871	75.80602	70.40016	-258.65678	-345.52513	661.28459	1
128	H	79.76631	75.36663	70.58837	-1826.06090	-1801.46097	-918.64554	1
129	C	77.86690	74.71224	69.84613	-541.23400	531.92970	-218.41428	1
130	H	78.26227	74.30562	68.87413	1311.73218	-2219.18200	882.19023	1
131	H	77.78218	73.84638	70.56249	-1048.71298	1223.58118	-2196.97971	1
132	H	76.82128	75.07950	69.65245	419.06414	1903.92898	1903.44670	1
133	C	78.91793	76.91484	69.37472	-423.86431	152.66566	-648.55262	1
134	H	79.47166	76.56817	68.45937	105.68386	-2342.50080	1387.51238	1
135	H	77.92019	77.30890	69.03585	-1695.63603	-1484.73621	-1531.02793	1
136	H	79.48129	77.79442	69.80355	-1853.57121	-487.39031	1936.59343	1
137	C	77.79593	75.24806	72.82130	539.71428	-510.58232	267.58633	1
138	O	76.88333	74.47127	72.56830	-15.93758	-278.34085	-624.49402	1
139	N	78.43484	75.37981	73.96966	-676.81886	12.05292	276.17960	1
140	H	79.18526	76.06861	73.91108	-1694.44250	-373.84189	-2100.66098	1
141	C	78.48811	74.24255	74.84808	412.33078	-664.70360	108.35451	1
142	H	78.36367	73.34496	74.20038	1765.77476	1294.44366	1621.76594	1
143	C	79.87158	74.34332	75.60364	-179.66635	-721.95667	-264.73915	1
144	H	80.72446	74.25512	74.89214	-607.34922	2587.87032	-598.10018	1
145	H	79.98177	75.34561	76.07615	-359.69332	-1479.13954	-2259.74260	1
146	C	79.90744	73.21408	76.68634	-240.01076	616.02425	431.85322	1
147	H	78.97385	73.23265	77.29554	-1359.17131	782.54425	2227.99181	1
148	H	79.94373	72.20603	76.21626	-820.36667	85.81767	-2596.78715	1
149	C	81.17772	73.46949	77.59345	-513.07015	236.18570	-551.87280	1
150	H	82.11617	73.36918	77.00081	1816.11944	-1183.11722	-1650.94321	1
151	H	81.17998	74.51125	77.98882	-1800.04429	-1361.53473	1526.34643	1
152	C	81.14067	72.44785	78.75347	726.08972	-253.19732	-179.64713	1
153	H	80.26311	72.54467	79.42200	1224.27271	-456.51798	-2390.90304	1
154	H	81.26266	71.39105	78.44338	1206.40339	-1150.93514	-2154.90344	1
155	N	82.37291	72.73593	79.67641	329.70796	-633.68968	-155.67358	1
156	H	82.45776	72.11201	80.53000	1348.31305	1938.76845	1359.00643	1
157	H	83.33636	72.62832	79.24362	2096.92035	1446.54551	-966.48890	1
158	H	82.43625	73.69907	80.11802	-1197.07217	-2303.53719	827.28733	1
159	C	77.28345	74.37998	75.93353	-378.01186	-556.17301	-413.96481	1
160	O	76.76296	73.37281	76.40852	-409.44433	-307.55053	-453.30833	1
161	N	77.09693	75.63840	76.27939	-429.02477	524.70884	274.08502	1
162	H	77.60074	76.33072	75.72929	1706.34263	-1425.96036	1574.38926	1
163	C	76.11187	75.93917	77.26811	-45.25864	-626.22952	478.93267	1
164	H	76.20293	75.06940	77.95985	1988.63164	570.90773	1772.87287	1
165	C	76.45008	77.34856	77.89261	551.77128	-20.49526	-564.54996	1
166	H	77.48859	77.37488	78.29305	1434.61535	-1753.10253	1513.99471	1
167	H	76.40607	78.14121	77.11197	-714.67738	1819.09770	1898.36494	1
168	C	75.39658	77.61795	79.01974	446.99263	-555.77305	338.97221	1
169	H	74.36513	77.51172	78.61007	1953.68466	1892.25957	-161.67766	1
170	H	75.48032	76.86859	79.83862	-403.03785	2688.07032	-188.43591	1
171	C	75.62041	79.08523	79.56346	567.86262	335.74681	434.04421	1
172	H	76.56471	79.15828	80.15064	-1080.02275	1568.26081	-1948.78900	1
173	H	75.72819	79.80810	78.72235	-919.54108	2111.34692	1456.13463	1
174	C	74.38792	79.44105	80.42784	195.81897	173.33862	-745.11536	1
175	H	73.43237	79.48409	79.86754	1405.67949	-2301.21089	-390.08113	1
176	H	74.26471	78.81928	81.33685	-940.37328	-1118.32446	2299.72133	1
177	N	74.59028	80.89763	80.96391	319.26422	656.36007	-42.02424	1
178	H	73.79770	81.28097	81.55562	1961.03633	619.91968	1787.09422	1

179	H	75.42505	81.06961	81.59655	854.14343	-2156.80752	1429.08711	1
180	H	74.70019	81.66692	80.24079	1237.02905	-1378.50857	-1998.28500	1
181	C	74.64145	75.95513	76.53237	532.53319	-268.57236	517.55729	1
182	O	73.97492	76.95375	76.42793	266.16714	-290.73804	-558.88002	1
183	N	74.36620	74.70190	76.18399	-226.25352	640.49678	-270.32839	1
184	H	75.09916	73.96793	76.31937	2007.69063	-1035.27229	1523.50231	1
185	C	73.16310	74.47074	75.46788	-540.76542	-573.33303	49.50000	1
186	H	72.64588	75.45920	75.44393	-2374.20950	-1036.76023	843.75774	1
187	C	73.62016	73.99745	74.00377	-77.09082	666.87422	-415.84136	1
188	H	74.37895	73.17387	74.10752	-985.81834	617.19825	2463.91927	1
189	O	74.24897	75.02085	73.22882	293.29899	-391.65602	-477.80926	1
190	H	75.15355	74.63001	73.05128	2528.72714	-681.76262	-751.27122	1
191	C	72.30396	73.40109	73.39689	252.47363	-605.14473	440.05134	1
192	H	72.45339	73.07580	72.34032	-2052.65063	1456.49051	-1043.51830	1
193	H	71.94795	72.50909	73.96828	-2152.98800	-1661.97574	-161.70652	1
194	H	71.47964	74.15314	73.39792	-473.12726	-1584.27339	2165.61725	1
195	C	72.29426	73.32953	76.25768	360.36307	488.46713	505.10056	1
196	O	71.12252	73.20801	75.98128	-200.08817	-528.03552	-385.82850	1
197	N	73.02221	72.61211	77.10381	-597.54095	-226.44775	355.20479	1
198	H	74.00691	72.83310	77.22992	2179.23655	-1300.70981	-991.33835	1
199	C	72.38744	71.60883	77.87778	-687.68921	297.39807	-249.45179	1
200	H	71.30523	71.77977	77.66624	-349.16256	-2467.37713	-1101.72831	1
201	C	72.90795	70.18361	77.36278	672.47345	361.54328	-201.62880	1
202	H	74.01717	70.12337	77.45697	1541.41502	582.18425	2169.97026	1
203	H	72.47198	69.37323	77.99201	-2534.67717	60.25153	997.72295	1
204	C	72.49320	69.98044	75.89834	574.26774	-389.43119	-377.02542	1
205	C	71.15758	69.58015	75.59257	688.82679	-287.33580	-257.96133	1
206	H	70.41079	69.44159	76.39519	331.14182	1470.38163	2269.80013	1
207	C	73.44781	70.17729	74.85523	-383.52382	-675.04808	144.24917	1
208	H	74.47778	70.50174	75.09039	4.09847	1517.59662	2262.86397	1
209	C	70.81904	69.35535	74.25914	-134.76730	428.45285	-649.50303	1
210	H	69.79109	69.02898	74.02378	-903.23433	1600.49020	2011.53387	1
211	C	73.05924	69.93945	73.53453	-335.53281	-615.00040	-364.39058	1
212	H	73.80893	70.08067	72.73648	1596.45398	-1369.33862	1732.02659	1
213	C	71.74283	69.51788	73.18623	585.48547	-340.24194	-406.23938	1
214	O	71.33623	69.26966	71.84928	-419.15649	-173.04408	-511.94141	1
215	H	72.19125	69.42668	71.38338	-1071.84350	1559.71507	-1960.13012	1
216	C	72.81519	71.86341	79.43280	291.41878	-183.13091	710.72246	1
217	O	72.57281	72.90926	79.98920	379.87695	523.47396	-222.23622	1
218	N	73.33688	70.75832	79.96863	564.30591	373.09380	277.24371	1
219	H	73.54648	69.96525	79.36252	-120.59931	-2436.07824	-1214.35098	1
220	C	74.00074	70.88465	81.22201	404.07514	-299.37480	608.84009	1
221	H	73.54698	71.77483	81.71881	-1071.07882	-841.69025	2359.66467	1
222	C	73.78205	69.49391	81.95040	-683.12807	68.71770	-390.13096	1
223	H	72.78418	69.07854	81.68518	2068.88918	1596.58590	770.89603	1
224	H	74.52297	68.74864	81.58261	1379.86429	2342.49779	-179.85638	1
225	C	73.90457	69.66519	83.49537	-176.39967	537.49466	550.97268	1
226	H	74.90946	70.03987	83.79241	-396.28051	1942.22168	1869.33314	1
227	H	73.17214	70.40960	83.87979	-94.44700	586.00678	-2659.20016	1
228	C	73.62533	68.20742	84.08877	-291.69381	-718.18079	-150.72929	1
229	H	72.63349	67.76400	83.81668	-2303.38776	1089.76242	964.62032	1
230	H	74.40956	67.44015	83.86511	884.16729	2568.80533	-207.74283	1
231	N	73.61420	68.41569	85.47411	-594.49522	-252.81478	342.29276	1
232	H	73.76284	69.36083	85.79124	-1735.17426	2084.05705	-263.71605	1
233	C	73.42198	67.49936	86.33392	595.23177	-271.52487	442.22352	1
234	N	73.22015	66.19788	85.86132	585.53813	-424.79750	-105.81303	1
235	H	73.18504	65.85558	84.90187	959.88797	1327.56823	-2177.11905	1
236	H	73.04527	65.38332	86.45049	1578.48647	16.27378	-2220.76233	1
237	N	73.46184	68.01438	87.63728	-452.17763	-390.33541	-421.51853	1
238	H	73.57844	68.96700	87.97975	470.26107	1974.25629	-1817.92087	1
239	H	73.30798	67.43844	88.46571	1856.67307	-1573.97321	-1224.35416	1
240	C	75.61035	71.01609	80.92535	-531.47271	-581.45780	-55.06206	1

241	O	76.12368	70.63455	79.89803	-243.00837	192.73507	609.52485	1
242	N	76.19603	71.50455	82.01377	343.49288	-644.25607	38.09164	1
243	H	75.60763	71.76653	82.80214	-1691.16043	-1535.97525	-1484.73099	1
244	C	77.60825	71.64035	82.00179	542.66492	350.14337	454.42563	1
245	H	77.93784	71.06554	81.10504	1209.57979	-2396.95920	463.86744	1
246	C	77.90860	73.19806	81.86999	-737.14309	145.93010	242.71942	1
247	H	77.31864	73.77842	82.61125	-1050.18303	159.36419	-2509.06125	1
248	C	79.44126	73.43825	82.07585	-706.77696	-252.88343	-245.16230	1
249	H	79.74212	74.46999	81.77619	-1624.64039	-1665.49085	1417.86935	1
250	H	79.72810	73.30675	83.16411	2566.10521	598.51109	693.22305	1
251	H	80.05682	72.72478	81.47869	-1972.69758	107.10018	-1876.34312	1
252	C	77.52868	73.63553	80.41353	412.85148	672.58832	-27.69222	1
253	H	77.70208	74.72472	80.24751	1447.02277	1762.76533	-1490.78944	1
254	H	78.12269	73.08192	79.64952	1320.77379	-145.20455	2378.68491	1
255	H	76.45290	73.43074	80.19875	-1512.10848	1470.52031	1724.75147	1
256	C	78.22626	71.06218	83.41672	-607.11113	499.56689	73.73769	1
257	O	79.11398	70.24175	83.34957	357.97126	460.81534	356.68785	1
258	N	77.63698	71.58421	84.48010	536.55407	-368.62270	332.76306	1
259	H	76.89107	72.25051	84.28566	524.38866	2297.69985	1367.20941	1
260	C	78.15382	71.43891	85.79228	46.50277	-774.29190	-147.97904	1
261	H	77.31259	71.76787	86.44128	1676.51875	1883.29066	1032.55549	1
262	C	78.61969	69.91697	86.06231	-559.41456	-34.19198	-556.30433	1
263	H	79.41789	69.64564	85.31887	-64.66664	395.18769	2695.05373	1
264	H	79.08879	69.81949	87.07100	-2703.44278	-60.40056	333.79418	1
265	C	77.44937	68.98195	85.92691	-519.76435	377.31045	459.42366	1
266	H	76.95298	69.18160	84.94997	-1746.74323	1667.50644	-1261.73691	1
267	C	77.92810	67.53476	85.93986	570.95554	16.46261	-545.27700	1
268	H	77.07630	66.81634	85.82131	2391.58273	28.05277	-1305.07271	1
269	H	78.65349	67.33280	85.10971	175.75588	917.63458	2559.43867	1
270	H	78.44518	67.28048	86.90099	-1063.97851	-2155.34650	1283.00462	1
271	C	76.43605	69.18545	87.04527	193.76014	2.62946	-765.53141	1
272	H	75.60785	68.43327	86.98471	507.39394	-846.55087	2539.60089	1
273	H	76.90704	69.07732	88.05624	1337.57841	1818.19054	1526.01994	1
274	H	75.96539	70.20102	87.00259	1100.88635	-1172.91350	-2199.08909	1
275	C	79.44043	72.38180	85.98354	-549.21115	475.64486	-309.38218	1
276	O	79.93919	73.04521	85.10465	556.06106	-390.37755	-78.24250	1
277	O	79.98262	72.40898	87.28843	-572.27940	-310.19032	-209.75862	1
278	H	79.33052	71.79916	87.73551	-1380.08193	2212.14486	790.85944	1

Listing 100: C00100.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.4309	0.0000	300.0000
3	H	73.12045	65.74689	66.44632	-2043.14101	-1757.64893	399.89339		1
4	N	73.52448	66.23757	67.24051	426.75047	490.45733	-334.42467		1
5	H	72.69606	66.57767	67.72394	442.25559	-1110.30854	-2448.52907		1
6	C	74.47122	67.22856	66.91027	415.32972	-666.39213	83.73172		1
7	H	75.07534	66.74717	66.11284	879.32219	2491.00447	667.35213		1
8	C	73.73967	68.56293	66.39403	31.35357	477.41777	628.23362		1
9	H	73.10518	68.98001	67.21277	1168.38489	2240.25337	-1019.71136		1
10	H	74.51152	69.34214	66.18323	-360.43770	2534.90498	931.67112		1
11	C	72.90431	68.30115	65.16521	463.18208	512.70242	-382.34388		1
12	H	72.11998	67.55415	65.42032	1725.29117	1863.52247	-987.07854		1
13	C	72.22064	69.58673	64.71586	710.42801	-144.27427	-313.15367		1
14	H	71.56845	69.41782	63.82033	364.20195	-1033.13725	2494.72524		1
15	H	71.57356	70.01739	65.52300	2567.61904	335.80679	847.48802		1
16	H	72.96827	70.37329	64.43590	-2587.99029	680.92867	-512.16411		1
17	C	73.74142	67.75051	64.01927	268.17616	741.64379	-40.42634		1
18	H	73.13374	67.62991	63.08522	1283.54314	-1945.37420	-1411.27812		1
19	H	74.59819	68.42926	63.77170	-1258.57796	1317.15249	-2026.02085		1
20	H	74.17295	66.74569	64.26292	-2502.84526	909.80597	575.92391		1

21	C	75.34635	67.59643	68.23677	619.36578	-458.64843	-172.09273	1
22	O	75.78593	68.72042	68.36565	-81.40433	433.87611	522.34594	1
23	N	75.52568	66.52039	68.99051	175.23996	-622.20190	341.55523	1
24	H	75.06474	65.68790	68.62216	-876.57256	-303.22879	-2561.90213	1
25	C	76.37099	66.42440	70.12906	-571.88214	-534.10783	-106.15033	1
26	H	76.74277	65.38039	70.06146	-2713.20841	-16.25800	-248.80809	1
27	C	77.52664	67.52323	70.07411	166.60354	288.16399	-716.09568	1
28	H	77.03534	68.54135	70.05493	-2097.85574	1636.78449	-586.18044	1
29	O	78.39346	67.44617	68.92285	-317.80580	-363.38227	484.43082	1
30	H	77.99388	68.14726	68.36304	1863.74748	-1451.84923	1357.29467	1
31	C	78.21381	67.31358	71.47343	503.80731	517.99032	318.51606	1
32	H	79.00986	68.07264	71.65565	640.61020	-2157.10410	-1536.29104	1
33	H	77.47541	67.39684	72.30896	1687.88455	465.60692	2087.56452	1
34	H	78.69110	66.30900	71.55006	-1293.07895	-1899.88581	-1463.57452	1
35	C	75.45303	66.66626	71.46278	-153.07550	-733.68902	248.70981	1
36	O	75.27210	67.79253	71.84561	186.15459	-480.78787	-449.34387	1
37	N	75.04237	65.50831	72.00301	-487.53139	543.18517	42.03850	1
38	C	74.17800	65.49163	73.14013	-699.35871	69.34393	360.10701	1
39	H	73.49584	66.36729	73.05024	2.81126	-221.99807	-2715.58072	1
40	C	73.50678	64.06003	73.00024	-507.46439	-592.59194	122.07761	1
41	H	73.06026	63.69584	73.95250	-1975.08116	525.87560	-1801.71556	1
42	H	72.69050	64.06371	72.24395	1588.27743	-1913.22100	1113.83566	1
43	C	74.72047	63.20455	72.52147	-613.62442	-457.55993	-194.14490	1
44	H	75.40128	62.97488	73.37450	1707.54637	-721.27992	1996.92523	1
45	H	74.43244	62.22919	72.06802	758.23357	2100.81767	1560.55011	1
46	C	75.41444	64.19544	71.49226	-352.41524	704.96076	49.21465	1
47	H	76.52803	64.13589	71.46789	1714.76886	-2070.42778	443.35792	1
48	H	75.01590	64.14448	70.45128	1224.15040	1801.50881	1636.97633	1
49	C	75.10867	65.54843	74.49851	566.85117	537.05831	117.62814	1
50	O	75.97961	64.74440	74.70114	-550.26779	-406.08867	4.21666	1
51	N	74.63105	66.50974	75.26798	566.34832	-425.77725	180.18749	1
52	H	73.79532	67.06617	75.02870	644.44502	2646.80550	-52.73430	1
53	C	75.28907	66.91742	76.46043	612.34801	-281.48662	411.56221	1
54	H	75.82180	66.03609	76.88304	1667.23498	-1490.75142	1556.16753	1
55	C	76.29050	68.10631	76.05937	-714.45746	-175.43074	286.98927	1
56	H	75.67712	68.92547	75.59193	-787.09484	1763.03619	-1922.46060	1
57	O	77.30207	67.78382	75.08882	-429.46514	516.51932	-128.40526	1
58	H	76.97774	68.27996	74.30956	1981.82785	436.16847	-1818.18182	1
59	C	76.85070	68.59399	77.44406	630.79189	-468.94448	76.03230	1
60	H	77.56103	69.44336	77.31532	-1775.71861	2062.30353	131.89849	1
61	H	76.03859	68.95081	78.12046	-1855.14608	88.94118	1993.53760	1
62	H	77.39929	67.78127	77.97476	-1504.82350	-780.94249	-2132.90992	1
63	C	73.99577	67.47518	77.28037	288.57638	618.62814	-397.00270	1
64	O	72.96232	67.68031	76.66366	321.70495	-185.26452	574.37218	1
65	N	74.23227	67.62539	78.57945	-447.05792	-446.53431	367.76425	1
66	H	75.16815	67.40636	78.92047	350.31316	1975.63644	-1843.31522	1
67	C	73.41377	68.56720	79.28261	-511.23061	374.03917	-471.51480	1
68	H	72.44487	68.41711	78.75141	2234.79579	-898.70890	-1273.45190	1
69	C	73.39894	68.10264	80.81287	529.53781	-159.34528	563.72604	1
70	H	72.53055	68.62143	81.30250	654.59388	2347.94251	1217.51488	1
71	H	73.16622	67.00588	80.82298	-1526.55661	2103.42026	817.87394	1
72	O	74.59219	68.39398	81.59264	-554.84278	14.12789	399.58769	1
73	H	75.07529	67.55765	81.46778	1297.06236	2061.84854	1220.68812	1
74	C	73.97857	70.06224	79.01625	-662.15484	-412.13544	123.62687	1
75	O	74.33131	70.41485	77.91767	-540.01537	-317.05804	274.91456	1
76	N	73.94722	70.82418	80.13740	-202.76299	-690.00100	-131.49145	1
77	H	73.61624	70.28212	80.93915	-702.62132	-2617.37191	281.70413	1
78	C	73.55264	72.24497	80.01070	-491.73914	576.34187	222.73509	1
79	H	72.59184	72.23489	79.44839	1977.17978	-1823.58850	-434.68928	1
80	C	73.44956	72.81402	81.40310	-649.50797	-328.66843	306.11224	1
81	H	74.26245	72.36309	82.01666	2075.07803	1452.16490	-1004.45904	1
82	C	73.64433	74.32025	81.40895	-615.18735	-489.99689	-70.96352	1

83	H	73.60930	74.74209	82.45091	-1226.32661	-1724.38906	-1716.47170	1
84	H	74.63846	74.61184	80.96160	2381.64273	-969.84735	900.46860	1
85	H	72.84938	74.84220	80.80827	2122.74991	1702.23946	-141.36228	1
86	C	72.12759	72.46356	82.06378	-501.86074	-479.61276	-376.42482	1
87	H	72.08284	72.83456	83.12471	993.79261	-2246.95401	-1177.81305	1
88	H	71.25794	72.91934	81.51479	42.71279	-626.15391	-2651.37258	1
89	H	71.95874	71.35184	82.09096	-2026.39012	-1590.33709	-887.82922	1
90	C	74.75583	73.01087	79.16657	-672.89153	382.57394	-156.34072	1
91	O	74.45999	73.80896	78.30431	410.04627	221.86223	500.35950	1
92	N	75.94179	72.70094	79.66600	-378.11782	-443.79414	-441.10984	1
93	H	75.88451	71.95903	80.36179	2404.15973	-568.14894	1149.30085	1
94	C	77.16856	73.09799	79.05985	-544.54484	466.16019	331.29119	1
95	H	77.90676	72.33316	79.38989	-1409.80988	-170.17955	2325.32679	1
96	C	76.84455	73.04633	77.50144	-184.48284	116.78282	-758.89137	1
97	H	76.25162	72.12652	77.28743	1893.78641	1861.14652	611.04528	1
98	H	76.18514	73.90379	77.20676	-2170.79665	-974.19311	1327.50117	1
99	C	78.15321	73.06501	76.64973	389.51668	672.81878	-138.49152	1
100	H	78.72851	73.99921	76.84312	510.64577	1933.03327	1851.02484	1
101	H	78.83721	72.24678	76.96724	-2302.30869	-1105.72939	-948.89774	1
102	C	77.86756	72.92316	75.12134	-559.93427	-126.34590	542.30857	1
103	O	78.81109	72.96356	74.35089	-670.36003	-111.83166	76.36448	1
104	N	76.57187	72.79042	74.80582	-216.06729	-537.07037	446.51379	1
105	H	75.75710	72.71238	75.42743	-1251.96487	1074.12894	-2168.52500	1
106	H	76.21821	72.62977	73.85480	-2451.83023	-720.73851	944.84612	1
107	C	77.54248	74.59012	79.56110	546.24052	-563.88337	-85.11809	1
108	O	76.67387	75.41602	79.81601	71.70702	-307.40463	606.69673	1
109	N	78.86372	74.75571	79.60211	479.90863	-504.50129	222.86849	1
110	C	79.42674	76.02988	79.96499	75.51268	-600.91904	506.73700	1
111	H	78.83110	76.36398	80.84511	-2033.61562	1795.30103	254.89480	1
112	C	80.94773	75.69669	80.24809	523.79067	517.99274	284.45581	1
113	H	81.61862	76.56843	80.07383	1599.61665	-1127.00911	1895.98173	1
114	H	81.10922	75.37424	81.30128	-1881.83093	1275.82488	-1501.55016	1
115	C	81.19377	74.52299	79.24888	-600.05639	-404.05026	316.64485	1
116	H	81.30004	74.90593	78.20865	-2597.05260	496.36221	657.73249	1
117	H	82.10932	73.93006	79.47004	-1666.24518	1294.38985	-1723.90591	1
118	C	79.84738	73.69653	79.43104	493.57570	-129.95376	-602.56394	1
119	H	79.56197	73.06072	78.56418	-1469.08415	-637.84797	2204.22581	1
120	H	79.80439	73.08644	80.36450	-1038.97840	1068.88701	-2280.71789	1
121	C	79.24413	77.04361	78.69329	188.88100	241.05089	-727.87821	1
122	O	80.17554	77.38622	78.00887	531.88613	-49.19943	427.07960	1
123	N	77.96439	77.39985	78.60420	708.14833	26.93417	-179.73509	1
124	H	77.23730	76.97271	79.22488	-2232.69501	-1179.09831	1023.94816	1
125	C	77.64453	78.29130	77.53122	-738.32412	259.92548	104.42456	1
126	H	78.39083	78.04374	76.73992	2028.89123	1260.02983	1311.33324	1
127	C	76.12484	78.07163	77.11678	-258.65678	-345.52513	661.28459	1
128	H	75.44018	78.36049	77.94695	-1826.06090	-1801.46097	-918.64554	1
129	C	75.85734	78.96664	75.85729	-541.23400	531.92970	-218.41428	1
130	H	74.89230	78.70845	75.35600	1311.73218	-2219.18200	882.19023	1
131	H	75.81164	80.05557	76.13063	-1048.71298	1223.58118	-2196.97971	1
132	H	76.66196	78.84743	75.09306	419.06414	1903.92898	1903.44670	1
133	C	75.90493	76.56077	76.77053	-423.86431	152.66566	-648.55262	1
134	H	74.85040	76.35813	76.46934	105.68386	-2342.50080	1387.51238	1
135	H	76.56904	76.22658	75.93307	-1695.63603	-1484.73621	-1531.02793	1
136	H	76.12244	75.91087	77.65458	-1853.57121	-487.39031	1936.59343	1
137	C	77.78867	79.83838	78.02634	539.71428	-510.58232	267.58633	1
138	O	77.73408	80.72109	77.16954	-15.93758	-278.34085	-624.49402	1
139	N	77.87669	79.94913	79.33055	-676.81886	12.05292	276.17960	1
140	H	77.87978	79.05966	79.82783	-1694.44250	-373.84189	-2100.66098	1
141	C	78.06279	81.17841	80.01704	412.33078	-664.70360	108.35451	1
142	H	78.39613	80.87280	81.03383	1765.77476	1294.44366	1621.76594	1
143	C	79.14456	82.01150	79.21528	-179.66635	-721.95667	-264.73915	1
144	H	80.03037	81.37623	78.98781	-607.34922	2587.87032	-598.10018	1

145	H	78.74366	82.32583	78.22074	-359.69332	-1479.13954	-2259.74260	1
146	C	79.55031	83.25522	80.07238	-240.01076	616.02425	431.85322	1
147	H	78.67106	83.91308	80.25543	-1359.17131	782.54425	2227.99181	1
148	H	79.91663	82.94557	81.07666	-820.36667	85.81767	-2596.78715	1
149	C	80.68082	84.02200	79.27382	-513.07015	236.18570	-551.87280	1
150	H	81.56267	83.36198	79.10502	1816.11944	-1183.11722	-1650.94321	1
151	H	80.32245	84.31038	78.25890	-1800.04429	-1361.53473	1526.34643	1
152	C	81.08225	85.27269	80.08898	726.08972	-253.19732	-179.64713	1
153	H	80.28848	86.04114	80.17570	1224.27271	-456.51798	-2390.90304	1
154	H	81.50899	85.05555	81.08843	1206.40339	-1150.93514	-2154.90344	1
155	N	82.24275	85.98514	79.31412	329.70796	-633.68968	-155.67358	1
156	H	82.60881	86.87739	79.75576	1348.31305	1938.76845	1359.00643	1
157	H	83.14162	85.43653	79.18083	2096.92035	1446.54551	-966.48890	1
158	H	82.03687	86.31135	78.32530	-1197.07217	-2303.53719	827.28733	1
159	C	76.63413	81.98590	80.07350	-378.01186	-556.17301	-413.96481	1
160	O	76.27538	82.47965	81.11291	-409.44433	-307.55053	-453.30833	1
161	N	76.06126	82.05364	78.87883	-429.02477	524.70884	274.08502	1
162	H	76.53669	81.67915	78.02676	1706.34263	-1425.96036	1574.38926	1
163	C	74.68212	82.44299	78.84741	-45.25864	-626.22952	478.93267	1
164	H	74.19231	81.98319	79.73450	1988.63164	570.90773	1772.87287	1
165	C	74.75696	84.01611	78.98766	551.77128	-20.49526	-564.54996	1
166	H	75.32578	84.27378	79.91196	1434.61535	-1753.10253	1513.99471	1
167	H	75.34267	84.44811	78.14555	-714.67738	1819.09770	1898.36494	1
168	C	73.31958	84.63024	79.03470	446.99263	-555.77305	338.97221	1
169	H	72.74534	84.38236	78.11330	1953.68466	1892.25957	-161.67766	1
170	H	72.73200	84.22103	79.88686	-403.03785	2688.07032	-188.43591	1
171	C	73.53074	86.19186	79.18210	567.86262	335.74681	434.04421	1
172	H	74.10418	86.42227	80.10936	-1080.02275	1568.26081	-1948.78900	1
173	H	74.14865	86.58376	78.34189	-919.54108	2111.34692	1456.13463	1
174	C	72.15387	86.89294	79.21103	195.81897	173.33862	-745.11536	1
175	H	71.57343	86.81274	78.27030	1405.67949	-2301.21089	-390.08113	1
176	H	71.51474	86.62392	80.07549	-940.37328	-1118.32446	2299.72133	1
177	N	72.42710	88.42686	79.38198	319.26422	656.36007	-42.02424	1
178	H	71.56725	89.04684	79.41311	1961.03633	619.91968	1787.09422	1
179	H	72.93463	88.73112	80.26323	854.14343	-2156.80752	1429.08711	1
180	H	72.99892	88.90274	78.62490	1237.02905	-1378.50857	-1998.28500	1
181	C	74.08464	81.97472	77.39814	532.53319	-268.57236	517.55729	1
182	O	74.76049	82.06761	76.39603	266.16714	-290.73804	-558.88002	1
183	N	72.81029	81.63984	77.53653	-226.25352	640.49678	-270.32839	1
184	H	72.43298	81.66772	78.48252	2007.69063	-1035.27229	1523.50231	1
185	C	72.06110	81.02487	76.49708	-540.76542	-573.33303	49.50000	1
186	H	71.03181	80.96932	76.91560	-2374.20950	-1036.76023	843.75774	1
187	C	72.12825	82.04019	75.25907	-77.09082	666.87422	-415.84136	1
188	H	73.22021	82.27938	75.07536	-985.81834	617.19825	2463.91927	1
189	O	71.47146	83.29528	75.54120	293.29899	-391.65602	-477.80926	1
190	H	72.24250	83.89466	75.57094	2528.72714	-681.76262	-751.27122	1
191	C	71.60231	81.31312	73.97076	252.47363	-605.14473	440.05134	1
192	H	71.58345	82.01514	73.10403	-2052.65063	1456.49051	-1043.51830	1
193	H	72.26644	80.44234	73.67075	-2152.98800	-1661.97574	-161.70652	1
194	H	70.56002	80.93719	74.10242	-473.12726	-1584.27339	2165.61725	1
195	C	72.65608	79.52616	76.29831	360.36307	488.46713	505.10056	1
196	O	73.49787	79.04365	77.02734	-200.08817	-528.03552	-385.82850	1
197	N	71.97999	78.90667	75.33161	-597.54095	-226.44775	355.20479	1
198	H	71.26282	79.41915	74.82137	2179.23655	-1300.70981	-991.33835	1
199	C	72.54893	77.71771	74.79489	-687.68921	297.39807	-249.45179	1
200	H	72.99647	77.17670	75.65871	-349.16256	-2467.37713	-1101.72831	1
201	C	71.42106	76.93548	73.97850	672.47345	361.54328	-201.62880	1
202	H	71.11635	77.54168	73.09572	1541.41502	582.18425	2169.97026	1
203	H	71.84008	75.98016	73.58656	-2534.67717	60.25153	997.72295	1
204	C	70.20356	76.66973	74.87476	574.26774	-389.43119	-377.02542	1
205	C	70.25445	75.66407	75.88590	688.82679	-287.33580	-257.96133	1
206	H	71.16792	75.06096	76.03979	331.14182	1470.38163	2269.80013	1

207	C	69.02348	77.44930	74.68121	-383.52382	-675.04808	144.24917	1
208	H	68.98160	78.22031	73.88997	4.09847	1517.59662	2262.86397	1
209	C	69.12309	75.46198	76.67591	-134.76730	428.45285	-649.50303	1
210	H	69.15760	74.68205	77.45629	-903.23433	1600.49020	2011.53387	1
211	C	67.91845	77.20968	75.50073	-335.53281	-615.00040	-364.39058	1
212	H	67.00950	77.81565	75.34047	1596.45398	-1369.33862	1732.02659	1
213	C	67.92287	76.21483	76.52171	585.48547	-340.24194	-406.23938	1
214	O	66.80467	75.96523	77.35918	-419.15649	-173.04408	-511.94141	1
215	H	66.16386	76.61091	76.97750	-1071.84350	1559.71507	-1960.13012	1
216	C	73.63547	78.12481	73.64168	291.41878	-183.13091	710.72246	1
217	O	73.50916	79.09838	72.92535	379.87695	523.47396	-222.23622	1
218	N	74.52308	77.14504	73.58117	564.30591	373.09380	277.24371	1
219	H	74.43336	76.38129	74.24838	-120.59931	-2436.07824	-1214.35098	1
220	C	75.68787	77.28686	72.76055	404.07514	-299.37480	608.84009	1
221	H	76.01771	78.34163	72.89619	-1071.07882	-841.69025	2359.66467	1
222	C	76.73304	76.20166	73.24105	-683.12807	68.71770	-390.13096	1
223	H	76.86391	76.23440	74.35049	2068.88918	1596.58590	770.89603	1
224	H	76.35619	75.17674	73.01999	1379.86429	2342.49779	-179.85638	1
225	C	78.08965	76.45631	72.51170	-176.39967	537.49466	550.97268	1
226	H	77.95121	76.47833	71.40539	-396.28051	1942.22168	1869.33314	1
227	H	78.51351	77.44846	72.78312	-94.44700	586.00678	-2659.20016	1
228	C	79.05942	75.26622	72.95498	-291.69381	-718.18079	-150.72929	1
229	H	79.23872	75.18720	74.05756	-2303.38776	1089.76242	964.62032	1
230	H	78.76853	74.24766	72.58173	884.16729	2568.80533	-207.74283	1
231	N	80.30427	75.57526	72.39510	-594.49522	-252.81478	342.29276	1
232	H	80.36123	76.42489	71.85682	-1735.17426	2084.05705	-263.71605	1
233	C	81.35098	74.86441	72.53291	595.23177	-271.52487	442.22352	1
234	N	81.25552	73.68922	73.27801	585.53813	-424.79750	-105.81303	1
235	H	80.40009	73.29055	73.73211	959.88797	1327.56823	-2177.11905	1
236	H	82.04677	73.05728	73.43966	1578.48647	16.27378	-2220.76233	1
237	N	82.45332	75.43357	71.87342	-452.17763	-390.33541	-421.51853	1
238	H	82.53636	76.29132	71.33084	470.26107	1974.25629	-1817.92087	1
239	H	83.38316	75.01352	71.87940	1856.67307	-1573.97321	-1224.35416	1
240	C	75.31631	76.99126	71.20058	-531.47271	-581.45780	-55.06206	1
241	O	76.10200	77.28107	70.32731	-243.00837	192.73507	609.52485	1
242	N	74.15684	76.34286	71.07064	343.49288	-644.25607	38.09164	1
243	H	73.66470	76.17196	71.94693	-1691.16043	-1535.97525	-1484.73099	1
244	C	73.59836	76.05812	69.75748	542.66492	350.14337	454.42563	1
245	H	74.34526	76.52792	69.07132	1209.57979	-2396.95920	463.86744	1
246	C	73.53686	74.54344	69.60767	-737.14309	145.93010	242.71942	1
247	H	72.83287	74.15430	70.37607	-1050.18303	159.36419	-2509.06125	1
248	C	73.02694	74.12122	68.24361	-706.77696	-252.88343	-245.16230	1
249	H	72.95446	73.00169	68.15436	-1624.64039	-1665.49085	1417.86935	1
250	H	72.00009	74.54584	68.03512	2566.10521	598.51109	693.22305	1
251	H	73.70610	74.47703	67.42024	-1972.69758	107.10018	-1876.34312	1
252	C	74.89381	73.91175	69.86337	412.85148	672.58832	-27.69222	1
253	H	74.85332	72.78915	69.80885	1447.02277	1762.76533	-1490.78944	1
254	H	75.65452	74.25567	69.10945	1320.77379	-145.20455	2378.68491	1
255	H	75.29244	74.18809	70.87814	-1512.10848	1470.52031	1724.75147	1
256	C	72.09421	76.76606	69.66120	-607.11113	499.56689	73.73769	1
257	O	71.36410	76.45143	68.75177	357.97126	460.81534	356.68785	1
258	N	71.87080	77.63047	70.64446	536.55407	-368.62270	332.76306	1
259	H	72.66926	77.76732	71.26641	524.38866	2297.69985	1367.20941	1
260	C	70.93785	78.69352	70.49531	46.50277	-774.29190	-147.97904	1
261	H	71.18107	79.34599	71.36253	1676.51875	1883.29066	1032.55549	1
262	C	71.12123	79.43743	69.07525	-559.41456	-34.19198	-556.30433	1
263	H	71.21596	78.67825	68.25865	-64.66664	395.18769	2695.05373	1
264	H	70.19448	80.01904	68.84855	-2703.44278	-60.40056	333.79418	1
265	C	72.31932	80.34740	69.10352	-519.76435	377.31045	459.42366	1
266	H	73.24020	79.72594	69.18063	-1746.74323	1667.50644	-1261.73691	1
267	C	72.38138	81.16677	67.81973	570.95554	16.46261	-545.27700	1
268	H	73.26386	81.85722	67.81123	2391.58273	28.05277	-1305.07271	1

269	H	72.46101	80.51358	66.91287	175.75588	917.63458	2559.43867	1
270	H	71.46564	81.80017	67.69174	-1063.97851	-2155.34650	1283.00462	1
271	C	72.27765	81.29103	70.29826	193.76014	2.62946	-765.53141	1
272	H	73.05906	82.09014	70.22249	507.39394	-846.55087	2539.60089	1
273	H	71.28440	81.80339	70.38514	1337.57841	1818.19054	1526.01994	1
274	H	72.46244	80.74746	71.26111	1100.88635	-1172.91350	-2199.08909	1
275	C	69.42846	78.15472	70.55160	-549.21115	475.64486	-309.38218	1
276	O	68.52112	78.75029	70.02888	556.06106	-390.37755	-78.24250	1
277	O	69.16726	77.07853	71.43709	-572.27940	-310.19032	-209.75862	1
278	H	70.10405	76.75654	71.56041	-1380.08193	2212.14486	790.85944	1

Listing 101: C00101.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.4272	0.0000	300.0000
3	H	80.89296	72.09404	75.93576	-2043.14101	-1757.64893	399.89339		1
4	N	80.99881	72.36087	74.95719	426.75047	490.45733	-334.42467		1
5	H	80.09531	72.80438	74.78961	442.25559	-1110.30854	-2448.52907		1
6	C	82.05539	73.28458	74.75225	415.32972	-666.39213	83.73172		1
7	H	81.84519	74.11841	75.45545	879.32219	2491.00447	667.35213		1
8	C	83.47614	72.59016	75.04960	31.35357	477.41777	628.23362		1
9	H	83.59961	71.71554	74.36665	1168.38489	2240.25337	-1019.71136		1
10	H	84.29365	73.30294	74.78266	-360.43770	2534.90498	931.67112		1
11	C	83.61601	72.15211	76.48550	463.18208	512.70242	-382.34388		1
12	H	82.77190	71.47126	76.73416	1725.29117	1863.52247	-987.07854		1
13	C	84.92173	71.38760	76.66928	710.42801	-144.27427	-313.15367		1
14	H	85.04951	71.03230	77.72427	364.20195	-1033.13725	2494.72524		1
15	H	84.97151	70.48560	76.00624	2567.61904	335.80679	847.48802		1
16	H	85.81016	72.02575	76.42550	-2587.99029	680.92867	-512.16411		1
17	C	83.58738	73.33625	77.44171	268.17616	741.64379	-40.42634		1
18	H	83.72267	73.01364	78.50699	1283.54314	-1945.37420	-1411.27812		1
19	H	84.40333	74.06989	77.21358	-1258.57796	1317.15249	-2026.02085		1
20	H	82.61683	73.89288	77.38956	-2502.84526	909.80597	575.92391		1
21	C	82.04423	73.77232	73.20055	619.36578	-458.64843	-172.09273		1
22	O	82.60170	74.81117	72.91499	-81.40433	433.87611	522.34594		1
23	N	81.45744	72.90057	72.38038	175.23996	-622.20190	341.55523		1
24	H	81.04308	72.07249	72.80474	-876.57256	-303.22879	-2561.90213		1
25	C	81.46562	73.17905	70.98683	-571.88214	-534.10783	-106.15033		1
26	H	81.95911	74.18047	70.92695	-2713.20841	-16.25800	-248.80809		1
27	C	82.32469	72.02881	70.26595	166.60354	288.16399	-716.09568		1
28	H	81.86527	71.02543	70.49368	-2097.85574	1636.78449	-586.18044		1
29	O	83.69365	71.90424	70.68324	-317.80580	-363.38227	484.43082		1
30	H	83.69497	70.99857	71.05540	1863.74748	-1451.84923	1357.29467		1
31	C	82.09321	72.37933	68.75158	503.80731	517.99032	318.51606		1
32	H	82.49686	71.58630	68.08014	640.61020	-2157.10410	-1536.29104		1
33	H	81.00831	72.50254	68.51273	1687.88455	465.60692	2087.56452		1
34	H	82.59878	73.33452	68.47795	-1293.07895	-1899.88581	-1463.57452		1
35	C	79.92964	73.18959	70.42779	-153.07550	-733.68902	248.70981		1
36	O	79.69314	74.02716	69.59531	186.15459	-480.78787	-449.34387		1
37	N	79.16008	72.15823	70.80738	-487.53139	543.18517	42.03850		1
38	C	77.73536	72.29682	70.70806	-699.35871	69.34393	360.10701		1
39	H	77.61273	73.21727	70.08969	2.81126	-221.99807	-2715.58072		1
40	C	77.32326	70.94364	69.98659	-507.46439	-592.59194	122.07761		1
41	H	76.25956	70.66481	70.15401	-1975.08116	525.87560	-1801.71556		1
42	H	77.44901	71.03244	68.88465	1588.27743	-1913.22100	1113.83566		1
43	C	78.33142	69.90626	70.57589	-613.62442	-457.55993	-194.14490		1
44	H	77.99891	69.51220	71.56214	1707.54637	-721.27992	1996.92523		1
45	H	78.47415	69.01700	69.92168	758.23357	2100.81767	1560.55011		1
46	C	79.64471	70.78266	70.72519	-352.41524	704.96076	49.21465		1
47	H	80.22702	70.57473	71.65294	1714.76886	-2070.42778	443.35792		1
48	H	80.32286	70.74996	69.83952	1224.15040	1801.50881	1636.97633		1

49	C	77.11383	72.49255	72.20661	566.85117	537.05831	117.62814	1
50	O	77.16308	73.61360	72.72496	-550.26779	-406.08867	4.21666	1
51	N	76.59832	71.38923	72.67443	566.34832	-425.77725	180.18749	1
52	H	76.65347	70.58213	72.05797	644.44502	2646.80550	-52.73430	1
53	C	76.12895	71.22796	74.00666	612.34801	-281.48662	411.56221	1
54	H	75.90588	70.13964	74.06701	1667.23498	-1490.75142	1556.16753	1
55	C	77.33775	71.61915	74.98337	-714.45746	-175.43074	286.98927	1
56	H	77.77758	72.60294	74.66408	-787.09484	1763.03619	-1922.46060	1
57	O	78.40646	70.65379	74.97183	-429.46514	516.51932	-128.40526	1
58	H	79.16375	71.20479	74.70275	1981.82785	436.16847	-1818.18182	1
59	C	76.62005	71.81192	76.36608	630.79189	-468.94448	76.03230	1
60	H	77.35888	72.01438	77.17832	-1775.71861	2062.30353	131.89849	1
61	H	75.90688	72.67333	76.35142	-1855.14608	88.94118	1993.53760	1
62	H	76.05033	70.90069	76.66084	-1504.82350	-780.94249	-2132.90992	1
63	C	74.74463	72.08364	74.15540	288.57638	618.62814	-397.00270	1
64	O	73.74809	71.43639	74.37035	321.70495	-185.26452	574.37218	1
65	N	74.87945	73.41225	74.08210	-447.05792	-446.53431	367.76425	1
66	H	75.81352	73.80904	73.81386	350.31316	1975.63644	-1843.31522	1
67	C	73.66962	74.08304	73.70892	-511.23061	374.03917	-471.51480	1
68	H	72.84642	73.45200	74.13148	2234.79579	-898.70890	-1273.45190	1
69	C	73.72073	75.56696	74.30174	529.53781	-159.34528	563.72604	1
70	H	72.87229	76.14314	73.84159	654.59388	2347.94251	1217.51488	1
71	H	73.46539	75.47736	75.39113	-1526.55661	2103.42026	817.87394	1
72	O	74.94015	76.32169	74.08970	-554.84278	14.12789	399.58769	1
73	H	75.54714	75.81805	74.66163	1297.06236	2061.84854	1220.68812	1
74	C	73.52394	74.18550	72.08704	-662.15484	-412.13544	123.62687	1
75	O	72.40750	74.10109	71.62696	-540.01537	-317.05804	274.91456	1
76	N	74.68246	74.34338	71.46740	-202.76299	-690.00100	-131.49145	1
77	H	75.55136	74.37280	72.02189	-702.62132	-2617.37191	281.70413	1
78	C	74.71943	74.67132	70.08403	-491.73914	576.34187	222.73509	1
79	H	75.76799	74.47455	69.76854	1977.17978	-1823.58850	-434.68928	1
80	C	73.64233	73.77310	69.32829	-649.50797	-328.66843	306.11224	1
81	H	72.61386	74.16042	69.53203	2075.07803	1452.16490	-1004.45904	1
82	C	73.92771	73.72589	67.78837	-615.18735	-489.99689	-70.96352	1
83	H	73.17885	73.09315	67.25660	-1226.32661	-1724.38906	-1716.47170	1
84	H	73.89216	74.73540	67.31883	2381.64273	-969.84735	900.46860	1
85	H	74.93466	73.29800	67.57360	2122.74991	1702.23946	-141.36228	1
86	C	73.75908	72.28498	69.80542	-501.86074	-479.61276	-376.42482	1
87	H	73.02045	71.62639	69.29090	993.79261	-2246.95401	-1177.81305	1
88	H	74.77405	71.87151	69.60628	42.71279	-626.15391	-2651.37258	1
89	H	73.57057	72.20274	70.90354	-2026.39012	-1590.33709	-887.82922	1
90	C	74.30984	76.24367	69.94481	-672.89153	382.57394	-156.34072	1
91	O	73.67683	76.87844	70.78916	410.04627	221.86223	500.35950	1
92	N	74.66027	76.65650	68.74343	-378.11782	-443.79414	-441.10984	1
93	H	75.21791	76.00662	68.19396	2404.15973	-568.14894	1149.30085	1
94	C	74.58528	78.06459	68.45007	-544.54484	466.16019	331.29119	1
95	H	75.21926	78.49785	69.25561	-1409.80988	-170.17955	2325.32679	1
96	C	75.20946	78.25564	67.01085	-184.48284	116.78282	-758.89137	1
97	H	76.16739	77.69589	66.91294	1893.78641	1861.14652	611.04528	1
98	H	74.53471	77.84675	66.22493	-2170.79665	-974.19311	1327.50117	1
99	C	75.42676	79.79064	66.81954	389.51668	672.81878	-138.49152	1
100	H	74.46101	80.33137	66.95923	510.64577	1933.03327	1851.02484	1
101	H	76.07239	80.18880	67.63323	-2302.30869	-1105.72939	-948.89774	1
102	C	76.05665	80.16549	65.42585	-559.93427	-126.34590	542.30857	1
103	O	76.24142	81.32353	65.15186	-670.36003	-111.83166	76.36448	1
104	N	76.35624	79.10351	64.64681	-216.06729	-537.07037	446.51379	1
105	H	76.23707	78.10041	64.82945	-1251.96487	1074.12894	-2168.52500	1
106	H	76.79038	79.17876	63.72037	-2451.83023	-720.73851	944.84612	1
107	C	73.08341	78.69448	68.54011	546.24052	-563.88337	-85.11809	1
108	O	73.07374	79.88665	68.72015	71.70702	-307.40463	606.69673	1
109	N	72.04986	77.88421	68.33333	479.90863	-504.50129	222.86849	1
110	C	70.68137	78.29489	68.58754	75.51268	-600.91904	506.73700	1

111	H	70.61271	79.35292	68.23310	-2033.61562	1795.30103	254.89480	1
112	C	69.83717	77.24561	67.71187	523.79067	517.99274	284.45581	1
113	H	68.79310	77.12690	68.07642	1599.61665	-1127.00911	1895.98173	1
114	H	69.77039	77.56505	66.64872	-1881.83093	1275.82488	-1501.55016	1
115	C	70.69506	75.95812	67.86364	-600.05639	-404.05026	316.64485	1
116	H	70.51773	75.47478	68.85084	-2597.05260	496.36221	657.73249	1
117	H	70.48352	75.18780	67.08864	-1666.24518	1294.38985	-1723.90591	1
118	C	72.17164	76.55302	67.76832	493.57570	-129.95376	-602.56394	1
119	H	72.93246	76.01621	68.38323	-1469.08415	-637.84797	2204.22581	1
120	H	72.56253	76.68826	66.73192	-1038.97840	1068.88701	-2280.71789	1
121	C	70.30961	78.15387	70.11427	188.88100	241.05089	-727.87821	1
122	O	69.08730	78.14688	70.53734	531.88613	-49.19943	427.07960	1
123	N	71.31951	78.04744	70.92216	708.14833	26.93417	-179.73509	1
124	H	72.31948	77.94112	70.62435	-2232.69501	-1179.09831	1023.94816	1
125	C	70.97411	78.43627	72.25586	-738.32412	259.92548	104.42456	1
126	H	71.71290	77.96736	72.93987	2028.89123	1260.02983	1311.33324	1
127	C	71.01633	80.01999	72.25116	-258.65678	-345.52513	661.28459	1
128	H	70.35230	80.40589	71.44707	-1826.06090	-1801.46097	-918.64554	1
129	C	70.58718	80.62139	73.63333	-541.23400	531.92970	-218.41428	1
130	H	70.66563	81.73411	73.63728	1311.73218	-2219.18200	882.19023	1
131	H	69.52713	80.36552	73.87848	-1048.71298	1223.58118	-2196.97971	1
132	H	71.21938	80.24405	74.46937	419.06414	1903.92898	1903.44670	1
133	C	72.49423	80.47408	71.98983	-423.86431	152.66566	-648.55262	1
134	H	72.59938	81.58326	72.04091	105.68386	-2342.50080	1387.51238	1
135	H	73.19617	80.03708	72.73850	-1695.63603	-1484.73621	-1531.02793	1
136	H	72.84449	80.15387	70.97706	-1853.57121	-487.39031	1936.59343	1
137	C	69.39459	77.91125	72.39474	539.71428	-510.58232	267.58633	1
138	O	68.54292	78.51784	73.06272	-15.93758	-278.34085	-624.49402	1
139	N	69.61281	76.50182	72.60900	-676.81886	12.05292	276.17960	1
140	H	70.29299	76.08754	71.96286	-1694.44250	-373.84189	-2100.66098	1
141	C	68.34872	75.80361	72.64800	412.33078	-664.70360	108.35451	1
142	H	67.58330	76.57804	72.40826	1765.77476	1294.44366	1621.76594	1
143	C	68.42141	74.62285	71.60579	-179.66635	-721.95667	-264.73915	1
144	H	68.62147	75.00092	70.57755	-607.34922	2587.87032	-598.10018	1
145	H	69.26420	73.93447	71.84444	-359.69332	-1479.13954	-2259.74260	1
146	C	67.04418	73.88090	71.68805	-240.01076	616.02425	431.85322	1
147	H	66.82695	73.59197	72.74289	-1359.17131	782.54425	2227.99181	1
148	H	66.21447	74.55747	71.38407	-820.36667	85.81767	-2596.78715	1
149	C	67.08434	72.59493	70.77059	-513.07015	236.18570	-551.87280	1
150	H	67.21403	72.86887	69.69838	1816.11944	-1183.11722	-1650.94321	1
151	H	67.95318	71.94594	71.02729	-1800.04429	-1361.53473	1526.34643	1
152	C	65.74900	71.84819	71.00306	726.08972	-253.19732	-179.64713	1
153	H	65.61797	71.44951	72.02900	1224.27271	-456.51798	-2390.90304	1
154	H	64.84574	72.41529	70.70173	1206.40339	-1150.93514	-2154.90344	1
155	N	65.74072	70.58120	70.08584	329.70796	-633.68968	-155.67358	1
156	H	64.87467	69.97207	70.15457	1348.31305	1938.76845	1359.00643	1
157	H	65.79230	70.75072	69.04005	2096.92035	1446.54551	-966.48890	1
158	H	66.51159	69.86616	70.23271	-1197.07217	-2303.53719	827.28733	1
159	C	68.11033	75.14479	74.12037	-378.01186	-556.17301	-413.96481	1
160	O	66.97082	75.03632	74.50800	-409.44433	-307.55053	-453.30833	1
161	N	69.21306	74.61353	74.64509	-429.02477	524.70884	274.08502	1
162	H	70.11424	74.82799	74.21267	1706.34263	-1425.96036	1574.38926	1
163	C	69.17654	74.26116	76.04845	-45.25864	-626.22952	478.93267	1
164	H	68.78511	75.18908	76.52065	1988.63164	570.90773	1772.87287	1
165	C	68.18908	73.04184	76.24758	551.77128	-20.49526	-564.54996	1
166	H	67.43353	73.00494	75.42927	1434.61535	-1753.10253	1513.99471	1
167	H	68.75744	72.08674	76.17633	-714.67738	1819.09770	1898.36494	1
168	C	67.47815	73.15263	77.63802	446.99263	-555.77305	338.97221	1
169	H	68.18651	73.48379	78.43048	1953.68466	1892.25957	-161.67766	1
170	H	66.67515	73.92330	77.61885	-403.03785	2688.07032	-188.43591	1
171	C	66.89929	71.72288	77.98662	567.86262	335.74681	434.04421	1
172	H	65.85447	71.61272	77.61527	-1080.02275	1568.26081	-1948.78900	1

173	H	67.48515	70.92192	77.47984	-919.54108	2111.34692	1456.13463	1
174	C	66.97838	71.53496	79.51958	195.81897	173.33862	-745.11536	1
175	H	68.01019	71.46429	79.91896	1405.67949	-2301.21089	-390.08113	1
176	H	66.39246	72.26663	80.11111	-940.37328	-1118.32446	2299.72133	1
177	N	66.33680	70.14622	79.85580	319.26422	656.36007	-42.02424	1
178	H	66.38033	69.85499	80.87486	1961.03633	619.91968	1787.09422	1
179	H	65.30218	70.02908	79.64978	854.14343	-2156.80752	1429.08711	1
180	H	66.75427	69.29459	79.37916	1237.02905	-1378.50857	-1998.28500	1
181	C	70.69544	73.88565	76.43996	532.53319	-268.57236	517.55729	1
182	O	71.63385	74.15019	75.69514	266.16714	-290.73804	-558.88002	1
183	N	70.71940	73.34127	77.64326	-226.25352	640.49678	-270.32839	1
184	H	69.82136	73.20870	78.10458	2007.69063	-1035.27229	1523.50231	1
185	C	71.82554	72.58375	78.12278	-540.76542	-573.33303	49.50000	1
186	H	71.42912	72.10872	79.04765	-2374.20950	-1036.76023	843.75774	1
187	C	72.18132	71.49618	77.00054	-77.09082	666.87422	-415.84136	1
188	H	72.37167	72.02150	76.02016	-985.81834	617.19825	2463.91927	1
189	O	71.13994	70.54314	76.71709	293.29899	-391.65602	-477.80926	1
190	H	71.05630	70.64824	75.74718	2528.72714	-681.76262	-751.27122	1
191	C	73.53621	70.90614	77.53528	252.47363	-605.14473	440.05134	1
192	H	73.99059	70.21208	76.78970	-2052.65063	1456.49051	-1043.51830	1
193	H	74.28363	71.70723	77.74501	-2152.98800	-1661.97574	-161.70652	1
194	H	73.39016	70.33196	78.47930	-473.12726	-1584.27339	2165.61725	1
195	C	73.04175	73.61624	78.46737	360.36307	488.46713	505.10056	1
196	O	73.21646	73.87666	79.64898	-200.08817	-528.03552	-385.82850	1
197	N	73.67409	74.02936	77.39517	-597.54095	-226.44775	355.20479	1
198	H	73.25996	73.79701	76.46795	2179.23655	-1300.70981	-991.33835	1
199	C	74.72110	74.97880	77.45159	-687.68921	297.39807	-249.45179	1
200	H	74.92092	75.18799	76.38026	-349.16256	-2467.37713	-1101.72831	1
201	C	74.23084	76.26941	78.26893	672.47345	361.54328	-201.62880	1
202	H	73.99605	75.99975	79.32921	1541.41502	582.18425	2169.97026	1
203	H	75.05027	77.02463	78.30209	-2534.67717	60.25153	997.72295	1
204	C	72.99397	76.83218	77.56115	574.26774	-389.43119	-377.02542	1
205	C	73.13362	77.59489	76.37036	688.82679	-287.33580	-257.96133	1
206	H	74.13152	77.83102	75.95712	331.14182	1470.38163	2269.80013	1
207	C	71.70600	76.52590	78.07467	-383.52382	-675.04808	144.24917	1
208	H	71.59401	75.91814	78.99101	4.09847	1517.59662	2262.86397	1
209	C	71.98602	77.99755	75.71609	-134.76730	428.45285	-649.50303	1
210	H	72.10459	78.56699	74.78067	-903.23433	1600.49020	2011.53387	1
211	C	70.59986	76.97314	77.38007	-335.53281	-615.00040	-364.39058	1
212	H	69.60048	76.72851	77.77669	1596.45398	-1369.33862	1732.02659	1
213	C	70.68575	77.71011	76.18131	585.48547	-340.24194	-406.23938	1
214	O	69.55245	78.11087	75.49976	-419.15649	-173.04408	-511.94141	1
215	H	68.96842	78.34819	74.67335	-1071.84350	1559.71507	-1960.13012	1
216	C	76.06464	74.42691	78.20729	291.41878	-183.13091	710.72246	1
217	O	77.05745	74.25045	77.54252	379.87695	523.47396	-222.23622	1
218	N	75.83603	74.19518	79.48564	564.30591	373.09380	277.24371	1
219	H	74.85262	74.30906	79.84920	-120.59931	-2436.07824	-1214.35098	1
220	C	76.85049	74.37901	80.49638	404.07514	-299.37480	608.84009	1
221	H	76.98249	73.36597	80.93497	-1071.07882	-841.69025	2359.66467	1
222	C	78.19979	74.96447	79.93313	-683.12807	68.71770	-390.13096	1
223	H	78.48154	74.47518	78.96232	2068.88918	1596.58590	770.89603	1
224	H	78.10975	76.05479	79.71448	1379.86429	2342.49779	-179.85638	1
225	C	79.28968	74.68225	81.01869	-176.39967	537.49466	550.97268	1
226	H	79.13699	75.31289	81.92253	-396.28051	1942.22168	1869.33314	1
227	H	79.22031	73.63018	81.37267	-94.44700	586.00678	-2659.20016	1
228	C	80.71472	74.95815	80.35431	-291.69381	-718.18079	-150.72929	1
229	H	80.89841	74.43915	79.38020	-2303.38776	1089.76242	964.62032	1
230	H	81.00560	76.03260	80.23430	884.16729	2568.80533	-207.74283	1
231	N	81.56801	74.35199	81.28854	-594.49522	-252.81478	342.29276	1
232	H	81.12883	73.85541	82.04869	-1735.17426	2084.05705	-263.71605	1
233	C	82.83828	74.36687	81.23269	595.23177	-271.52487	442.22352	1
234	N	83.43668	75.05401	80.17205	585.53813	-424.79750	-105.81303	1

235	H	82.99974	75.56992	79.40912	959.88797	1327.56823	-2177.11905	1
236	H	84.44269	75.14276	80.02482	1578.48647	16.27378	-2220.76233	1
237	N	83.38993	73.65376	82.30670	-452.17763	-390.33541	-421.51853	1
238	H	82.94896	73.13910	83.06771	470.26107	1974.25629	-1817.92087	1
239	H	84.39469	73.53370	82.43886	1856.67307	-1573.97321	-1224.35416	1
240	C	76.15800	75.41345	81.54108	-531.47271	-581.45780	-55.06206	1
241	O	75.39024	76.28425	81.20286	-243.00837	192.73507	609.52485	1
242	N	76.63615	75.17666	82.76753	343.49288	-644.25607	38.09164	1
243	H	77.30476	74.41404	82.86406	-1691.16043	-1535.97525	-1484.73099	1
244	C	76.21785	76.00972	83.89572	542.66492	350.14337	454.42563	1
245	H	75.33139	76.54419	83.47408	1209.57979	-2396.95920	463.86744	1
246	C	75.89630	75.09743	85.07048	-737.14309	145.93010	242.71942	1
247	H	76.82032	74.53137	85.32284	-1050.18303	159.36419	-2509.06125	1
248	C	75.47245	75.87859	86.29852	-706.77696	-252.88343	-245.16230	1
249	H	75.30027	75.20497	87.18307	-1624.64039	-1665.49085	1417.86935	1
250	H	76.26228	76.63680	86.59483	2566.10521	598.51109	693.22305	1
251	H	74.51695	76.44513	86.12086	-1972.69758	107.10018	-1876.34312	1
252	C	74.82059	74.08951	84.70692	412.85148	672.58832	-27.69222	1
253	H	74.63155	73.35898	85.54050	1447.02277	1762.76533	-1490.78944	1
254	H	73.84271	74.59634	84.47934	1320.77379	-145.20455	2378.68491	1
255	H	75.10239	73.49656	83.79382	-1512.10848	1470.52031	1724.75147	1
256	C	77.47599	77.04241	84.21835	-607.11113	499.56689	73.73769	1
257	O	77.68233	77.44542	85.34236	357.97126	460.81534	356.68785	1
258	N	78.12199	77.35393	83.10805	536.55407	-368.62270	332.76306	1
259	H	77.77450	76.94539	82.24196	524.38866	2297.69985	1367.20941	1
260	C	79.09140	78.38614	83.14663	46.50277	-774.29190	-147.97904	1
261	H	78.88239	78.93660	84.09222	1676.51875	1883.29066	1032.55549	1
262	C	80.57281	77.73915	83.11402	-559.41456	-34.19198	-556.30433	1
263	H	80.69788	77.15771	82.16995	-64.66664	395.18769	2695.05373	1
264	H	81.34303	78.54633	83.08080	-2703.44278	-60.40056	333.79418	1
265	C	80.78490	76.84658	84.30644	-519.76435	377.31045	459.42366	1
266	H	79.95802	76.10099	84.33588	-1746.74323	1667.50644	-1261.73691	1
267	C	82.11010	76.10565	84.17181	570.95554	16.46261	-545.27700	1
268	H	82.27364	75.38751	85.01601	2391.58273	28.05277	-1305.07271	1
269	H	82.15766	75.51736	83.21998	175.75588	917.63458	2559.43867	1
270	H	82.97907	76.81278	84.16393	-1063.97851	-2155.34650	1283.00462	1
271	C	80.76974	77.63326	85.60950	193.76014	2.62946	-765.53141	1
272	H	81.03620	76.98691	86.48538	507.39394	-846.55087	2539.60089	1
273	H	81.49969	78.48361	85.59009	1337.57841	1818.19054	1526.01994	1
274	H	79.75151	78.06352	85.81592	1100.88635	-1172.91350	-2199.08909	1
275	C	78.94599	79.23150	81.77994	-549.21115	475.64486	-309.38218	1
276	O	78.57106	78.74573	80.74502	556.06106	-390.37755	-78.24250	1
277	O	79.45524	80.55108	81.81754	-572.27940	-310.19032	-209.75862	1
278	H	79.68511	80.60214	82.78629	-1380.08193	2212.14486	790.85944	1

Listing 102: C00102.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.4171	0.0000	300.0000
3	H	72.52675	84.15658	83.29686	-2043.14101	-1757.64893	399.89339		1
4	N	73.39020	83.63226	83.41829	426.75047	490.45733	-334.42467		1
5	H	73.27892	83.25107	84.35506	442.25559	-1110.30854	-2448.52907		1
6	C	74.57877	84.35892	83.19987	415.32972	-666.39213	83.73172		1
7	H	74.34545	84.96363	82.29762	879.32219	2491.00447	667.35213		1
8	C	74.89677	85.28865	84.47481	31.35357	477.41777	628.23362		1
9	H	75.18345	84.64275	85.33915	1168.38489	2240.25337	-1019.71136		1
10	H	75.79519	85.91532	84.25841	-360.43770	2534.90498	931.67112		1
11	C	73.71737	86.15344	84.84022	463.18208	512.70242	-382.34388		1
12	H	72.85060	85.49345	85.06782	1725.29117	1863.52247	-987.07854		1
13	C	74.03324	86.97579	86.08366	710.42801	-144.27427	-313.15367		1
14	H	73.15868	87.60132	86.39933	364.20195	-1033.13725	2494.72524		1

15	H	74.30811	86.32460	86.95319	2567.61904	335.80679	847.48802	1
16	H	74.89239	87.67344	85.90782	-2587.99029	680.92867	-512.16411	1
17	C	73.32767	87.08738	83.70288	268.17616	741.64379	-40.42634	1
18	H	72.47401	87.75409	83.99070	1283.54314	-1945.37420	-1411.27812	1
19	H	74.18010	87.75049	83.40394	-1258.57796	1317.15249	-2026.02085	1
20	H	73.01074	86.52177	82.78918	-2502.84526	909.80597	575.92391	1
21	C	75.82995	83.35278	82.98011	619.36578	-458.64843	-172.09273	1
22	O	76.96864	83.75351	83.16511	-81.40433	433.87611	522.34594	1
23	N	75.44493	82.15534	82.56492	175.23996	-622.20190	341.55523	1
24	H	74.44418	82.02908	82.42392	-876.57256	-303.22879	-2561.90213	1
25	C	76.41604	81.15839	82.26004	-571.88214	-534.10783	-106.15033	1
26	H	77.23476	81.32818	82.99106	-2713.20841	-16.25800	-248.80809	1
27	C	75.67400	79.74915	82.38744	166.60354	288.16399	-716.09568	1
28	H	74.79381	79.74529	81.68796	-2097.85574	1636.78449	-586.18044	1
29	O	75.14938	79.44518	83.69341	-317.80580	-363.38227	484.43082	1
30	H	74.19095	79.39323	83.50806	1863.74748	-1451.84923	1357.29467	1
31	C	76.77074	78.76220	81.84324	503.80731	517.99032	318.51606	1
32	H	76.40730	77.70865	81.84297	640.61020	-2157.10410	-1536.29104	1
33	H	77.06204	79.00972	80.79694	1687.88455	465.60692	2087.56452	1
34	H	77.69580	78.79495	82.46443	-1293.07895	-1899.88581	-1463.57452	1
35	C	76.87486	81.41841	80.71076	-153.07550	-733.68902	248.70981	1
36	O	76.06765	81.27404	79.83245	186.15459	-480.78787	-449.34387	1
37	N	78.18403	81.71294	80.62677	-487.53139	543.18517	42.03850	1
38	C	78.80821	82.03016	79.38392	-699.35871	69.34393	360.10701	1
39	H	77.99989	82.37813	78.69974	2.81126	-221.99807	-2715.58072	1
40	C	79.87789	83.11916	79.82150	-507.46439	-592.59194	122.07761	1
41	H	80.69643	83.24045	79.07647	-1975.08116	525.87560	-1801.71556	1
42	H	79.41367	84.12116	79.96086	1588.27743	-1913.22100	1113.83566	1
43	C	80.36426	82.52467	81.18049	-613.62442	-457.55993	-194.14490	1
44	H	81.07820	81.68653	81.01441	1707.54637	-721.27992	1996.92523	1
45	H	80.88679	83.26249	81.83056	758.23357	2100.81767	1560.55011	1
46	C	78.99977	82.00345	81.79984	-352.41524	704.96076	49.21465	1
47	H	79.08768	81.06786	82.40173	1714.76886	-2070.42778	443.35792	1
48	H	78.39996	82.77980	82.38129	1224.15040	1801.50881	1636.97633	1
49	C	79.63562	80.73657	78.79816	566.85117	537.05831	117.62814	1
50	O	80.64590	80.89343	78.15463	-550.26779	-406.08867	4.21666	1
51	N	79.05307	79.58373	79.15384	566.34832	-425.77725	180.18749	1
52	H	78.14525	79.72525	79.59609	644.44502	2646.80550	-52.73430	1
53	C	79.35014	78.43828	78.34698	612.34801	-281.48662	411.56221	1
54	H	80.42684	78.53434	78.07617	1667.23498	-1490.75142	1556.16753	1
55	C	78.98456	77.14389	79.21234	-714.45746	-175.43074	286.98927	1
56	H	77.88560	77.17556	79.44897	-787.09484	1763.03619	-1922.46060	1
57	O	79.65506	77.02095	80.48088	-429.46514	516.51932	-128.40526	1
58	H	78.90525	77.12262	81.10029	1981.82785	436.16847	-1818.18182	1
59	C	79.26772	75.97965	78.19346	630.79189	-468.94448	76.03230	1
60	H	79.03551	74.98327	78.63079	-1775.71861	2062.30353	131.89849	1
61	H	78.65628	76.07421	77.26542	-1855.14608	88.94118	1993.53760	1
62	H	80.33891	75.95788	77.88663	-1504.82350	-780.94249	-2132.90992	1
63	C	78.35248	78.49794	77.06546	288.57638	618.62814	-397.00270	1
64	O	77.22255	78.97489	77.13551	321.70495	-185.26452	574.37218	1
65	N	78.92892	77.89923	76.04760	-447.05792	-446.53431	367.76425	1
66	H	79.86148	77.50929	76.16622	350.31316	1975.63644	-1843.31522	1
67	C	78.17283	77.68849	74.84983	-511.23061	374.03917	-471.51480	1
68	H	77.66658	78.67129	74.71126	2234.79579	-898.70890	-1273.45190	1
69	C	79.20398	77.25543	73.71226	529.53781	-159.34528	563.72604	1
70	H	78.64567	77.31395	72.73923	654.59388	2347.94251	1217.51488	1
71	H	80.03051	78.00982	73.64093	-1526.55661	2103.42026	817.87394	1
72	O	79.76085	75.93689	73.86447	-554.84278	14.12789	399.58769	1
73	H	78.89847	75.42071	74.02827	1297.06236	2061.84854	1220.68812	1
74	C	77.11169	76.47951	75.06374	-662.15484	-412.13544	123.62687	1
75	O	77.28829	75.39465	74.53575	-540.01537	-317.05804	274.91456	1
76	N	76.14238	76.88200	75.85640	-202.76299	-690.00100	-131.49145	1

77	H	76.20705	77.85173	76.25604	-702.62132	-2617.37191	281.70413	1
78	C	74.86805	76.19346	75.93620	-491.73914	576.34187	222.73509	1
79	H	74.23133	76.93451	76.47467	1977.17978	-1823.58850	-434.68928	1
80	C	74.36450	75.90286	74.53270	-649.50797	-328.66843	306.11224	1
81	H	75.06369	75.16163	74.07766	2075.07803	1452.16490	-1004.45904	1
82	C	72.97164	75.30240	74.55468	-615.18735	-489.99689	-70.96352	1
83	H	72.63356	75.00486	73.52573	-1226.32661	-1724.38906	-1716.47170	1
84	H	72.93891	74.37758	75.21344	2381.64273	-969.84735	900.46860	1
85	H	72.21077	76.02674	74.95693	2122.74991	1702.23946	-141.36228	1
86	C	74.36039	77.13639	73.64723	-501.86074	-479.61276	-376.42482	1
87	H	74.01608	76.89895	72.60307	993.79261	-2246.95401	-1177.81305	1
88	H	73.67637	77.93259	74.05058	42.71279	-626.15391	-2651.37258	1
89	H	75.38566	77.59018	73.56620	-2026.39012	-1590.33709	-887.82922	1
90	C	75.04811	74.77961	76.83187	-672.89153	382.57394	-156.34072	1
91	O	74.23830	73.88502	76.67396	410.04627	221.86223	500.35950	1
92	N	75.99991	74.88379	77.72977	-378.11782	-443.79414	-441.10984	1
93	H	76.44970	75.78864	77.61068	2404.15973	-568.14894	1149.30085	1
94	C	76.33820	73.92897	78.73190	-544.54484	466.16019	331.29119	1
95	H	76.66023	74.55554	79.59206	-1409.80988	-170.17955	2325.32679	1
96	C	75.05207	73.04664	79.00407	-184.48284	116.78282	-758.89137	1
97	H	74.16208	73.71092	79.09317	1893.78641	1861.14652	611.04528	1
98	H	74.85018	72.39481	78.11748	-2170.79665	-974.19311	1327.50117	1
99	C	75.22001	72.17238	80.28616	389.51668	672.81878	-138.49152	1
100	H	76.06515	71.45779	80.16131	510.64577	1933.03327	1851.02484	1
101	H	75.51510	72.80486	81.15185	-2302.30869	-1105.72939	-948.89774	1
102	C	73.90299	71.38648	80.65071	-559.93427	-126.34590	542.30857	1
103	O	73.87447	70.68644	81.63027	-670.36003	-111.83166	76.36448	1
104	N	72.87560	71.60776	79.80166	-216.06729	-537.07037	446.51379	1
105	H	72.83104	72.19207	78.95878	-1251.96487	1074.12894	-2168.52500	1
106	H	71.93489	71.22077	79.93368	-2451.83023	-720.73851	944.84612	1
107	C	77.53095	72.95736	78.19403	546.24052	-563.88337	-85.11809	1
108	O	77.43632	72.35833	77.14496	71.70702	-307.40463	606.69673	1
109	N	78.51103	72.87854	79.10084	479.90863	-504.50129	222.86849	1
110	C	79.76628	72.27835	78.74726	75.51268	-600.91904	506.73700	1
111	H	79.98629	72.62824	77.71221	-2033.61562	1795.30103	254.89480	1
112	C	80.72262	72.81274	79.89621	523.79067	517.99274	284.45581	1
113	H	81.63796	72.19166	80.02105	1599.61665	-1127.00911	1895.98173	1
114	H	81.05873	73.85761	79.71028	-1881.83093	1275.82488	-1501.55016	1
115	C	79.74984	72.72815	81.11142	-600.05639	-404.05026	316.64485	1
116	H	79.59343	71.66258	81.40578	-2597.05260	496.36221	657.73249	1
117	H	80.10668	73.27263	82.01460	-1666.24518	1294.38985	-1723.90591	1
118	C	78.43448	73.35486	80.47391	493.57570	-129.95376	-602.56394	1
119	H	77.47687	73.00506	80.92118	-1469.08415	-637.84797	2204.22581	1
120	H	78.43741	74.47004	80.43522	-1038.97840	1068.88701	-2280.71789	1
121	C	79.61274	70.64629	78.83651	188.88100	241.05089	-727.87821	1
122	O	79.99239	70.05716	79.81383	531.88613	-49.19943	427.07960	1
123	N	79.14296	70.19173	77.67692	708.14833	26.93417	-179.73509	1
124	H	78.76428	70.91685	77.04056	-2232.69501	-1179.09831	1023.94816	1
125	C	78.81189	68.79124	77.41269	-738.32412	259.92548	104.42456	1
126	H	79.05515	68.67475	76.33053	2028.89123	1260.02983	1311.33324	1
127	C	79.54333	67.82257	78.31428	-258.65678	-345.52513	661.28459	1
128	H	79.33686	68.11661	79.37569	-1826.06090	-1801.46097	-918.64554	1
129	C	79.04668	66.40063	78.11420	-541.23400	531.92970	-218.41428	1
130	H	79.55957	65.67949	78.80754	1311.73218	-2219.18200	882.19023	1
131	H	77.94174	66.31894	78.30745	-1048.71298	1223.58118	-2196.97971	1
132	H	79.22826	66.03999	77.06511	419.06414	1903.92898	1903.44670	1
133	C	81.04709	67.86667	78.10855	-423.86431	152.66566	-648.55262	1
134	H	81.58248	67.16203	78.80256	105.68386	-2342.50080	1387.51238	1
135	H	81.33351	67.58384	77.05855	-1695.63603	-1484.73621	-1531.02793	1
136	H	81.44923	68.89933	78.30398	-1853.57121	-487.39031	1936.59343	1
137	C	77.17455	68.64921	77.69931	539.71428	-510.58232	267.58633	1
138	O	76.72691	68.67565	78.82094	-15.93758	-278.34085	-624.49402	1

139	N	76.53312	68.54954	76.54139	-676.81886	12.05292	276.17960	1
140	H	77.14767	68.54661	75.72834	-1694.44250	-373.84189	-2100.66098	1
141	C	75.30475	67.79105	76.47317	412.33078	-664.70360	108.35451	1
142	H	75.60161	66.72024	76.43421	1765.77476	1294.44366	1621.76594	1
143	C	74.44990	68.15507	77.74370	-179.66635	-721.95667	-264.73915	1
144	H	74.76608	67.55205	78.62760	-607.34922	2587.87032	-598.10018	1
145	H	74.65107	69.21522	78.02981	-359.69332	-1479.13954	-2259.74260	1
146	C	72.92871	67.92716	77.44055	-240.01076	616.02425	431.85322	1
147	H	72.64692	68.36335	76.45476	-1359.17131	782.54425	2227.99181	1
148	H	72.68103	66.84395	77.37936	-820.36667	85.81767	-2596.78715	1
149	C	72.15765	68.64346	78.61901	-513.07015	236.18570	-551.87280	1
150	H	72.46510	68.22719	79.60629	1816.11944	-1183.11722	-1650.94321	1
151	H	72.42976	69.72261	78.65371	-1800.04429	-1361.53473	1526.34643	1
152	C	70.63630	68.47109	78.39969	726.08972	-253.19732	-179.64713	1
153	H	70.24080	68.94520	77.47891	1224.27271	-456.51798	-2390.90304	1
154	H	70.27743	67.42494	78.47041	1206.40339	-1150.93514	-2154.90344	1
155	N	69.92299	69.21747	79.57631	329.70796	-633.68968	-155.67358	1
156	H	68.86943	69.10429	79.62685	1348.31305	1938.76845	1359.00643	1
157	H	70.21192	68.93223	80.55631	2096.92035	1446.54551	-966.48890	1
158	H	70.02192	70.27320	79.61949	-1197.07217	-2303.53719	827.28733	1
159	C	74.54500	68.25944	75.11222	-378.01186	-556.17301	-413.96481	1
160	O	73.83724	67.49645	74.49514	-409.44433	-307.55053	-453.30833	1
161	N	74.67786	69.57924	74.94298	-429.02477	524.70884	274.08502	1
162	H	75.35363	70.05844	75.54098	1706.34263	-1425.96036	1574.38926	1
163	C	74.31644	70.13429	73.67716	-45.25864	-626.22952	478.93267	1
164	H	73.85490	69.30215	73.09194	1988.63164	570.90773	1772.87287	1
165	C	73.29160	71.28463	74.06974	551.77128	-20.49526	-564.54996	1
166	H	72.46370	70.84787	74.67183	1434.61535	-1753.10253	1513.99471	1
167	H	73.77691	72.03212	74.73799	-714.67738	1819.09770	1898.36494	1
168	C	72.72413	71.96889	72.78724	446.99263	-555.77305	338.97221	1
169	H	73.47826	72.65693	72.34252	1953.68466	1892.25957	-161.67766	1
170	H	72.48550	71.22142	71.99738	-403.03785	2688.07032	-188.43591	1
171	C	71.41505	72.74536	73.22772	567.86262	335.74681	434.04421	1
172	H	70.58893	72.03501	73.46123	-1080.02275	1568.26081	-1948.78900	1
173	H	71.58121	73.32353	74.16346	-919.54108	2111.34692	1456.13463	1
174	C	71.03402	73.67825	72.05684	195.81897	173.33862	-745.11536	1
175	H	71.78552	74.45561	71.81468	1405.67949	-2301.21089	-390.08113	1
176	H	70.74688	73.13756	71.13508	-940.37328	-1118.32446	2299.72133	1
177	N	69.75034	74.48279	72.45449	319.26422	656.36007	-42.02424	1
178	H	69.33518	75.08538	71.68235	1961.03633	619.91968	1787.09422	1
179	H	68.88829	73.93173	72.73718	854.14343	-2156.80752	1429.08711	1
180	H	69.82030	75.19907	73.23642	1237.02905	-1378.50857	-1998.28500	1
181	C	75.69579	70.72433	73.05945	532.53319	-268.57236	517.55729	1
182	O	76.68567	70.93116	73.76904	266.16714	-290.73804	-558.88002	1
183	N	75.57471	70.90679	71.76128	-226.25352	640.49678	-270.32839	1
184	H	74.66456	70.69283	71.35704	2007.69063	-1035.27229	1523.50231	1
185	C	76.49237	71.81759	71.13779	-540.76542	-573.33303	49.50000	1
186	H	76.66481	72.61297	71.89904	-2374.20950	-1036.76023	843.75774	1
187	C	77.83329	71.02773	70.80783	-77.09082	666.87422	-415.84136	1
188	H	77.63649	70.20277	70.06128	-985.81834	617.19825	2463.91927	1
189	O	78.46437	70.30628	71.87835	293.29899	-391.65602	-477.80926	1
190	H	77.86111	70.57830	72.66078	2528.72714	-681.76262	-751.27122	1
191	C	78.69837	72.13263	70.10547	252.47363	-605.14473	440.05134	1
192	H	79.66638	71.71803	69.73800	-2052.65063	1456.49051	-1043.51830	1
193	H	78.17113	72.57800	69.22605	-2152.98800	-1661.97574	-161.70652	1
194	H	78.93900	72.96832	70.80441	-473.12726	-1584.27339	2165.61725	1
195	C	75.84774	72.34956	69.73445	360.36307	488.46713	505.10056	1
196	O	76.07681	73.48057	69.36925	-200.08817	-528.03552	-385.82850	1
197	N	75.21088	71.38199	69.08132	-597.54095	-226.44775	355.20479	1
198	H	75.11044	70.46702	69.51782	2179.23655	-1300.70981	-991.33835	1
199	C	74.76467	71.66293	67.76509	-687.68921	297.39807	-249.45179	1
200	H	75.38404	72.52373	67.42380	-349.16256	-2467.37713	-1101.72831	1

201	C	74.89076	70.32033	66.90634	672.47345	361.54328	-201.62880	1
202	H	74.25791	69.52153	67.35649	1541.41502	582.18425	2169.97026	1
203	H	74.50896	70.49684	65.87454	-2534.67717	60.25153	997.72295	1
204	C	76.36339	69.88716	66.87465	574.26774	-389.43119	-377.02542	1
205	C	77.25587	70.48848	65.93733	688.82679	-287.33580	-257.96133	1
206	H	76.89852	71.26255	65.23421	331.14182	1470.38163	2269.80013	1
207	C	76.83700	68.90016	67.79116	-383.52382	-675.04808	144.24917	1
208	H	76.15215	68.44077	68.52661	4.09847	1517.59662	2262.86397	1
209	C	78.58778	70.07526	65.92422	-134.76730	428.45285	-649.50303	1
210	H	79.27620	70.53408	65.19325	-903.23433	1600.49020	2011.53387	1
211	C	78.18062	68.52125	67.74012	-335.53281	-615.00040	-364.39058	1
212	H	78.53377	67.75298	68.45011	1596.45398	-1369.33862	1732.02659	1
213	C	79.10222	69.08405	66.80948	585.48547	-340.24194	-406.23938	1
214	O	80.46784	68.70275	66.74473	-419.15649	-173.04408	-511.94141	1
215	H	80.48290	68.01599	67.45234	-1071.84350	1559.71507	-1960.13012	1
216	C	73.16442	72.02022	67.86655	291.41878	-183.13091	710.72246	1
217	O	72.34081	71.19134	68.16358	379.87695	523.47396	-222.23622	1
218	N	73.01845	73.29728	67.56964	564.30591	373.09380	277.24371	1
219	H	73.79802	73.93682	67.32436	-120.59931	-2436.07824	-1214.35098	1
220	C	71.70347	73.88436	67.47323	404.07514	-299.37480	608.84009	1
221	H	71.19063	73.30361	66.67351	-1071.07882	-841.69025	2359.66467	1
222	C	70.97303	73.69461	68.86629	-683.12807	68.71770	-390.13096	1
223	H	71.16990	72.65494	69.22642	2068.88918	1596.58590	770.89603	1
224	H	71.41945	74.37055	69.63003	1379.86429	2342.49779	-179.85638	1
225	C	69.43740	73.93132	68.75121	-176.39967	537.49466	550.97268	1
226	H	69.16910	74.97618	69.02736	-396.28051	1942.22168	1869.33314	1
227	H	69.08706	73.79416	67.70424	-94.44700	586.00678	-2659.20016	1
228	C	68.72130	72.87357	69.72004	-291.69381	-718.18079	-150.72929	1
229	H	68.61411	71.85674	69.26254	-2303.38776	1089.76242	964.62032	1
230	H	69.14067	72.77506	70.75228	884.16729	2568.80533	-207.74283	1
231	N	67.45550	73.46084	69.82978	-594.49522	-252.81478	342.29276	1
232	H	67.11704	73.94644	69.01248	-1735.17426	2084.05705	-263.71605	1
233	C	66.70910	73.42610	70.86088	595.23177	-271.52487	442.22352	1
234	N	67.15229	72.73403	71.99048	585.53813	-424.79750	-105.81303	1
235	H	67.99929	72.18351	72.12673	959.88797	1327.56823	-2177.11905	1
236	H	66.61871	72.63431	72.85465	1578.48647	16.27378	-2220.76233	1
237	N	65.51489	74.12306	70.62512	-452.17763	-390.33541	-421.51853	1
238	H	65.22809	74.68859	69.82816	470.26107	1974.25629	-1817.92087	1
239	H	64.80831	74.27725	71.34464	1856.67307	-1573.97321	-1224.35416	1
240	C	72.12619	75.38018	67.05554	-531.47271	-581.45780	-55.06206	1
241	O	73.27837	75.60218	66.71049	-243.00837	192.73507	609.52485	1
242	N	71.09523	76.23340	67.03810	343.49288	-644.25607	38.09164	1
243	H	70.22625	75.84776	67.40961	-1691.16043	-1535.97525	-1484.73099	1
244	C	71.37457	77.67311	67.10541	542.66492	350.14337	454.42563	1
245	H	72.39235	77.74723	66.65035	1209.57979	-2396.95920	463.86744	1
246	C	70.27920	78.37870	66.32906	-737.14309	145.93010	242.71942	1
247	H	69.29672	78.02989	66.71724	-1050.18303	159.36419	-2509.06125	1
248	C	70.34688	79.88440	66.50325	-706.77696	-252.88343	-245.16230	1
249	H	69.52058	80.40490	65.94457	-1624.64039	-1665.49085	1417.86935	1
250	H	70.25783	80.17909	67.58608	2566.10521	598.51109	693.22305	1
251	H	71.32057	80.30124	66.12392	-1972.69758	107.10018	-1876.34312	1
252	C	70.33130	78.01923	64.85456	412.85148	672.58832	-27.69222	1
253	H	69.47213	78.46655	64.28296	1447.02277	1762.76533	-1490.78944	1
254	H	71.27979	78.38572	64.37355	1320.77379	-145.20455	2378.68491	1
255	H	70.29442	76.90489	64.70368	-1512.10848	1470.52031	1724.75147	1
256	C	71.39766	78.08561	68.71524	-607.11113	499.56689	73.73769	1
257	O	72.44316	78.39279	69.23415	357.97126	460.81534	356.68785	1
258	N	70.19235	78.05903	69.25851	536.55407	-368.62270	332.76306	1
259	H	69.39253	77.75385	68.70657	524.38866	2297.69985	1367.20941	1
260	C	70.11098	78.15613	70.67834	46.50277	-774.29190	-147.97904	1
261	H	71.12300	77.84506	71.02602	1676.51875	1883.29066	1032.55549	1
262	C	69.77525	79.68253	71.10176	-559.41456	-34.19198	-556.30433	1

263	H	69.05146	80.12061	70.37452	-64.66664	395.18769	2695.05373	1
264	H	69.27127	79.71534	72.09662	-2703.44278	-60.40056	333.79418	1
265	C	71.05000	80.47603	71.13678	-519.76435	377.31045	459.42366	1
266	H	71.60585	80.29385	70.18701	-1746.74323	1667.50644	-1261.73691	1
267	C	70.74266	81.96509	71.24747	570.95554	16.46261	-545.27700	1
268	H	71.67844	82.58106	71.25757	2391.58273	28.05277	-1305.07271	1
269	H	70.11689	82.32476	70.39066	175.75588	917.63458	2559.43867	1
270	H	70.18192	82.20015	72.18859	-1063.97851	-2155.34650	1283.00462	1
271	C	71.93303	80.05763	72.30590	193.76014	2.62946	-765.53141	1
272	H	72.86359	80.67888	72.36134	507.39394	-846.55087	2539.60089	1
273	H	71.40173	80.16842	73.28597	1337.57841	1818.19054	1526.01994	1
274	H	72.25750	78.98903	72.22210	1100.88635	-1172.91350	-2199.08909	1
275	C	68.90090	77.20870	71.13351	-549.21115	475.64486	-309.38218	1
276	O	68.22824	76.58078	70.35557	556.06106	-390.37755	-78.24250	1
277	O	68.67460	77.09986	72.53010	-572.27940	-310.19032	-209.75862	1
278	H	69.36233	77.74917	72.84405	-1380.08193	2212.14486	790.85944	1

Listing 103: C00103.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.4116	0.0000	300.0000
3	H	64.93624	68.23730	61.77167	-2043.14101	-1757.64893	399.89339		1
4	N	64.51992	69.12593	61.49110	426.75047	490.45733	-334.42467		1
5	H	63.96207	69.40573	62.31453	442.25559	-1110.30854	-2448.52907		1
6	C	65.47518	70.10983	61.14455	415.32972	-666.39213	83.73172		1
7	H	66.46259	69.62414	61.30203	879.32219	2491.00447	667.35213		1
8	C	65.27296	70.57809	59.61557	31.35357	477.41777	628.23362		1
9	H	64.27486	71.06618	59.50775	1168.38489	2240.25337	-1019.71136		1
10	H	66.02546	71.35609	59.34283	-360.43770	2534.90498	931.67112		1
11	C	65.38033	69.39425	58.69191	463.18208	512.70242	-382.34388		1
12	H	64.60761	68.65010	58.99024	1725.29117	1863.52247	-987.07854		1
13	C	65.11997	69.82451	57.25307	710.42801	-144.27427	-313.15367		1
14	H	65.15823	68.95509	56.54738	364.20195	-1033.13725	2494.72524		1
15	H	64.11318	70.30250	57.13834	2567.61904	335.80679	847.48802		1
16	H	65.88121	70.56811	56.90218	-2587.99029	680.92867	-512.16411		1
17	C	66.74938	68.73274	58.77704	268.17616	741.64379	-40.42634		1
18	H	66.84505	67.88698	58.04826	1283.54314	-1945.37420	-1411.27812		1
19	H	67.57329	69.45828	58.55314	-1258.57796	1317.15249	-2026.02085		1
20	H	66.94512	68.31196	59.79661	-2502.84526	909.80597	575.92391		1
21	C	65.14383	71.28036	62.21463	619.36578	-458.64843	-172.09273		1
22	O	64.39332	71.03628	63.15982	-81.40433	433.87611	522.34594		1
23	N	65.79385	72.37856	61.90021	175.23996	-622.20190	341.55523		1
24	H	66.38443	72.31225	61.07147	-876.57256	-303.22879	-2561.90213		1
25	C	65.69716	73.63717	62.55135	-571.88214	-534.10783	-106.15033		1
26	H	65.96825	74.33840	61.73136	-2713.20841	-16.25800	-248.80809		1
27	C	64.21095	73.89822	63.07362	166.60354	288.16399	-716.09568		1
28	H	63.88618	73.05434	63.74943	-2097.85574	1636.78449	-586.18044		1
29	O	63.19821	73.94395	62.04596	-317.80580	-363.38227	484.43082		1
30	H	62.70303	73.12437	62.24503	1863.74748	-1451.84923	1357.29467		1
31	C	64.39405	75.21569	63.91072	503.80731	517.99032	318.51606		1
32	H	63.45171	75.49973	64.43447	640.61020	-2157.10410	-1536.29104		1
33	H	65.18872	75.10649	64.68853	1687.88455	465.60692	2087.56452		1
34	H	64.68097	76.07391	63.25991	-1293.07895	-1899.88581	-1463.57452		1
35	C	66.98963	73.73327	63.55970	-153.07550	-733.68902	248.70981		1
36	O	67.96274	74.22918	63.05066	186.15459	-480.78787	-449.34387		1
37	N	66.84579	73.26841	64.80868	-487.53139	543.18517	42.03850		1
38	C	67.92597	73.36254	65.74394	-699.35871	69.34393	360.10701		1
39	H	68.45030	74.31687	65.51046	2.81126	-221.99807	-2715.58072		1
40	C	67.16143	73.28081	67.12927	-507.46439	-592.59194	122.07761		1
41	H	67.82460	72.97783	67.97047	-1975.08116	525.87560	-1801.71556		1
42	H	66.70791	74.25750	67.41069	1588.27743	-1913.22100	1113.83566		1

43	C	66.06862	72.21800	66.79285	-613.62442	-457.55993	-194.14490	1
44	H	66.51245	71.19462	66.73381	1707.54637	-721.27992	1996.92523	1
45	H	65.23963	72.17208	67.53456	758.23357	2100.81767	1560.55011	1
46	C	65.60943	72.73755	65.36413	-352.41524	704.96076	49.21465	1
47	H	65.22120	71.95300	64.64390	1714.76886	-2070.42778	443.35792	1
48	H	64.89593	73.59612	65.40281	1224.15040	1801.50881	1636.97633	1
49	C	68.91262	72.05005	65.61391	566.85117	537.05831	117.62814	1
50	O	68.62149	71.00402	66.14402	-550.26779	-406.08867	4.21666	1
51	N	69.99726	72.36397	64.92083	566.34832	-425.77725	180.18749	1
52	H	70.07284	73.29170	64.50361	644.44502	2646.80550	-52.73430	1
53	C	71.07188	71.43943	64.89947	612.34801	-281.48662	411.56221	1
54	H	70.77365	70.60604	65.57869	1667.23498	-1490.75142	1556.16753	1
55	C	71.25910	70.99964	63.36605	-714.45746	-175.43074	286.98927	1
56	H	71.40468	71.93379	62.75710	-787.09484	1763.03619	-1922.46060	1
57	O	70.14973	70.30826	62.76920	-429.46514	516.51932	-128.40526	1
58	H	69.82066	70.98422	62.14282	1981.82785	436.16847	-1818.18182	1
59	C	72.60864	70.19619	63.42680	630.79189	-468.94448	76.03230	1
60	H	72.92721	69.85764	62.41369	-1775.71861	2062.30353	131.89849	1
61	H	73.43696	70.81418	63.84520	-1855.14608	88.94118	1993.53760	1
62	H	72.51454	69.28672	64.06455	-1504.82350	-780.94249	-2132.90992	1
63	C	72.41378	72.27222	65.33948	288.57638	618.62814	-397.00270	1
64	O	72.88962	73.11472	64.57465	321.70495	-185.26452	574.37218	1
65	N	72.84786	71.86785	66.49889	-447.05792	-446.53431	367.76425	1
66	H	72.27943	71.15998	66.96152	350.31316	1975.63644	-1843.31522	1
67	C	74.10190	72.27245	67.05409	-511.23061	374.03917	-471.51480	1
68	H	74.36907	71.31559	67.55705	2234.79579	-898.70890	-1273.45190	1
69	C	75.10712	72.64992	65.86905	529.53781	-159.34528	563.72604	1
70	H	76.15100	72.42656	66.22522	654.59388	2347.94251	1217.51488	1
71	H	74.88457	71.93977	65.02757	-1526.55661	2103.42026	817.87394	1
72	O	75.10183	74.00596	65.39354	-554.84278	14.12789	399.58769	1
73	H	74.23818	73.95690	64.82419	1297.06236	2061.84854	1220.68812	1
74	C	73.86490	73.39916	68.18304	-662.15484	-412.13544	123.62687	1
75	O	72.91749	73.34184	68.95880	-540.01537	-317.05804	274.91456	1
76	N	74.90157	74.22253	68.23026	-202.76299	-690.00100	-131.49145	1
77	H	75.56818	74.09025	67.46448	-702.62132	-2617.37191	281.70413	1
78	C	74.89532	75.50023	68.93524	-491.73914	576.34187	222.73509	1
79	H	75.77609	76.03615	68.50758	1977.17978	-1823.58850	-434.68928	1
80	C	73.57661	76.21116	68.66654	-649.50797	-328.66843	306.11224	1
81	H	72.74690	75.48649	68.85027	2075.07803	1452.16490	-1004.45904	1
82	C	73.38105	77.39327	69.59215	-615.18735	-489.99689	-70.96352	1
83	H	72.42197	77.93893	69.37298	-1226.32661	-1724.38906	-1716.47170	1
84	H	73.34549	77.07022	70.69350	2381.64273	-969.84735	900.46860	1
85	H	74.21797	78.13863	69.49258	2122.74991	1702.23946	-141.36228	1
86	C	73.48740	76.64770	67.21552	-501.86074	-479.61276	-376.42482	1
87	H	72.48895	77.10618	66.97521	993.79261	-2246.95401	-1177.81305	1
88	H	74.27464	77.41070	66.96348	42.71279	-626.15391	-2651.37258	1
89	H	73.63652	75.77617	66.51762	-2026.39012	-1590.33709	-887.82922	1
90	C	75.11012	75.20311	70.55770	-672.89153	382.57394	-156.34072	1
91	O	76.11235	75.61184	71.08325	410.04627	221.86223	500.35950	1
92	N	74.10354	74.52904	71.08157	-378.11782	-443.79414	-441.10984	1
93	H	73.33958	74.16072	70.47088	2404.15973	-568.14894	1149.30085	1
94	C	74.11647	74.30874	72.49446	-544.54484	466.16019	331.29119	1
95	H	73.27406	73.59462	72.63786	-1409.80988	-170.17955	2325.32679	1
96	C	75.55158	73.66553	72.75761	-184.48284	116.78282	-758.89137	1
97	H	76.04768	73.43731	71.78613	1893.78641	1861.14652	611.04528	1
98	H	76.21803	74.40748	73.25610	-2170.79665	-974.19311	1327.50117	1
99	C	75.41030	72.36179	73.60211	389.51668	672.81878	-138.49152	1
100	H	74.70861	72.50475	74.45487	510.64577	1933.03327	1851.02484	1
101	H	74.92808	71.56539	72.99278	-2302.30869	-1105.72939	-948.89774	1
102	C	76.80769	71.86438	74.14592	-559.93427	-126.34590	542.30857	1
103	O	76.85897	71.04948	75.03084	-670.36003	-111.83166	76.36448	1
104	N	77.86118	72.41369	73.50437	-216.06729	-537.07037	446.51379	1

105	H	77.87069	73.07962	72.72313	-1251.96487	1074.12894	-2168.52500	1
106	H	78.83901	72.15635	73.67185	-2451.83023	-720.73851	944.84612	1
107	C	73.85718	75.73159	73.22374	546.24052	-563.88337	-85.11809	1
108	O	73.33442	76.62978	72.59654	71.70702	-307.40463	606.69673	1
109	N	74.20235	75.74710	74.52054	479.90863	-504.50129	222.86849	1
110	C	74.04118	76.93797	75.29886	75.51268	-600.91904	506.73700	1
111	H	73.19265	77.50317	74.84581	-2033.61562	1795.30103	254.89480	1
112	C	73.80594	76.34957	76.75604	523.79067	517.99274	284.45581	1
113	H	73.99127	77.09989	77.55993	1599.61665	-1127.00911	1895.98173	1
114	H	72.76033	75.98490	76.88687	-1881.83093	1275.82488	-1501.55016	1
115	C	74.82786	75.17165	76.76810	-600.05639	-404.05026	316.64485	1
116	H	75.86045	75.54514	76.95004	-2597.05260	496.36221	657.73249	1
117	H	74.62479	74.41144	77.55557	-1666.24518	1294.38985	-1723.90591	1
118	C	74.67238	74.60488	75.29084	493.57570	-129.95376	-602.56394	1
119	H	75.63202	74.25961	74.83910	-1469.08415	-637.84797	2204.22581	1
120	H	73.89631	73.81092	75.16686	-1038.97840	1068.88701	-2280.71789	1
121	C	75.44934	77.77526	75.31071	188.88100	241.05089	-727.87821	1
122	O	75.81409	78.38508	76.31273	531.88613	-49.19943	427.07960	1
123	N	76.03124	77.69382	74.13891	708.14833	26.93417	-179.73509	1
124	H	75.50555	77.11757	73.47862	-2232.69501	-1179.09831	1023.94816	1
125	C	77.20062	78.44874	73.73445	-738.32412	259.92548	104.42456	1
126	H	77.28810	78.24268	72.63963	2028.89123	1260.02983	1311.33324	1
127	C	76.96449	79.91980	74.07074	-258.65678	-345.52513	661.28459	1
128	H	76.65135	79.97653	75.14142	-1826.06090	-1801.46097	-918.64554	1
129	C	78.22881	80.73993	73.90791	-541.23400	531.92970	-218.41428	1
130	H	78.06241	81.82028	74.17527	1311.73218	-2219.18200	882.19023	1
131	H	79.05709	80.35609	74.56700	-1048.71298	1223.58118	-2196.97971	1
132	H	78.60753	80.71185	72.84880	419.06414	1903.92898	1903.44670	1
133	C	75.83894	80.50713	73.24143	-423.86431	152.66566	-648.55262	1
134	H	75.62040	81.57276	73.52960	105.68386	-2342.50080	1387.51238	1
135	H	76.08673	80.50215	72.14408	-1695.63603	-1484.73621	-1531.02793	1
136	H	74.88661	79.92097	73.37019	-1853.57121	-487.39031	1936.59343	1
137	C	78.52357	77.88172	74.57442	539.71428	-510.58232	267.58633	1
138	O	79.42504	77.38331	73.95325	-15.93758	-278.34085	-624.49402	1
139	N	78.44273	78.09677	75.87903	-676.81886	12.05292	276.17960	1
140	H	77.57190	78.48392	76.31082	-1694.44250	-373.84189	-2100.66098	1
141	C	79.70740	78.02344	76.55688	412.33078	-664.70360	108.35451	1
142	H	80.43826	78.35918	75.78435	1765.77476	1294.44366	1621.76594	1
143	C	79.67070	78.91400	77.86270	-179.66635	-721.95667	-264.73915	1
144	H	79.34827	79.95557	77.63922	-607.34922	2587.87032	-598.10018	1
145	H	78.91708	78.51608	78.57828	-359.69332	-1479.13954	-2259.74260	1
146	C	81.10484	78.88694	78.49226	-240.01076	616.02425	431.85322	1
147	H	81.51917	77.84736	78.46444	-1359.17131	782.54425	2227.99181	1
148	H	81.81616	79.51120	77.90590	-820.36667	85.81767	-2596.78715	1
149	C	80.99962	79.38624	79.98744	-513.07015	236.18570	-551.87280	1
150	H	80.77529	80.47699	80.03150	1816.11944	-1183.11722	-1650.94321	1
151	H	80.14720	78.88305	80.50129	-1800.04429	-1361.53473	1526.34643	1
152	C	82.31977	79.05866	80.72499	726.08972	-253.19732	-179.64713	1
153	H	82.51841	77.97496	80.84788	1224.27271	-456.51798	-2390.90304	1
154	H	83.22183	79.56632	80.32800	1206.40339	-1150.93514	-2154.90344	1
155	N	82.15513	79.59990	82.18405	329.70796	-633.68968	-155.67358	1
156	H	82.87917	79.30101	82.90134	1348.31305	1938.76845	1359.00643	1
157	H	82.16521	80.65353	82.30138	2096.92035	1446.54551	-966.48890	1
158	H	81.24570	79.34767	82.66675	-1197.07217	-2303.53719	827.28733	1
159	C	80.00058	76.47221	76.99458	-378.01186	-556.17301	-413.96481	1
160	O	81.13496	76.15338	77.29966	-409.44433	-307.55053	-453.30833	1
161	N	78.89448	75.74635	77.06040	-429.02477	524.70884	274.08502	1
162	H	78.05706	76.22078	76.72417	1706.34263	-1425.96036	1574.38926	1
163	C	78.98766	74.33463	77.21412	-45.25864	-626.22952	478.93267	1
164	H	78.01297	73.96873	76.81985	1988.63164	570.90773	1772.87287	1
165	C	80.25044	73.83621	76.40261	551.77128	-20.49526	-564.54996	1
166	H	80.27673	74.30261	75.39034	1434.61535	-1753.10253	1513.99471	1

167	H	81.19864	74.15778	76.91454	-714.67738	1819.09770	1898.36494	1
168	C	80.19514	72.27404	76.31112	446.99263	-555.77305	338.97221	1
169	H	80.13140	71.82832	77.33121	1953.68466	1892.25957	-161.67766	1
170	H	79.28693	71.92899	75.76691	-403.03785	2688.07032	-188.43591	1
171	C	81.51998	71.80748	75.58476	567.86262	335.74681	434.04421	1
172	H	81.54366	72.16069	74.52809	-1080.02275	1568.26081	-1948.78900	1
173	H	82.41663	72.25463	76.07321	-919.54108	2111.34692	1456.13463	1
174	C	81.57711	70.26415	75.66136	195.81897	173.33862	-745.11536	1
175	H	81.64832	69.85761	76.69015	1405.67949	-2301.21089	-390.08113	1
176	H	80.77308	69.74358	75.10396	-940.37328	-1118.32446	2299.72133	1
177	N	82.90675	69.80914	74.97020	319.26422	656.36007	-42.02424	1
178	H	83.08289	68.76319	74.96048	1961.03633	619.91968	1787.09422	1
179	H	83.02641	70.04991	73.94344	854.14343	-2156.80752	1429.08711	1
180	H	83.81450	70.16857	75.38716	1237.02905	-1378.50857	-1998.28500	1
181	C	79.21497	73.97046	78.79938	532.53319	-268.57236	517.55729	1
182	O	80.11646	73.19230	79.14286	266.16714	-290.73804	-558.88002	1
183	N	78.33044	74.57670	79.53927	-226.25352	640.49678	-270.32839	1
184	H	77.69027	75.10819	78.95102	2007.69063	-1035.27229	1523.50231	1
185	C	78.09806	74.35402	80.93724	-540.76542	-573.33303	49.50000	1
186	H	77.28182	73.59374	80.95329	-2374.20950	-1036.76023	843.75774	1
187	C	79.41336	73.77074	81.63407	-77.09082	666.87422	-415.84136	1
188	H	80.29746	74.27139	81.14298	-985.81834	617.19825	2463.91927	1
189	O	79.62018	72.37038	81.44699	293.29899	-391.65602	-477.80926	1
190	H	80.12963	72.40071	80.54433	2528.72714	-681.76262	-751.27122	1
191	C	79.30170	74.23965	83.12866	252.47363	-605.14473	440.05134	1
192	H	80.13461	73.83751	83.75188	-2052.65063	1456.49051	-1043.51830	1
193	H	79.32345	75.35313	83.21747	-2152.98800	-1661.97574	-161.70652	1
194	H	78.33700	73.90084	83.59148	-473.12726	-1584.27339	2165.61725	1
195	C	77.55763	75.71457	81.60869	360.36307	488.46713	505.10056	1
196	O	77.10332	75.62923	82.76160	-200.08817	-528.03552	-385.82850	1
197	N	77.70618	76.78261	80.86089	-597.54095	-226.44775	355.20479	1
198	H	78.15261	76.60109	79.96235	2179.23655	-1300.70981	-991.33835	1
199	C	77.22209	78.07709	81.15452	-687.68921	297.39807	-249.45179	1
200	H	77.22666	78.60028	80.17341	-349.16256	-2467.37713	-1101.72831	1
201	C	75.78597	78.01231	81.86099	672.47345	361.54328	-201.62880	1
202	H	75.83386	77.35450	82.76431	1541.41502	582.18425	2169.97026	1
203	H	75.52020	79.03367	82.21851	-2534.67717	60.25153	997.72295	1
204	C	74.68851	77.49214	80.92339	574.26774	-389.43119	-377.02542	1
205	C	74.08609	78.36415	79.96663	688.82679	-287.33580	-257.96133	1
206	H	74.46097	79.39392	79.82437	331.14182	1470.38163	2269.80013	1
207	C	74.21974	76.15261	81.08596	-383.52382	-675.04808	144.24917	1
208	H	74.70240	75.47600	81.81498	4.09847	1517.59662	2262.86397	1
209	C	72.99158	77.89358	79.24015	-134.76730	428.45285	-649.50303	1
210	H	72.50879	78.57360	78.51613	-903.23433	1600.49020	2011.53387	1
211	C	73.12167	75.72946	80.33274	-335.53281	-615.00040	-364.39058	1
212	H	72.75203	74.69934	80.47891	1596.45398	-1369.33862	1732.02659	1
213	C	72.45830	76.58036	79.40121	585.48547	-340.24194	-406.23938	1
214	O	71.33709	76.16134	78.63432	-419.15649	-173.04408	-511.94141	1
215	H	71.18877	75.27174	79.03329	-1071.84350	1559.71507	-1960.13012	1
216	C	78.21216	78.79816	82.23832	291.41878	-183.13091	710.72246	1
217	O	78.74767	79.85089	81.99653	379.87695	523.47396	-222.23622	1
218	N	78.15100	78.09650	83.37368	564.30591	373.09380	277.24371	1
219	H	77.63088	77.19344	83.28687	-120.59931	-2436.07824	-1214.35098	1
220	C	79.31494	78.10254	84.23866	404.07514	-299.37480	608.84009	1
221	H	80.14751	77.77443	83.57755	-1071.07882	-841.69025	2359.66467	1
222	C	79.50957	79.59454	84.71443	-683.12807	68.71770	-390.13096	1
223	H	79.44653	80.28632	83.82999	2068.88918	1596.58590	770.89603	1
224	H	78.67599	79.89945	85.38750	1379.86429	2342.49779	-179.85638	1
225	C	80.88323	79.76400	85.43572	-176.39967	537.49466	550.97268	1
226	H	80.88425	79.25919	86.43037	-396.28051	1942.22168	1869.33314	1
227	H	81.71596	79.30269	84.86079	-94.44700	586.00678	-2659.20016	1
228	C	81.05144	81.35078	85.53684	-291.69381	-718.18079	-150.72929	1

229	H	81.07005	81.89399	84.55777	-2303.38776	1089.76242	964.62032	1
230	H	80.29594	81.85717	86.18758	884.16729	2568.80533	-207.74283	1
231	N	82.29275	81.55336	86.14793	-594.49522	-252.81478	342.29276	1
232	H	82.73552	80.74478	86.55537	-1735.17426	2084.05705	-263.71605	1
233	C	82.87230	82.68189	86.23379	595.23177	-271.52487	442.22352	1
234	N	82.23143	83.79143	85.67013	585.53813	-424.79750	-105.81303	1
235	H	81.33442	83.84850	85.18966	959.88797	1327.56823	-2177.11905	1
236	H	82.59553	84.74456	85.68418	1578.48647	16.27378	-2220.76233	1
237	N	84.09446	82.57797	86.91240	-452.17763	-390.33541	-421.51853	1
238	H	84.56088	81.77566	87.33293	470.26107	1974.25629	-1817.92087	1
239	H	84.70087	83.37959	87.09123	1856.67307	-1573.97321	-1224.35416	1
240	C	79.09407	77.11956	85.49500	-531.47271	-581.45780	-55.06206	1
241	O	79.89931	77.19601	86.39885	-243.00837	192.73507	609.52485	1
242	N	78.06135	76.27958	85.42043	343.49288	-644.25607	38.09164	1
243	H	77.42053	76.17201	84.62463	-1691.16043	-1535.97525	-1484.73099	1
244	C	77.66540	75.65889	86.65222	542.66492	350.14337	454.42563	1
245	H	78.60339	75.26982	87.10733	1209.57979	-2396.95920	463.86744	1
246	C	76.94916	76.74021	87.56531	-737.14309	145.93010	242.71942	1
247	H	76.11975	77.22667	87.00771	-1050.18303	159.36419	-2509.06125	1
248	C	76.40844	75.98356	88.82707	-706.77696	-252.88343	-245.16230	1
249	H	75.88742	76.67436	89.53070	-1624.64039	-1665.49085	1417.86935	1
250	H	75.67884	75.18858	88.54189	2566.10521	598.51109	693.22305	1
251	H	77.23157	75.48831	89.39369	-1972.69758	107.10018	-1876.34312	1
252	C	77.96948	77.81661	88.07710	412.85148	672.58832	-27.69222	1
253	H	77.54315	78.42401	88.91064	1447.02277	1762.76533	-1490.78944	1
254	H	78.90965	77.34325	88.45203	1320.77379	-145.20455	2378.68491	1
255	H	78.25708	78.52813	87.26620	-1512.10848	1470.52031	1724.75147	1
256	C	76.53052	74.54769	86.25642	-607.11113	499.56689	73.73769	1
257	O	75.44780	74.87819	85.82296	357.97126	460.81534	356.68785	1
258	N	76.97745	73.32959	86.53113	536.55407	-368.62270	332.76306	1
259	H	77.91201	73.17983	86.91188	524.38866	2297.69985	1367.20941	1
260	C	76.08439	72.24313	86.34890	46.50277	-774.29190	-147.97904	1
261	H	75.06863	72.70037	86.31951	1676.51875	1883.29066	1032.55549	1
262	C	76.45025	71.48213	84.96888	-559.41456	-34.19198	-556.30433	1
263	H	77.50494	71.12171	85.01800	-64.66664	395.18769	2695.05373	1
264	H	75.81994	70.56815	84.85761	-2703.44278	-60.40056	333.79418	1
265	C	76.26771	72.39744	83.79010	-519.76435	377.31045	459.42366	1
266	H	76.88750	73.31689	83.94734	-1746.74323	1667.50644	-1261.73691	1
267	C	76.73570	71.69856	82.51975	570.95554	16.46261	-545.27700	1
268	H	76.54546	72.32620	81.60567	2391.58273	28.05277	-1305.07271	1
269	H	77.83738	71.48297	82.54947	175.75588	917.63458	2559.43867	1
270	H	76.20964	70.72124	82.36673	-1063.97851	-2155.34650	1283.00462	1
271	C	74.81914	72.83595	83.63077	193.76014	2.62946	-765.53141	1
272	H	74.65299	73.36291	82.65593	507.39394	-846.55087	2539.60089	1
273	H	74.11239	71.96681	83.66451	1337.57841	1818.19054	1526.01994	1
274	H	74.52343	73.55517	84.44807	1100.88635	-1172.91350	-2199.08909	1
275	C	76.34016	71.20535	87.55617	-549.21115	475.64486	-309.38218	1
276	O	77.31170	71.24027	88.26498	556.06106	-390.37755	-78.24250	1
277	O	75.38747	70.16618	87.68700	-572.27940	-310.19032	-209.75862	1
278	H	74.75582	70.44525	86.96798	-1380.08193	2212.14486	790.85944	1

Listing 104: C00104.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.2750	1100
		0.2500	300.00	0.00	0.00	0.00	-1293.4101	0.0000	300.0000
3	H	82.12460	73.63974	69.98136	-2043.14101	-1757.64893	399.89339		1
4	N	82.03970	74.60119	69.65854	426.75047	490.45733	-334.42467		1
5	H	81.51859	75.02698	70.42186	442.25559	-1110.30854	-2448.52907		1
6	C	83.25334	75.22933	69.30725	415.32972	-666.39213	83.73172		1
7	H	83.94269	74.41160	69.00958	879.32219	2491.00447	667.35213		1
8	C	82.95368	76.27109	68.11889	31.35357	477.41777	628.23362		1

9	H	82.14134	76.97658	68.42440	1168.38489	2240.25337	-1019.71136	1
10	H	83.84960	76.90386	67.90712	-360.43770	2534.90498	931.67112	1
11	C	82.55048	75.47495	66.90118	463.18208	512.70242	-382.34388	1
12	H	81.73260	74.78017	67.19857	1725.29117	1863.52247	-987.07854	1
13	C	82.03429	76.40171	65.80849	710.42801	-144.27427	-313.15367	1
14	H	81.72523	75.83091	64.89490	364.20195	-1033.13725	2494.72524	1
15	H	81.14589	76.99307	66.15052	2567.61904	335.80679	847.48802	1
16	H	82.81880	77.13656	65.48957	-2587.99029	680.92867	-512.16411	1
17	C	83.71758	74.65955	66.36246	268.17616	741.64379	-40.42634	1
18	H	83.44311	74.11632	65.42146	1283.54314	-1945.37420	-1411.27812	1
19	H	84.59888	75.31093	66.12464	-1258.57796	1317.15249	-2026.02085	1
20	H	84.06540	73.88890	67.09753	-2502.84526	909.80597	575.92391	1
21	C	83.77750	76.06238	70.60964	619.36578	-458.64843	-172.09273	1
22	O	84.91988	75.98486	71.00794	-81.40433	433.87611	522.34594	1
23	N	82.77819	76.80568	71.09083	175.23996	-622.20190	341.55523	1
24	H	81.87654	76.78083	70.61643	-876.57256	-303.22879	-2561.90213	1
25	C	82.89861	77.33704	72.40204	-571.88214	-534.10783	-106.15033	1
26	H	83.98610	77.26087	72.64022	-2713.20841	-16.25800	-248.80809	1
27	C	82.27714	78.81330	72.35440	166.60354	288.16399	-716.09568	1
28	H	81.15619	78.71649	72.28836	-2097.85574	1636.78449	-586.18044	1
29	O	82.66683	79.63282	71.23833	-317.80580	-363.38227	484.43082	1
30	H	81.85113	79.61660	70.69902	1863.74748	-1451.84923	1357.29467	1
31	C	82.68612	79.36176	73.76995	503.80731	517.99032	318.51606	1
32	H	82.19086	80.33604	73.98965	640.61020	-2157.10410	-1536.29104	1
33	H	82.41386	78.64974	74.59994	1687.88455	465.60692	2087.56452	1
34	H	83.78650	79.53285	73.82735	-1293.07895	-1899.88581	-1463.57452	1
35	C	81.90641	76.45433	73.36299	-153.07550	-733.68902	248.70981	1
36	O	80.75468	76.78970	73.44585	186.15459	-480.78787	-449.34387	1
37	N	82.51319	75.35533	73.84550	-487.53139	543.18517	42.03850	1
38	C	81.90392	74.61815	74.90315	-699.35871	69.34393	360.10701	1
39	H	80.89969	75.06930	75.08314	2.81126	-221.99807	-2715.58072	1
40	C	81.88715	73.15281	74.28205	-507.46439	-592.59194	122.07761	1
41	H	81.74459	72.35846	75.04812	-1975.08116	525.87560	-1801.71556	1
42	H	81.06183	73.03366	73.54379	1588.27743	-1913.22100	1113.83566	1
43	C	83.28117	73.09297	73.58231	-613.62442	-457.55993	-194.14490	1
44	H	84.09721	72.89728	74.31290	1707.54637	-721.27992	1996.92523	1
45	H	83.35865	72.29773	72.80590	758.23357	2100.81767	1560.55011	1
46	C	83.38436	74.55667	72.98183	-352.41524	704.96076	49.21465	1
47	H	84.40617	75.00271	73.00819	1714.76886	-2070.42778	443.35792	1
48	H	82.95907	74.67895	71.95636	1224.15040	1801.50881	1636.97633	1
49	C	82.85179	74.54819	76.24372	566.85117	537.05831	117.62814	1
50	O	82.43791	73.93068	77.19745	-550.26779	-406.08867	4.21666	1
51	N	84.02691	75.15164	76.10373	566.34832	-425.77725	180.18749	1
52	H	84.17946	75.68068	75.24759	644.44502	2646.80550	-52.73430	1
53	C	84.97221	75.02346	77.15776	612.34801	-281.48662	411.56221	1
54	H	84.65328	74.10210	77.69622	1667.23498	-1490.75142	1556.16753	1
55	C	86.44351	74.97795	76.53230	-714.45746	-175.43074	286.98927	1
56	H	86.57639	75.87923	75.87350	-787.09484	1763.03619	-1922.46060	1
57	O	86.72632	73.82274	75.72426	-429.46514	516.51932	-128.40526	1
58	H	86.88759	74.23318	74.85173	1981.82785	436.16847	-1818.18182	1
59	C	87.32464	75.16429	77.82168	630.79189	-468.94448	76.03230	1
60	H	88.40622	75.26470	77.56782	-1775.71861	2062.30353	131.89849	1
61	H	87.02667	76.08337	78.38521	-1855.14608	88.94118	1993.53760	1
62	H	87.22939	74.30027	78.52087	-1504.82350	-780.94249	-2132.90992	1
63	C	84.87380	76.37912	78.08531	288.57638	618.62814	-397.00270	1
64	O	85.33706	77.44766	77.68263	321.70495	-185.26452	574.37218	1
65	N	84.34370	76.04626	79.23399	-447.05792	-446.53431	367.76425	1
66	H	84.06118	75.06520	79.25218	350.31316	1975.63644	-1843.31522	1
67	C	83.98957	76.85904	80.33667	-511.23061	374.03917	-471.51480	1
68	H	83.53539	76.09623	81.00934	2234.79579	-898.70890	-1273.45190	1
69	C	85.30708	77.51122	80.97550	529.53781	-159.34528	563.72604	1
70	H	85.06225	77.85654	82.01730	654.59388	2347.94251	1217.51488	1

71	H	86.04922	76.67906	81.08290	-1526.55661	2103.42026	817.87394	1
72	O	85.89167	78.65180	80.29857	-554.84278	14.12789	399.58769	1
73	H	86.08772	78.24658	79.42701	1297.06236	2061.84854	1220.68812	1
74	C	82.91242	78.02580	79.97070	-662.15484	-412.13544	123.62687	1
75	O	81.95988	78.19387	80.68635	-540.01537	-317.05804	274.91456	1
76	N	83.28655	78.75063	78.91432	-202.76299	-690.00100	-131.49145	1
77	H	84.14385	78.46854	78.37308	-702.62132	-2617.37191	281.70413	1
78	C	82.36590	79.75936	78.39117	-491.73914	576.34187	222.73509	1
79	H	81.80738	80.13133	79.28163	1977.17978	-1823.58850	-434.68928	1
80	C	83.23116	80.80037	77.70179	-649.50797	-328.66843	306.11224	1
81	H	83.92684	80.26556	77.01728	2075.07803	1452.16490	-1004.45904	1
82	C	82.40355	81.76359	76.87337	-615.18735	-489.99689	-70.96352	1
83	H	83.05164	82.49181	76.31019	-1226.32661	-1724.38906	-1716.47170	1
84	H	81.77599	81.21713	76.11475	2381.64273	-969.84735	900.46860	1
85	H	81.70043	82.36693	77.51326	2122.74991	1702.23946	-141.36228	1
86	C	84.07043	81.54949	78.72079	-501.86074	-479.61276	-376.42482	1
87	H	84.80031	82.25228	78.23302	993.79261	-2246.95401	-1177.81305	1
88	H	83.43009	82.16122	79.41590	42.71279	-626.15391	-2651.37258	1
89	H	84.66324	80.83702	79.36233	-2026.39012	-1590.33709	-887.82922	1
90	C	81.37913	78.94526	77.32245	-672.89153	382.57394	-156.34072	1
91	O	81.83110	78.20239	76.47806	410.04627	221.86223	500.35950	1
92	N	80.13124	79.31700	77.52442	-378.11782	-443.79414	-441.10984	1
93	H	79.99768	80.00646	78.26187	2404.15973	-568.14894	1149.30085	1
94	C	79.04292	78.75662	76.80253	-544.54484	466.16019	331.29119	1
95	H	78.15852	79.30784	77.19669	-1409.80988	-170.17955	2325.32679	1
96	C	79.33977	79.05981	75.26608	-184.48284	116.78282	-758.89137	1
97	H	79.63706	80.12687	75.15032	1893.78641	1861.14652	611.04528	1
98	H	80.21249	78.45804	74.91146	-2170.79665	-974.19311	1327.50117	1
99	C	78.07942	78.72762	74.41390	389.51668	672.81878	-138.49152	1
100	H	77.90049	77.61993	74.41624	510.64577	1933.03327	1851.02484	1
101	H	77.17240	79.15365	74.89857	-2302.30869	-1105.72939	-948.89774	1
102	C	78.16276	79.22233	72.92029	-559.93427	-126.34590	542.30857	1
103	O	77.31730	78.85927	72.14457	-670.36003	-111.83166	76.36448	1
104	N	79.18147	80.06852	72.65532	-216.06729	-537.07037	446.51379	1
105	H	79.91315	80.44354	73.27038	-1251.96487	1074.12894	-2168.52500	1
106	H	79.30820	80.53550	71.75003	-2451.83023	-720.73851	944.84612	1
107	C	78.92171	77.14448	76.98736	546.24052	-563.88337	-85.11809	1
108	O	78.42473	76.54392	76.05996	71.70702	-307.40463	606.69673	1
109	N	79.22599	76.67081	78.19893	479.90863	-504.50129	222.86849	1
110	C	79.56038	75.28940	78.40345	75.51268	-600.91904	506.73700	1
111	H	80.24974	74.98298	77.58192	-2033.61562	1795.30103	254.89480	1
112	C	80.21905	75.33754	79.84711	523.79067	517.99274	284.45581	1
113	H	80.25440	74.34079	80.34183	1599.61665	-1127.00911	1895.98173	1
114	H	81.26433	75.72024	79.80745	-1881.83093	1275.82488	-1501.55016	1
115	C	79.27546	76.35561	80.55823	-600.05639	-404.05026	316.64485	1
116	H	78.28335	75.90450	80.77917	-2597.05260	496.36221	657.73249	1
117	H	79.67618	76.74677	81.51931	-1666.24518	1294.38985	-1723.90591	1
118	C	79.18647	77.46416	79.42154	493.57570	-129.95376	-602.56394	1
119	H	78.25996	78.08379	79.41500	-1469.08415	-637.84797	2204.22581	1
120	H	80.08316	78.12834	79.38079	-1038.97840	1068.88701	-2280.71789	1
121	C	78.20944	74.37465	78.45721	188.88100	241.05089	-727.87821	1
122	O	78.28000	73.22391	78.81322	531.88613	-49.19943	427.07960	1
123	N	77.11457	75.07237	78.14387	708.14833	26.93417	-179.73509	1
124	H	77.29228	76.02107	77.80169	-2232.69501	-1179.09831	1023.94816	1
125	C	75.79776	74.45449	78.17514	-738.32412	259.92548	104.42456	1
126	H	76.01296	73.45628	78.62769	2028.89123	1260.02983	1311.33324	1
127	C	74.88559	75.33402	79.01440	-258.65678	-345.52513	661.28459	1
128	H	75.07247	76.39670	78.74618	-1826.06090	-1801.46097	-918.64554	1
129	C	73.42242	75.02743	78.75876	-541.23400	531.92970	-218.41428	1
130	H	72.74269	75.62140	79.43138	1311.73218	-2219.18200	882.19023	1
131	H	73.12810	75.26217	77.69322	-1048.71298	1223.58118	-2196.97971	1
132	H	73.19394	73.93643	78.93169	419.06414	1903.92898	1903.44670	1

133	C	75.17727	75.17851	80.49658	-423.86431	152.66566	-648.55262	1
134	H	74.49889	75.81936	81.12464	105.68386	-2342.50080	1387.51238	1
135	H	75.03300	74.11382	80.83134	-1695.63603	-1484.73621	-1531.02793	1
136	H	76.23601	75.46402	80.74274	-1853.57121	-487.39031	1936.59343	1
137	C	75.22583	74.29754	76.61181	539.71428	-510.58232	267.58633	1
138	O	75.13468	73.16003	76.15306	-15.93758	-278.34085	-624.49402	1
139	N	74.86203	75.44009	76.08380	-676.81886	12.05292	276.17960	1
140	H	75.05850	76.21680	76.71296	-1694.44250	-373.84189	-2100.66098	1
141	C	74.45978	75.65237	74.74187	412.33078	-664.70360	108.35451	1
142	H	74.46716	76.76125	74.64921	1765.77476	1294.44366	1621.76594	1
143	C	75.54543	74.94525	73.83271	-179.66635	-721.95667	-264.73915	1
144	H	76.57052	75.28716	74.10593	-607.34922	2587.87032	-598.10018	1
145	H	75.54232	73.84357	74.01183	-359.69332	-1479.13954	-2259.74260	1
146	C	75.21398	75.28262	72.34133	-240.01076	616.02425	431.85322	1
147	H	74.18528	74.94291	72.08348	-1359.17131	782.54425	2227.99181	1
148	H	75.22744	76.38279	72.16901	-820.36667	85.81767	-2596.78715	1
149	C	76.29044	74.56201	71.43533	-513.07015	236.18570	-551.87280	1
150	H	77.30643	74.98081	71.62168	1816.11944	-1183.11722	-1650.94321	1
151	H	76.35772	73.47809	71.68470	-1800.04429	-1361.53473	1526.34643	1
152	C	75.87599	74.75808	69.95772	726.08972	-253.19732	-179.64713	1
153	H	74.92372	74.26517	69.67664	1224.27271	-456.51798	-2390.90304	1
154	H	75.87429	75.81213	69.61430	1206.40339	-1150.93514	-2154.90344	1
155	N	76.96248	74.05884	69.07485	329.70796	-633.68968	-155.67358	1
156	H	76.80076	74.08845	68.02667	1348.31305	1938.76845	1359.00643	1
157	H	77.94571	74.45086	69.14534	2096.92035	1446.54551	-966.48890	1
158	H	77.12665	73.02204	69.23376	-1197.07217	-2303.53719	827.28733	1
159	C	72.97781	75.03430	74.38205	-378.01186	-556.17301	-413.96481	1
160	O	72.26625	75.65446	73.63156	-409.44433	-307.55053	-453.30833	1
161	N	72.79878	73.81511	74.86741	-429.02477	524.70884	274.08502	1
162	H	73.55044	73.37788	75.44497	1706.34263	-1425.96036	1574.38926	1
163	C	71.46480	73.30162	74.89363	-45.25864	-626.22952	478.93267	1
164	H	71.00678	73.75761	73.98509	1988.63164	570.90773	1772.87287	1
165	C	71.66102	71.73456	74.83196	551.77128	-20.49526	-564.54996	1
166	H	72.40928	71.50291	74.04067	1434.61535	-1753.10253	1513.99471	1
167	H	72.12621	71.37526	75.77781	-714.67738	1819.09770	1898.36494	1
168	C	70.34504	70.93513	74.55250	446.99263	-555.77305	338.97221	1
169	H	69.71381	70.88074	75.46867	1953.68466	1892.25957	-161.67766	1
170	H	69.72133	71.42614	73.76563	-403.03785	2688.07032	-188.43591	1
171	C	70.73126	69.46673	74.10769	567.86262	335.74681	434.04421	1
172	H	71.31020	69.46680	73.15552	-1080.02275	1568.26081	-1948.78900	1
173	H	71.38380	68.97278	74.86361	-919.54108	2111.34692	1456.13463	1
174	C	69.38582	68.71949	73.95237	195.81897	173.33862	-745.11536	1
175	H	68.75859	68.71062	74.86567	1405.67949	-2301.21089	-390.08113	1
176	H	68.78295	69.03917	73.07848	-940.37328	-1118.32446	2299.72133	1
177	N	69.68663	67.20546	73.70067	319.26422	656.36007	-42.02424	1
178	H	68.83175	66.58174	73.62404	1961.03633	619.91968	1787.09422	1
179	H	70.20441	66.95887	72.80806	854.14343	-2156.80752	1429.08711	1
180	H	70.25415	66.69288	74.43705	1237.02905	-1378.50857	-1998.28500	1
181	C	70.73896	73.83924	76.25965	532.53319	-268.57236	517.55729	1
182	O	71.17383	74.77615	76.89585	266.16714	-290.73804	-558.88002	1
183	N	69.58239	73.20772	76.41486	-226.25352	640.49678	-270.32839	1
184	H	69.39090	72.52561	75.68249	2007.69063	-1035.27229	1523.50231	1
185	C	68.95134	73.00600	77.68231	-540.76542	-573.33303	49.50000	1
186	H	68.80648	71.90546	77.74500	-2374.20950	-1036.76023	843.75774	1
187	C	69.75302	73.59650	78.92568	-77.09082	666.87422	-415.84136	1
188	H	70.13522	74.63000	78.66265	-985.81834	617.19825	2463.91927	1
189	O	70.88846	72.80551	79.33305	293.29899	-391.65602	-477.80926	1
190	H	71.62099	73.36740	79.00943	2528.72714	-681.76262	-751.27122	1
191	C	68.59675	73.76014	79.97923	252.47363	-605.14473	440.05134	1
192	H	68.95502	74.24204	80.91802	-2052.65063	1456.49051	-1043.51830	1
193	H	67.76401	74.39195	79.57114	-2152.98800	-1661.97574	-161.70652	1
194	H	68.15222	72.77658	80.25666	-473.12726	-1584.27339	2165.61725	1

195	C	67.51627	73.78073	77.58174	360.36307	488.46713	505.10056	1
196	O	66.50147	73.28458	78.01746	-200.08817	-528.03552	-385.82850	1
197	N	67.71090	75.02494	77.11616	-597.54095	-226.44775	355.20479	1
198	H	68.65000	75.22310	76.76201	2179.23655	-1300.70981	-991.33835	1
199	C	66.54887	75.70818	76.65513	-687.68921	297.39807	-249.45179	1
200	H	65.75109	75.32296	77.32856	-349.16256	-2467.37713	-1101.72831	1
201	C	66.79683	77.28126	76.78036	672.47345	361.54328	-201.62880	1
202	H	67.65167	77.59681	76.13826	1541.41502	582.18425	2169.97026	1
203	H	65.89532	77.82605	76.41510	-2534.67717	60.25153	997.72295	1
204	C	67.07809	77.62003	78.25298	574.26774	-389.43119	-377.02542	1
205	C	65.99712	77.68792	79.18255	688.82679	-287.33580	-257.96133	1
206	H	64.96002	77.48648	78.85679	331.14182	1470.38163	2269.80013	1
207	C	68.41683	77.85460	78.68942	-383.52382	-675.04808	144.24917	1
208	H	69.26103	77.78108	77.97953	4.09847	1517.59662	2262.86397	1
209	C	66.27282	78.02176	80.50891	-134.76730	428.45285	-649.50303	1
210	H	65.43331	78.08125	81.22389	-903.23433	1600.49020	2011.53387	1
211	C	68.64267	78.18914	80.02756	-335.53281	-615.00040	-364.39058	1
212	H	69.68108	78.38117	80.34961	1596.45398	-1369.33862	1732.02659	1
213	C	67.58940	78.29345	80.98258	585.48547	-340.24194	-406.23938	1
214	O	67.81085	78.63919	82.34129	-419.15649	-173.04408	-511.94141	1
215	H	68.78669	78.77842	82.32028	-1071.84350	1559.71507	-1960.13012	1
216	C	66.24342	75.33715	75.09721	291.41878	-183.13091	710.72246	1
217	O	65.37652	75.93343	74.49774	379.87695	523.47396	-222.23622	1
218	N	66.98436	74.32379	74.66021	564.30591	373.09380	277.24371	1
219	H	67.69476	73.94974	75.28833	-120.59931	-2436.07824	-1214.35098	1
220	C	66.82614	73.85661	73.32780	404.07514	-299.37480	608.84009	1
221	H	65.81190	74.22550	73.04296	-1071.07882	-841.69025	2359.66467	1
222	C	67.98971	74.49326	72.46048	-683.12807	68.71770	-390.13096	1
223	H	68.11568	75.57577	72.68902	2068.88918	1596.58590	770.89603	1
224	H	68.96377	74.01349	72.70760	1379.86429	2342.49779	-179.85638	1
225	C	67.62480	74.27040	70.96029	-176.39967	537.49466	550.97268	1
226	H	67.42894	73.19295	70.74838	-396.28051	1942.22168	1869.33314	1
227	H	66.70145	74.81885	70.66727	-94.44700	586.00678	-2659.20016	1
228	C	68.90912	74.80547	70.17527	-291.69381	-718.18079	-150.72929	1
229	H	69.16509	75.88145	70.35321	-2303.38776	1089.76242	964.62032	1
230	H	69.84153	74.20735	70.33646	884.16729	2568.80533	-207.74283	1
231	N	68.56251	74.67459	68.82625	-594.49522	-252.81478	342.29276	1
232	H	67.66118	74.27385	68.61578	-1735.17426	2084.05705	-263.71605	1
233	C	69.32038	75.02602	67.86771	595.23177	-271.52487	442.22352	1
234	N	70.56399	75.57041	68.20932	585.53813	-424.79750	-105.81303	1
235	H	70.97066	75.73083	69.13035	959.88797	1327.56823	-2177.11905	1
236	H	71.26894	75.88710	67.54360	1578.48647	16.27378	-2220.76233	1
237	N	68.71987	74.78533	66.62485	-452.17763	-390.33541	-421.51853	1
238	H	67.82196	74.36500	66.38901	470.26107	1974.25629	-1817.92087	1
239	H	69.17354	74.99298	65.73461	1856.67307	-1573.97321	-1224.35416	1
240	C	67.03331	72.23189	73.34599	-531.47271	-581.45780	-55.06206	1
241	O	67.75927	71.66887	72.55861	-243.00837	192.73507	609.52485	1
242	N	66.30318	71.68406	74.31868	343.49288	-644.25607	38.09164	1
243	H	65.75910	72.35650	74.85611	-1691.16043	-1535.97525	-1484.73099	1
244	C	66.11349	70.23538	74.39177	542.66492	350.14337	454.42563	1
245	H	67.05343	69.88179	73.90528	1209.57979	-2396.95920	463.86744	1
246	C	65.96875	69.86173	75.85620	-737.14309	145.93010	242.71942	1
247	H	65.07060	70.38697	76.25632	-1050.18303	159.36419	-2509.06125	1
248	C	65.76419	68.37321	76.05967	-706.77696	-252.88343	-245.16230	1
249	H	65.69421	68.10841	77.15122	-1624.64039	-1665.49085	1417.86935	1
250	H	64.80628	68.02429	75.56705	2566.10521	598.51109	693.22305	1
251	H	66.60770	67.77105	75.62164	-1972.69758	107.10018	-1876.34312	1
252	C	67.16339	70.33777	76.66459	412.85148	672.58832	-27.69222	1
253	H	67.04740	70.10745	77.75931	1447.02277	1762.76533	-1490.78944	1
254	H	68.11825	69.85423	76.32308	1320.77379	-145.20455	2378.68491	1
255	H	67.29445	71.45099	76.56727	-1512.10848	1470.52031	1724.75147	1
256	C	64.78242	69.80123	73.49982	-607.11113	499.56689	73.73769	1

257	O	63.95967	69.03135	73.95089	357.97126	460.81534	356.68785	1
258	N	64.81429	70.33033	72.29098	536.55407	-368.62270	332.76306	1
259	H	65.60168	70.94160	72.07344	524.38866	2297.69985	1367.20941	1
260	C	63.81851	69.93927	71.35965	46.50277	-774.29190	-147.97904	1
261	H	63.45612	68.94871	71.72200	1676.51875	1883.29066	1032.55549	1
262	C	62.65049	71.05431	71.32581	-559.41456	-34.19198	-556.30433	1
263	H	63.10631	72.03682	71.05354	-64.66664	395.18769	2695.05373	1
264	H	61.91988	70.82123	70.51364	-2703.44278	-60.40056	333.79418	1
265	C	61.95135	71.14621	72.65527	-519.76435	377.31045	459.42366	1
266	H	62.71933	71.34072	73.43872	-1746.74323	1667.50644	-1261.73691	1
267	C	60.95309	72.29788	72.65731	570.95554	16.46261	-545.27700	1
268	H	60.43779	72.39336	73.64713	2391.58273	28.05277	-1305.07271	1
269	H	61.45017	73.28008	72.44698	175.75588	917.63458	2559.43867	1
270	H	60.15608	72.15678	71.88285	-1063.97851	-2155.34650	1283.00462	1
271	C	61.22823	69.85355	73.00639	193.76014	2.62946	-765.53141	1
272	H	60.57861	69.97800	73.91135	507.39394	-846.55087	2539.60089	1
273	H	60.56891	69.50102	72.17158	1337.57841	1818.19054	1526.01994	1
274	H	61.95878	69.02743	73.23879	1100.88635	-1172.91350	-2199.08909	1
275	C	64.51094	69.95744	69.90085	-549.21115	475.64486	-309.38218	1
276	O	65.21367	70.86498	69.53959	556.06106	-390.37755	-78.24250	1
277	O	64.12997	68.93956	68.99797	-572.27940	-310.19032	-209.75862	1
278	H	63.55869	68.39310	69.60449	-1380.08193	2212.14486	790.85944	1

Listing 105: C00105.xmolout

1		276								
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100	
		0.2500	300.00	0.00	0.00	0.00	-1293.4091	0.0000	300.0000	
3	H	84.27790	65.94794	78.59807	-2043.14101	-1757.64893	399.89339		1	
4	N	85.20849	65.60722	78.36149	426.75047	490.45733	-334.42467		1	
5	H	85.04235	64.88523	77.65077	442.25559	-1110.30854	-2448.52907		1	
6	C	86.15143	66.55530	77.91544	415.32972	-666.39213	83.73172		1	
7	H	85.77898	67.56870	78.17727	879.32219	2491.00447	667.35213		1	
8	C	87.57316	66.21808	78.59554	31.35357	477.41777	628.23362		1	
9	H	87.89757	65.19831	78.27717	1168.38489	2240.25337	-1019.71136		1	
10	H	88.35905	66.92144	78.22806	-360.43770	2534.90498	931.67112		1	
11	C	87.44427	66.28291	80.09597	463.18208	512.70242	-382.34388		1	
12	H	86.57957	65.64776	80.39468	1725.29117	1863.52247	-987.07854		1	
13	C	88.70180	65.73511	80.75887	710.42801	-144.27427	-313.15367		1	
14	H	88.61678	65.73968	81.87624	364.20195	-1033.13725	2494.72524		1	
15	H	88.90901	64.67922	80.44549	2567.61904	335.80679	847.48802		1	
16	H	89.60530	66.34252	80.49310	-2587.99029	680.92867	-512.16411		1	
17	C	87.19180	67.70521	80.57611	268.17616	741.64379	-40.42634		1	
18	H	87.12199	67.75720	81.69350	1283.54314	-1945.37420	-1411.27812		1	
19	H	88.01445	68.39877	80.26280	-1258.57796	1317.15249	-2026.02085		1	
20	H	86.23445	68.11836	80.16575	-2502.84526	909.80597	575.92391		1	
21	C	86.26910	66.25119	76.31845	619.36578	-458.64843	-172.09273		1	
22	O	85.93190	65.17209	75.84736	-81.40433	433.87611	522.34594		1	
23	N	86.76550	67.32262	75.72858	175.23996	-622.20190	341.55523		1	
24	H	86.98590	68.10191	76.34911	-876.57256	-303.22879	-2561.90213		1	
25	C	87.06286	67.45076	74.34533	-571.88214	-534.10783	-106.15033		1	
26	H	87.90678	68.17578	74.35874	-2713.20841	-16.25800	-248.80809		1	
27	C	87.48642	66.05260	73.69302	166.60354	288.16399	-716.09568		1	
28	H	86.69599	65.27422	73.91338	-2097.85574	1636.78449	-586.18044		1	
29	O	88.72380	65.51147	74.19423	-317.80580	-363.38227	484.43082		1	
30	H	88.38888	64.74434	74.70289	1863.74748	-1451.84923	1357.29467		1	
31	C	87.44935	66.39547	72.15948	503.80731	517.99032	318.51606		1	
32	H	87.66348	65.49747	71.53469	640.61020	-2157.10410	-1536.29104		1	
33	H	86.45331	66.78907	71.84663	1687.88455	465.60692	2087.56452		1	
34	H	88.20788	67.16966	71.89779	-1293.07895	-1899.88581	-1463.57452		1	
35	C	85.83441	68.24345	73.60260	-153.07550	-733.68902	248.70981		1	
36	O	86.16287	69.32028	73.17368	186.15459	-480.78787	-449.34387		1	

37	N	84.64478	67.63235	73.51606	-487.53139	543.18517	42.03850	1
38	C	83.54486	68.31394	72.89880	-699.35871	69.34393	360.10701	1
39	H	83.94492	68.83145	71.99694	2.81126	-221.99807	-2715.58072	1
40	C	82.54799	67.11020	72.60764	-507.46439	-592.59194	122.07761	1
41	H	81.49824	67.44627	72.45225	-1975.08116	525.87560	-1801.71556	1
42	H	82.84428	66.55264	71.69140	1588.27743	-1913.22100	1113.83566	1
43	C	82.72991	66.23223	73.88416	-613.62442	-457.55993	-194.14490	1
44	H	82.10276	66.61383	74.72204	1707.54637	-721.27992	1996.92523	1
45	H	82.43544	65.16940	73.73436	758.23357	2100.81767	1560.55011	1
46	C	84.27513	66.40784	74.21360	-352.41524	704.96076	49.21465	1
47	H	84.48578	66.59006	75.29899	1714.76886	-2070.42778	443.35792	1
48	H	84.93700	65.59439	73.83362	1224.15040	1801.50881	1636.97633	1
49	C	82.89342	69.37618	73.95731	566.85117	537.05831	117.62814	1
50	O	82.12652	70.23636	73.53513	-550.26779	-406.08867	4.21666	1
51	N	83.27601	69.13683	75.18907	566.34832	-425.77725	180.18749	1
52	H	83.97403	68.40679	75.29511	644.44502	2646.80550	-52.73430	1
53	C	82.72955	69.81067	76.31822	612.34801	-281.48662	411.56221	1
54	H	81.65779	69.94372	76.04742	1667.23498	-1490.75142	1556.16753	1
55	C	83.02194	68.91803	77.60568	-714.45746	-175.43074	286.98927	1
56	H	84.12725	68.93560	77.81358	-787.09484	1763.03619	-1922.46060	1
57	O	82.67102	67.52549	77.50753	-429.46514	516.51932	-128.40526	1
58	H	83.54255	67.09566	77.62399	1981.82785	436.16847	-1818.18182	1
59	C	82.27414	69.75823	78.70556	630.79189	-468.94448	76.03230	1
60	H	82.42413	69.32586	79.72200	-1775.71861	2062.30353	131.89849	1
61	H	82.64004	70.81375	78.73607	-1855.14608	88.94118	1993.53760	1
62	H	81.17552	69.79168	78.51966	-1504.82350	-780.94249	-2132.90992	1
63	C	83.53366	71.23897	76.40262	288.57638	618.62814	-397.00270	1
64	O	84.28321	71.51173	77.30827	321.70495	-185.26452	574.37218	1
65	N	83.18843	71.94404	75.33412	-447.05792	-446.53431	367.76425	1
66	H	82.54923	71.54189	74.60553	350.31316	1975.63644	-1843.31522	1
67	C	83.77876	73.22701	75.17139	-511.23061	374.03917	-471.51480	1
68	H	84.37170	73.35097	76.10994	2234.79579	-898.70890	-1273.45190	1
69	C	84.68669	73.13111	73.86003	529.53781	-159.34528	563.72604	1
70	H	85.30370	74.06484	73.79477	654.59388	2347.94251	1217.51488	1
71	H	85.40261	72.27995	74.00465	-1526.55661	2103.42026	817.87394	1
72	O	83.96995	72.95930	72.58157	-554.84278	14.12789	399.58769	1
73	H	83.70067	72.02840	72.69908	1297.06236	2061.84854	1220.68812	1
74	C	82.50916	74.25016	75.08106	-662.15484	-412.13544	123.62687	1
75	O	81.77617	74.37086	76.02805	-540.01537	-317.05804	274.91456	1
76	N	82.43799	74.87010	73.89840	-202.76299	-690.00100	-131.49145	1
77	H	83.12027	74.60397	73.17514	-702.62132	-2617.37191	281.70413	1
78	C	81.57021	76.04158	73.75392	-491.73914	576.34187	222.73509	1
79	H	81.68193	76.58622	74.72014	1977.17978	-1823.58850	-434.68928	1
80	C	82.00761	76.81514	72.52921	-649.50797	-328.66843	306.11224	1
81	H	82.07091	76.10306	71.67563	2075.07803	1452.16490	-1004.45904	1
82	C	80.99628	77.88922	72.16899	-615.18735	-489.99689	-70.96352	1
83	H	81.28459	78.43796	71.23093	-1226.32661	-1724.38906	-1716.47170	1
84	H	79.97276	77.45150	72.00270	2381.64273	-969.84735	900.46860	1
85	H	80.89722	78.65287	72.98854	2122.74991	1702.23946	-141.36228	1
86	C	83.38300	77.43321	72.70713	-501.86074	-479.61276	-376.42482	1
87	H	83.71724	77.97712	71.78124	993.79261	-2246.95401	-1177.81305	1
88	H	83.39535	78.17514	73.55222	42.71279	-626.15391	-2651.37258	1
89	H	84.16086	76.65420	72.93781	-2026.39012	-1590.33709	-887.82922	1
90	C	79.99612	75.51929	73.55068	-672.89153	382.57394	-156.34072	1
91	O	79.09894	76.10963	74.10147	410.04627	221.86223	500.35950	1
92	N	79.91082	74.59062	72.58577	-378.11782	-443.79414	-441.10984	1
93	H	80.87079	74.31654	72.36931	2404.15973	-568.14894	1149.30085	1
94	C	78.85797	73.61168	72.61428	-544.54484	466.16019	331.29119	1
95	H	79.09245	73.01936	71.70247	-1409.80988	-170.17955	2325.32679	1
96	C	79.09572	72.76509	73.92823	-184.48284	116.78282	-758.89137	1
97	H	80.18252	72.59924	74.11157	1893.78641	1861.14652	611.04528	1
98	H	78.70545	73.29337	74.82820	-2170.79665	-974.19311	1327.50117	1

99	C	78.34247	71.41550	73.66601	389.51668	672.81878	-138.49152	1
100	H	77.25205	71.63022	73.56085	510.64577	1933.03327	1851.02484	1
101	H	78.63165	70.99774	72.67541	-2302.30869	-1105.72939	-948.89774	1
102	C	78.56590	70.32122	74.74512	-559.93427	-126.34590	542.30857	1
103	O	78.14619	69.17708	74.53615	-670.36003	-111.83166	76.36448	1
104	N	79.17957	70.74421	75.84536	-216.06729	-537.07037	446.51379	1
105	H	79.55632	71.67970	76.04991	-1251.96487	1074.12894	-2168.52500	1
106	H	79.41137	70.15112	76.65354	-2451.83023	-720.73851	944.84612	1
107	C	77.37645	74.27671	72.57782	546.24052	-563.88337	-85.11809	1
108	O	76.52763	73.77846	73.27079	71.70702	-307.40463	606.69673	1
109	N	77.24011	75.21142	71.62818	479.90863	-504.50129	222.86849	1
110	C	76.21619	76.21007	71.67014	75.51268	-600.91904	506.73700	1
111	H	76.06443	76.50014	72.73472	-2033.61562	1795.30103	254.89480	1
112	C	76.83660	77.32272	70.71980	523.79067	517.99274	284.45581	1
113	H	76.07640	78.04113	70.33974	1599.61665	-1127.00911	1895.98173	1
114	H	77.61544	77.92308	71.24069	-1881.83093	1275.82488	-1501.55016	1
115	C	77.45668	76.43247	69.60004	-600.05639	-404.05026	316.64485	1
116	H	76.66074	76.00709	68.94432	-2597.05260	496.36221	657.73249	1
117	H	78.17317	76.96927	68.93806	-1666.24518	1294.38985	-1723.90591	1
118	C	78.13728	75.29966	70.48185	493.57570	-129.95376	-602.56394	1
119	H	78.19781	74.29137	70.00890	-1469.08415	-637.84797	2204.22581	1
120	H	79.13574	75.57372	70.89658	-1038.97840	1068.88701	-2280.71789	1
121	C	74.85750	75.65018	70.94749	188.88100	241.05089	-727.87821	1
122	O	74.90965	74.94740	69.96292	531.88613	-49.19943	427.07960	1
123	N	73.79381	76.18365	71.53652	708.14833	26.93417	-179.73509	1
124	H	74.00665	76.78553	72.33175	-2232.69501	-1179.09831	1023.94816	1
125	C	72.41912	75.88046	71.16701	-738.32412	259.92548	104.42456	1
126	H	71.81937	76.64764	71.71400	2028.89123	1260.02983	1311.33324	1
127	C	72.28047	75.99669	69.65776	-258.65678	-345.52513	661.28459	1
128	H	73.06357	75.33631	69.19690	-1826.06090	-1801.46097	-918.64554	1
129	C	70.92372	75.54644	69.15214	-541.23400	531.92970	-218.41428	1
130	H	70.80362	75.74288	68.05080	1311.73218	-2219.18200	882.19023	1
131	H	70.76483	74.44097	69.30970	-1048.71298	1223.58118	-2196.97971	1
132	H	70.08624	76.07994	69.68131	419.06414	1903.92898	1903.44670	1
133	C	72.54725	77.41426	69.18301	-423.86431	152.66566	-648.55262	1
134	H	72.52460	77.48831	68.06094	105.68386	-2342.50080	1387.51238	1
135	H	71.78059	78.13528	69.57949	-1695.63603	-1484.73621	-1531.02793	1
136	H	73.55576	77.77733	69.52323	-1853.57121	-487.39031	1936.59343	1
137	C	72.04056	74.35081	71.70554	539.71428	-510.58232	267.58633	1
138	O	70.96087	73.87975	71.43717	-15.93758	-278.34085	-624.49402	1
139	N	72.99853	73.81364	72.43709	-676.81886	12.05292	276.17960	1
140	H	73.84715	74.35926	72.56104	-1694.44250	-373.84189	-2100.66098	1
141	C	72.75880	72.54494	73.05775	412.33078	-664.70360	108.35451	1
142	H	72.20519	71.95312	72.29270	1765.77476	1294.44366	1621.76594	1
143	C	74.17455	71.96450	73.44932	-179.66635	-721.95667	-264.73915	1
144	H	74.82752	71.86720	72.55237	-607.34922	2587.87032	-598.10018	1
145	H	74.71863	72.67070	74.12142	-359.69332	-1479.13954	-2259.74260	1
146	C	73.94604	70.57728	74.14107	-240.01076	616.02425	431.85322	1
147	H	73.19203	70.67108	74.95826	-1359.17131	782.54425	2227.99181	1
148	H	73.51993	69.84415	73.41986	-820.36667	85.81767	-2596.78715	1
149	C	75.31092	70.05478	74.73512	-513.07015	236.18570	-551.87280	1
150	H	76.04955	69.84346	73.92560	1816.11944	-1183.11722	-1650.94321	1
151	H	75.78763	70.82594	75.38326	-1800.04429	-1361.53473	1526.34643	1
152	C	75.00227	68.76734	75.54632	726.08972	-253.19732	-179.64713	1
153	H	74.35281	68.91887	76.43317	1224.27271	-456.51798	-2390.90304	1
154	H	74.61414	67.92772	74.93415	1206.40339	-1150.93514	-2154.90344	1
155	N	76.35100	68.26061	76.10490	329.70796	-633.68968	-155.67358	1
156	H	76.34590	67.30430	76.56084	1348.31305	1938.76845	1359.00643	1
157	H	77.17951	68.21224	75.34005	2096.92035	1446.54551	-966.48890	1
158	H	76.76467	68.84488	76.88593	-1197.07217	-2303.53719	827.28733	1
159	C	71.83239	72.75457	74.38771	-378.01186	-556.17301	-413.96481	1
160	O	71.32592	71.79212	74.92114	-409.44433	-307.55053	-453.30833	1

161	N	71.85736	74.01446	74.82576	-429.02477	524.70884	274.08502	1
162	H	72.29595	74.68267	74.19375	1706.34263	-1425.96036	1574.38926	1
163	C	70.77471	74.42195	75.68975	-45.25864	-626.22952	478.93267	1
164	H	69.89432	73.96049	75.19109	1988.63164	570.90773	1772.87287	1
165	C	71.04818	73.75539	77.08842	551.77128	-20.49526	-564.54996	1
166	H	71.25896	72.66736	76.95042	1434.61535	-1753.10253	1513.99471	1
167	H	71.97518	74.17565	77.53981	-714.67738	1819.09770	1898.36494	1
168	C	69.82285	73.94606	78.04793	446.99263	-555.77305	338.97221	1
169	H	69.52810	75.01607	78.12917	1953.68466	1892.25957	-161.67766	1
170	H	68.92453	73.41097	77.66715	-403.03785	2688.07032	-188.43591	1
171	C	70.28406	73.37361	79.44776	567.86262	335.74681	434.04421	1
172	H	70.46159	72.27536	79.38101	-1080.02275	1568.26081	-1948.78900	1
173	H	71.26107	73.81670	79.74874	-919.54108	2111.34692	1456.13463	1
174	C	69.20695	73.69047	80.51071	195.81897	173.33862	-745.11536	1
175	H	69.06833	74.76985	80.72252	1405.67949	-2301.21089	-390.08113	1
176	H	68.22483	73.20848	80.33431	-940.37328	-1118.32446	2299.72133	1
177	N	69.71007	73.08821	81.86705	319.26422	656.36007	-42.02424	1
178	H	69.08891	73.26650	82.70794	1961.03633	619.91968	1787.09422	1
179	H	69.83481	72.03481	81.91613	854.14343	-2156.80752	1429.08711	1
180	H	70.64378	73.43747	82.23089	1237.02905	-1378.50857	-1998.28500	1
181	C	70.76478	76.05380	75.61760	532.53319	-268.57236	517.55729	1
182	O	70.64281	76.57251	74.52991	266.16714	-290.73804	-558.88002	1
183	N	70.94324	76.60553	76.80993	-226.25352	640.49678	-270.32839	1
184	H	71.11772	75.96836	77.58562	2007.69063	-1035.27229	1523.50231	1
185	C	70.60391	77.94516	77.13268	-540.76542	-573.33303	49.50000	1
186	H	71.09006	78.12723	78.11615	-2374.20950	-1036.76023	843.75774	1
187	C	71.15832	78.89067	75.96993	-77.09082	666.87422	-415.84136	1
188	H	70.67426	78.57846	74.99473	-985.81834	617.19825	2463.91927	1
189	O	72.58606	78.82916	75.76661	293.29899	-391.65602	-477.80926	1
190	H	72.62406	78.28477	74.95371	2528.72714	-681.76262	-751.27122	1
191	C	70.59211	80.29576	76.38641	252.47363	-605.14473	440.05134	1
192	H	70.84000	81.07544	75.62826	-2052.65063	1456.49051	-1043.51830	1
193	H	69.47969	80.27787	76.48357	-2152.98800	-1661.97574	-161.70652	1
194	H	71.01092	80.63531	77.36215	-473.12726	-1584.27339	2165.61725	1
195	C	68.97043	78.02528	77.24538	360.36307	488.46713	505.10056	1
196	O	68.24014	77.63482	76.36692	-200.08817	-528.03552	-385.82850	1
197	N	68.64562	78.69467	78.35796	-597.54095	-226.44775	355.20479	1
198	H	69.39519	78.89138	79.02052	2179.23655	-1300.70981	-991.33835	1
199	C	67.29408	78.49618	78.81125	-687.68921	297.39807	-249.45179	1
200	H	67.10647	77.40222	78.75864	-349.16256	-2467.37713	-1101.72831	1
201	C	67.12479	79.13426	80.25792	672.47345	361.54328	-201.62880	1
202	H	67.47253	80.19266	80.23688	1541.41502	582.18425	2169.97026	1
203	H	66.03925	79.15383	80.51151	-2534.67717	60.25153	997.72295	1
204	C	67.88724	78.35527	81.34145	574.26774	-389.43119	-377.02542	1
205	C	67.27846	77.20736	81.93174	688.82679	-287.33580	-257.96133	1
206	H	66.29569	76.84522	81.57898	331.14182	1470.38163	2269.80013	1
207	C	69.15706	78.81996	81.79898	-383.52382	-675.04808	144.24917	1
208	H	69.63229	79.70553	81.33944	4.09847	1517.59662	2262.86397	1
209	C	67.93682	76.57153	82.98444	-134.76730	428.45285	-649.50303	1
210	H	67.45746	75.69606	83.45570	-903.23433	1600.49020	2011.53387	1
211	C	69.77430	78.15016	82.85906	-335.53281	-615.00040	-364.39058	1
212	H	70.74686	78.52845	83.21939	1596.45398	-1369.33862	1732.02659	1
213	C	69.19315	77.01288	83.49240	585.48547	-340.24194	-406.23938	1
214	O	69.81227	76.32729	84.57072	-419.15649	-173.04408	-511.94141	1
215	H	70.58797	76.91795	84.71964	-1071.84350	1559.71507	-1960.13012	1
216	C	66.29018	79.34745	77.85694	291.41878	-183.13091	710.72246	1
217	O	65.14380	79.00022	77.68177	379.87695	523.47396	-222.23622	1
218	N	66.86343	80.51261	77.52384	564.30591	373.09380	277.24371	1
219	H	67.85288	80.60563	77.75235	-120.59931	-2436.07824	-1214.35098	1
220	C	66.25294	81.26625	76.48357	404.07514	-299.37480	608.84009	1
221	H	65.20977	80.87807	76.41933	-1071.07882	-841.69025	2359.66467	1
222	C	66.39391	82.78338	76.90597	-683.12807	68.71770	-390.13096	1

223	H	66.04812	82.92365	77.95515	2068.88918	1596.58590	770.89603	1
224	H	67.46442	83.08941	76.89919	1379.86429	2342.49779	-179.85638	1
225	C	65.55880	83.66697	75.92762	-176.39967	537.49466	550.97268	1
226	H	65.92249	83.57297	74.88008	-396.28051	1942.22168	1869.33314	1
227	H	64.48979	83.35843	75.91022	-94.44700	586.00678	-2659.20016	1
228	C	65.73071	85.15645	76.47973	-291.69381	-718.18079	-150.72929	1
229	H	65.38568	85.32055	77.53257	-2303.38776	1089.76242	964.62032	1
230	H	66.76420	85.57918	76.39528	884.16729	2568.80533	-207.74283	1
231	N	64.89445	85.91261	75.64826	-594.49522	-252.81478	342.29276	1
232	H	64.42799	85.42071	74.90237	-1735.17426	2084.05705	-263.71605	1
233	C	64.69355	87.16060	75.78341	595.23177	-271.52487	442.22352	1
234	N	65.35641	87.81604	76.82748	585.53813	-424.79750	-105.81303	1
235	H	65.99918	87.44071	77.52381	959.88797	1327.56823	-2177.11905	1
236	H	65.27449	88.81102	77.03835	1578.48647	16.27378	-2220.76233	1
237	N	63.80648	87.63796	74.80854	-452.17763	-390.33541	-421.51853	1
238	H	63.30836	87.15723	74.06089	470.26107	1974.25629	-1817.92087	1
239	H	63.50596	88.61257	74.76304	1856.67307	-1573.97321	-1224.35416	1
240	C	67.15924	81.02428	75.12712	-531.47271	-581.45780	-55.06206	1
241	O	68.26239	81.49687	74.98162	-243.00837	192.73507	609.52485	1
242	N	66.45796	80.26722	74.29555	343.49288	-644.25607	38.09164	1
243	H	65.52875	79.94689	74.56760	-1691.16043	-1535.97525	-1484.73099	1
244	C	67.01357	80.01086	73.01086	542.66492	350.14337	454.42563	1
245	H	68.11212	80.09021	73.18494	1209.57979	-2396.95920	463.86744	1
246	C	66.51116	78.56633	72.58425	-737.14309	145.93010	242.71942	1
247	H	65.39987	78.53034	72.59331	-1050.18303	159.36419	-2509.06125	1
248	C	67.06042	78.18566	71.16770	-706.77696	-252.88343	-245.16230	1
249	H	66.75799	77.15285	70.87367	-1624.64039	-1665.49085	1417.86935	1
250	H	66.67504	78.88134	70.38207	2566.10521	598.51109	693.22305	1
251	H	68.17435	78.23005	71.13335	-1972.69758	107.10018	-1876.34312	1
252	C	67.10403	77.53983	73.61092	412.85148	672.58832	-27.69222	1
253	H	66.75133	76.50109	73.40933	1447.02277	1762.76533	-1490.78944	1
254	H	68.22005	77.52218	73.58373	1320.77379	-145.20455	2378.68491	1
255	H	66.81169	77.79664	74.66030	-1512.10848	1470.52031	1724.75147	1
256	C	66.51290	81.14857	71.93355	-607.11113	499.56689	73.73769	1
257	O	66.95223	81.10234	70.80516	357.97126	460.81534	356.68785	1
258	N	65.70245	82.04111	72.47830	536.55407	-368.62270	332.76306	1
259	H	65.49492	81.88215	73.46251	524.38866	2297.69985	1367.20941	1
260	C	65.04469	83.06173	71.74949	46.50277	-774.29190	-147.97904	1
261	H	64.72133	83.77593	72.53857	1676.51875	1883.29066	1032.55549	1
262	C	66.04883	83.71223	70.66796	-559.41456	-34.19198	-556.30433	1
263	H	66.35679	82.91941	69.93418	-64.66664	395.18769	2695.05373	1
264	H	65.54077	84.50756	70.07160	-2703.44278	-60.40056	333.79418	1
265	C	67.25812	84.25941	71.37816	-519.76435	377.31045	459.42366	1
266	H	67.65570	83.46270	72.04803	-1746.74323	1667.50644	-1261.73691	1
267	C	68.33924	84.62061	70.36682	570.95554	16.46261	-545.27700	1
268	H	69.26390	85.00668	70.86810	2391.58273	28.05277	-1305.07271	1
269	H	68.64041	83.73304	69.75200	175.75588	917.63458	2559.43867	1
270	H	67.99146	85.41349	69.65563	-1063.97851	-2155.34650	1283.00462	1
271	C	66.91136	85.47763	72.22271	193.76014	2.62946	-765.53141	1
272	H	67.81903	85.90389	72.72268	507.39394	-846.55087	2539.60089	1
273	H	66.46015	86.29454	71.60262	1337.57841	1818.19054	1526.01994	1
274	H	66.17682	85.22991	73.03172	1100.88635	-1172.91350	-2199.08909	1
275	C	63.77475	82.42495	70.99414	-549.21115	475.64486	-309.38218	1
276	O	63.41411	81.28376	71.11359	556.06106	-390.37755	-78.24250	1
277	O	63.02006	83.33420	70.20886	-572.27940	-310.19032	-209.75862	1
278	H	63.54743	84.15974	70.38367	-1380.08193	2212.14486	790.85944	1

Listing 106: C00106.xmolout

1	276								
2	150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100	
	0.2500	300.00	0.00	0.00	0.00	-1293.4080	0.0000	300.0000	

3	H	66.75474	82.77873	74.13355	-2043.14101	-1757.64893	399.89339	1
4	N	66.97021	83.51154	74.80742	426.75047	490.45733	-334.42467	1
5	H	67.01164	82.98131	75.67613	442.25559	-1110.30854	-2448.52907	1
6	C	68.16879	84.19791	74.50639	415.32972	-666.39213	83.73172	1
7	H	68.02805	84.42142	73.42805	879.32219	2491.00447	667.35213	1
8	C	68.26860	85.52872	75.40338	31.35357	477.41777	628.23362	1
9	H	68.30693	85.24745	76.48349	1168.38489	2240.25337	-1019.71136	1
10	H	69.21497	86.08255	75.19039	-360.43770	2534.90498	931.67112	1
11	C	67.07609	86.41212	75.13285	463.18208	512.70242	-382.34388	1
12	H	66.15488	85.79637	75.24088	1725.29117	1863.52247	-987.07854	1
13	C	67.02543	87.55045	76.14412	710.42801	-144.27427	-313.15367	1
14	H	66.13246	88.20813	75.98324	364.20195	-1033.13725	2494.72524	1
15	H	66.97230	87.16860	77.19636	2567.61904	335.80679	847.48802	1
16	H	67.93373	88.20321	76.07398	-2587.99029	680.92867	-512.16411	1
17	C	67.11654	86.98788	73.72419	268.17616	741.64379	-40.42634	1
18	H	66.25942	87.68596	73.53929	1283.54314	-1945.37420	-1411.27812	1
19	H	68.05966	87.56507	73.54117	-1258.57796	1317.15249	-2026.02085	1
20	H	67.06142	86.18502	72.94482	-2502.84526	909.80597	575.92391	1
21	C	69.36560	83.11083	74.72152	619.36578	-458.64843	-172.09273	1
22	O	69.28094	82.00197	74.24444	-81.40433	433.87611	522.34594	1
23	N	70.36845	83.64458	75.41104	175.23996	-622.20190	341.55523	1
24	H	70.24004	84.57634	75.80042	-876.57256	-303.22879	-2561.90213	1
25	C	71.67764	83.08266	75.41293	-571.88214	-534.10783	-106.15033	1
26	H	72.24395	83.78466	76.06620	-2713.20841	-16.25800	-248.80809	1
27	C	71.57607	81.59419	76.00221	166.60354	288.16399	-716.09568	1
28	H	71.06657	80.96492	75.21765	-2097.85574	1636.78449	-586.18044	1
29	O	70.79895	81.44428	77.20301	-317.80580	-363.38227	484.43082	1
30	H	70.00129	81.00036	76.84600	1863.74748	-1451.84923	1357.29467	1
31	C	73.08596	81.17904	76.15071	503.80731	517.99032	318.51606	1
32	H	73.18687	80.11480	76.46348	640.61020	-2157.10410	-1536.29104	1
33	H	73.66482	81.29657	75.19707	1687.88455	465.60692	2087.56452	1
34	H	73.60069	81.79464	76.92434	-1293.07895	-1899.88581	-1463.57452	1
35	C	72.23211	83.03645	73.88934	-153.07550	-733.68902	248.70981	1
36	O	72.48665	81.94280	73.40947	186.15459	-480.78787	-449.34387	1
37	N	72.35014	84.24001	73.32837	-487.53139	543.18517	42.03850	1
38	C	72.97810	84.39341	72.04598	-699.35871	69.34393	360.10701	1
39	H	72.71482	83.49357	71.44351	2.81126	-221.99807	-2715.58072	1
40	C	72.36887	85.76974	71.53273	-507.46439	-592.59194	122.07761	1
41	H	73.00245	86.26005	70.76020	-1975.08116	525.87560	-1801.71556	1
42	H	71.36343	85.62753	71.07752	1588.27743	-1913.22100	1113.83566	1
43	C	72.27800	86.57999	72.86273	-613.62442	-457.55993	-194.14490	1
44	H	73.27997	86.95247	73.17834	1707.54637	-721.27992	1996.92523	1
45	H	71.61048	87.46910	72.80162	758.23357	2100.81767	1560.55011	1
46	C	71.73772	85.45735	73.84832	-352.41524	704.96076	49.21465	1
47	H	72.02963	85.58158	74.91695	1714.76886	-2070.42778	443.35792	1
48	H	70.63886	85.27874	73.78438	1224.15040	1801.50881	1636.97633	1
49	C	74.58693	84.56333	72.22811	566.85117	537.05831	117.62814	1
50	O	75.31826	84.50104	71.24353	-550.26779	-406.08867	4.21666	1
51	N	74.91793	84.81566	73.47776	566.34832	-425.77725	180.18749	1
52	H	74.15360	84.83581	74.14783	644.44502	2646.80550	-52.73430	1
53	C	76.21329	85.35219	73.75586	612.34801	-281.48662	411.56221	1
54	H	76.44079	85.91594	72.82230	1667.23498	-1490.75142	1556.16753	1
55	C	76.11967	86.23064	75.08048	-714.45746	-175.43074	286.98927	1
56	H	75.95115	85.54852	75.95837	-787.09484	1763.03619	-1922.46060	1
57	O	75.05467	87.20002	75.11650	-429.46514	516.51932	-128.40526	1
58	H	74.57611	86.92738	75.92467	1981.82785	436.16847	-1818.18182	1
59	C	77.58568	86.80065	75.14413	630.79189	-468.94448	76.03230	1
60	H	77.76018	87.37737	76.08197	-1775.71861	2062.30353	131.89849	1
61	H	78.34788	85.98314	75.10693	-1855.14608	88.94118	1993.53760	1
62	H	77.79340	87.48812	74.29136	-1504.82350	-780.94249	-2132.90992	1
63	C	77.22873	84.07693	73.96120	288.57638	618.62814	-397.00270	1
64	O	77.66350	83.80269	75.04688	321.70495	-185.26452	574.37218	1

65	N	77.33969	83.46442	72.78509	-447.05792	-446.53431	367.76425	1
66	H	76.75254	83.83727	71.99661	350.31316	1975.63644	-1843.31522	1
67	C	78.52136	82.76124	72.41815	-511.23061	374.03917	-471.51480	1
68	H	78.19306	82.31332	71.45366	2234.79579	-898.70890	-1273.45190	1
69	C	79.70605	83.80897	72.14467	529.53781	-159.34528	563.72604	1
70	H	80.51643	83.22511	71.63152	654.59388	2347.94251	1217.51488	1
71	H	79.33037	84.56932	71.40663	-1526.55661	2103.42026	817.87394	1
72	O	80.23675	84.52967	73.28420	-554.84278	14.12789	399.58769	1
73	H	80.70431	83.79584	73.73283	1297.06236	2061.84854	1220.68812	1
74	C	78.92906	81.63463	73.51013	-662.15484	-412.13544	123.62687	1
75	O	80.07608	81.26782	73.58959	-540.01537	-317.05804	274.91456	1
76	N	77.84693	81.13892	74.09649	-202.76299	-690.00100	-131.49145	1
77	H	76.90320	81.54171	73.95797	-702.62132	-2617.37191	281.70413	1
78	C	77.93534	80.08536	75.05442	-491.73914	576.34187	222.73509	1
79	H	78.72699	79.36440	74.75141	1977.17978	-1823.58850	-434.68928	1
80	C	78.23320	80.78408	76.45895	-649.50797	-328.66843	306.11224	1
81	H	77.81840	81.81712	76.46173	2075.07803	1452.16490	-1004.45904	1
82	C	77.62378	79.91545	77.61044	-615.18735	-489.99689	-70.96352	1
83	H	77.84854	80.34508	78.61485	-1226.32661	-1724.38906	-1716.47170	1
84	H	76.51411	79.84007	77.52164	2381.64273	-969.84735	900.46860	1
85	H	78.02650	78.87533	77.59619	2122.74991	1702.23946	-141.36228	1
86	C	79.78251	80.80579	76.67989	-501.86074	-479.61276	-376.42482	1
87	H	80.05618	81.31210	77.63564	993.79261	-2246.95401	-1177.81305	1
88	H	80.20656	79.77454	76.71584	42.71279	-626.15391	-2651.37258	1
89	H	80.29978	81.34990	75.85133	-2026.39012	-1590.33709	-887.82922	1
90	C	76.39518	79.57402	74.96691	-672.89153	382.57394	-156.34072	1
91	O	75.55267	80.40115	74.65009	410.04627	221.86223	500.35950	1
92	N	76.27750	78.28987	75.22106	-378.11782	-443.79414	-441.10984	1
93	H	77.08634	77.68033	75.45057	2404.15973	-568.14894	1149.30085	1
94	C	74.99846	77.72747	75.60353	-544.54484	466.16019	331.29119	1
95	H	74.70104	78.30458	76.50892	-1409.80988	-170.17955	2325.32679	1
96	C	73.96876	77.98634	74.41712	-184.48284	116.78282	-758.89137	1
97	H	74.08179	79.03587	74.04320	1893.78641	1861.14652	611.04528	1
98	H	74.19338	77.33147	73.54513	-2170.79665	-974.19311	1327.50117	1
99	C	72.52045	77.74730	74.93829	389.51668	672.81878	-138.49152	1
100	H	72.37190	76.67062	75.16840	510.64577	1933.03327	1851.02484	1
101	H	72.38597	78.28375	75.90221	-2302.30869	-1105.72939	-948.89774	1
102	C	71.39157	78.22319	73.92594	-559.93427	-126.34590	542.30857	1
103	O	70.42361	77.52535	73.75526	-670.36003	-111.83166	76.36448	1
104	N	71.59429	79.44851	73.40626	-216.06729	-537.07037	446.51379	1
105	H	72.34002	80.18438	73.50714	-1251.96487	1074.12894	-2168.52500	1
106	H	70.84093	79.86616	72.84041	-2451.83023	-720.73851	944.84612	1
107	C	75.44336	76.22707	75.91649	546.24052	-563.88337	-85.11809	1
108	O	76.64768	75.95764	75.94284	71.70702	-307.40463	606.69673	1
109	N	74.42779	75.44123	76.25493	479.90863	-504.50129	222.86849	1
110	C	74.58171	74.00652	76.16710	75.51268	-600.91904	506.73700	1
111	H	75.54999	73.80771	76.68094	-2033.61562	1795.30103	254.89480	1
112	C	73.33705	73.43045	76.95061	523.79067	517.99274	284.45581	1
113	H	72.85247	72.57712	76.41948	1599.61665	-1127.00911	1895.98173	1
114	H	73.64583	73.03268	77.94385	-1881.83093	1275.82488	-1501.55016	1
115	C	72.38645	74.66126	77.10406	-600.05639	-404.05026	316.64485	1
116	H	71.75824	74.79487	76.19488	-2597.05260	496.36221	657.73249	1
117	H	71.68698	74.57700	77.96558	-1666.24518	1294.38985	-1723.90591	1
118	C	73.44894	75.83127	77.26664	493.57570	-129.95376	-602.56394	1
119	H	73.07884	76.86085	77.06537	-1469.08415	-637.84797	2204.22581	1
120	H	74.00371	75.82161	78.23522	-1038.97840	1068.88701	-2280.71789	1
121	C	74.65061	73.52503	74.60894	188.88100	241.05089	-727.87821	1
122	O	75.24438	72.49043	74.34310	531.88613	-49.19943	427.07960	1
123	N	73.94961	74.31315	73.81330	708.14833	26.93417	-179.73509	1
124	H	73.54820	75.12605	74.27878	-2232.69501	-1179.09831	1023.94816	1
125	C	73.71352	74.04369	72.44329	-738.32412	259.92548	104.42456	1
126	H	73.42048	75.02884	72.01746	2028.89123	1260.02983	1311.33324	1

127	C	75.01762	73.42145	71.78088	-258.65678	-345.52513	661.28459	1
128	H	75.27722	72.45095	72.27551	-1826.06090	-1801.46097	-918.64554	1
129	C	74.72941	73.21432	70.25464	-541.23400	531.92970	-218.41428	1
130	H	75.59365	72.74123	69.73162	1311.73218	-2219.18200	882.19023	1
131	H	73.83972	72.55678	70.09422	-1048.71298	1223.58118	-2196.97971	1
132	H	74.51838	74.18200	69.74190	419.06414	1903.92898	1903.44670	1
133	C	76.21175	74.42787	71.91580	-423.86431	152.66566	-648.55262	1
134	H	77.14529	74.02054	71.46064	105.68386	-2342.50080	1387.51238	1
135	H	75.99027	75.39877	71.41412	-1695.63603	-1484.73621	-1531.02793	1
136	H	76.43198	74.64877	72.98737	-1853.57121	-487.39031	1936.59343	1
137	C	72.50186	72.94721	72.28223	539.71428	-510.58232	267.58633	1
138	O	71.89173	72.90807	71.23821	-15.93758	-278.34085	-624.49402	1
139	N	72.40484	72.12628	73.31902	-676.81886	12.05292	276.17960	1
140	H	73.04582	72.27182	74.09900	-1694.44250	-373.84189	-2100.66098	1
141	C	71.18593	71.37857	73.47978	412.33078	-664.70360	108.35451	1
142	H	70.40293	72.13357	73.24667	1765.77476	1294.44366	1621.76594	1
143	C	71.21778	70.24188	72.38713	-179.66635	-721.95667	-264.73915	1
144	H	71.36561	70.68821	71.37532	-607.34922	2587.87032	-598.10018	1
145	H	72.08735	69.56387	72.54059	-359.69332	-1479.13954	-2259.74260	1
146	C	69.86276	69.45977	72.46264	-240.01076	616.02425	431.85322	1
147	H	69.70821	69.02782	73.47688	-1359.17131	782.54425	2227.99181	1
148	H	69.00118	70.14112	72.28397	-820.36667	85.81767	-2596.78715	1
149	C	69.91887	68.32139	71.36706	-513.07015	236.18570	-551.87280	1
150	H	70.07593	68.75588	70.35295	1816.11944	-1183.11722	-1650.94321	1
151	H	70.78566	67.64389	71.54456	-1800.04429	-1361.53473	1526.34643	1
152	C	68.58742	67.53707	71.42681	726.08972	-253.19732	-179.64713	1
153	H	68.42347	66.97657	72.36870	1224.27271	-456.51798	-2390.90304	1
154	H	67.68765	68.13555	71.18078	1206.40339	-1150.93514	-2154.90344	1
155	N	68.64404	66.43778	70.31268	329.70796	-633.68968	-155.67358	1
156	H	67.78806	65.81592	70.23683	1348.31305	1938.76845	1359.00643	1
157	H	68.74507	66.77369	69.31083	2096.92035	1446.54551	-966.48890	1
158	H	69.42037	65.71721	70.38158	-1197.07217	-2303.53719	827.28733	1
159	C	71.15330	70.87012	75.03072	-378.01186	-556.17301	-413.96481	1
160	O	70.86480	71.66533	75.89249	-409.44433	-307.55053	-453.30833	1
161	N	71.47242	69.59170	75.16291	-429.02477	524.70884	274.08502	1
162	H	71.75188	68.95820	74.39888	1706.34263	-1425.96036	1574.38926	1
163	C	71.48292	69.01466	76.47717	-45.25864	-626.22952	478.93267	1
164	H	71.91623	69.76476	77.17765	1988.63164	570.90773	1772.87287	1
165	C	69.97469	68.66479	76.83108	551.77128	-20.49526	-564.54996	1
166	H	69.36737	69.59598	76.88419	1434.61535	-1753.10253	1513.99471	1
167	H	69.51484	68.05339	76.02325	-714.67738	1819.09770	1898.36494	1
168	C	69.94426	67.90223	78.19468	446.99263	-555.77305	338.97221	1
169	H	70.49406	66.93612	78.11750	1953.68466	1892.25957	-161.67766	1
170	H	70.45963	68.49042	78.98667	-403.03785	2688.07032	-188.43591	1
171	C	68.43120	67.65167	78.58372	567.86262	335.74681	434.04421	1
172	H	67.86779	68.61184	78.63053	-1080.02275	1568.26081	-1948.78900	1
173	H	67.91801	67.03502	77.81049	-919.54108	2111.34692	1456.13463	1
174	C	68.41950	66.93934	79.95603	195.81897	173.33862	-745.11536	1
175	H	68.86517	65.92447	79.95324	1405.67949	-2301.21089	-390.08113	1
176	H	68.84248	67.53614	80.78871	-940.37328	-1118.32446	2299.72133	1
177	N	66.92245	66.71370	80.35573	319.26422	656.36007	-42.02424	1
178	H	66.76528	66.24402	81.29368	1961.03633	619.91968	1787.09422	1
179	H	66.31044	67.57605	80.44875	854.14343	-2156.80752	1429.08711	1
180	H	66.34103	66.09825	79.71568	1237.02905	-1378.50857	-1998.28500	1
181	C	72.37154	67.68505	76.19782	532.53319	-268.57236	517.55729	1
182	O	72.51558	67.31903	75.02202	266.16714	-290.73804	-558.88002	1
183	N	72.78783	67.15755	77.32038	-226.25352	640.49678	-270.32839	1
184	H	72.53492	67.68243	78.15869	2007.69063	-1035.27229	1523.50231	1
185	C	73.50181	65.94407	77.46029	-540.76542	-573.33303	49.50000	1
186	H	73.47317	65.74477	78.55438	-2374.20950	-1036.76023	843.75774	1
187	C	72.75376	64.81807	76.60109	-77.09082	666.87422	-415.84136	1
188	H	72.66534	65.17220	75.53494	-985.81834	617.19825	2463.91927	1

189	O	71.41353	64.51840	77.03294	293.29899	-391.65602	-477.80926	1
190	H	70.89809	64.81818	76.25704	2528.72714	-681.76262	-751.27122	1
191	C	73.78450	63.63276	76.65768	252.47363	-605.14473	440.05134	1
192	H	73.44299	62.76464	76.04718	-2052.65063	1456.49051	-1043.51830	1
193	H	74.78697	63.93412	76.26964	-2152.98800	-1661.97574	-161.70652	1
194	H	73.92897	63.26752	77.70123	-473.12726	-1584.27339	2165.61725	1
195	C	75.04477	66.15519	76.94315	360.36307	488.46713	505.10056	1
196	O	75.95960	65.80969	77.64863	-200.08817	-528.03552	-385.82850	1
197	N	75.06847	66.59390	75.68870	-597.54095	-226.44775	355.20479	1
198	H	74.17150	66.83977	75.20460	2179.23655	-1300.70981	-991.33835	1
199	C	76.30126	67.13437	75.22935	-687.68921	297.39807	-249.45179	1
200	H	77.07381	66.61633	75.84344	-349.16256	-2467.37713	-1101.72831	1
201	C	76.37727	66.82224	73.66040	672.47345	361.54328	-201.62880	1
202	H	75.56095	67.35299	73.11965	1541.41502	582.18425	2169.97026	1
203	H	77.34154	67.18101	73.23290	-2534.67717	60.25153	997.72295	1
204	C	76.23295	65.30163	73.51061	574.26774	-389.43119	-377.02542	1
205	C	77.36677	64.46048	73.72081	688.82679	-287.33580	-257.96133	1
206	H	78.35884	64.89483	73.94089	331.14182	1470.38163	2269.80013	1
207	C	74.95034	64.73198	73.24607	-383.52382	-675.04808	144.24917	1
208	H	74.06711	65.38034	73.10211	4.09847	1517.59662	2262.86397	1
209	C	77.19218	63.07827	73.65904	-134.76730	428.45285	-649.50303	1
210	H	78.06825	62.42735	73.82531	-903.23433	1600.49020	2011.53387	1
211	C	74.82698	63.34168	73.19280	-335.53281	-615.00040	-364.39058	1
212	H	73.83016	62.91287	72.98962	1596.45398	-1369.33862	1732.02659	1
213	C	75.93307	62.46522	73.39507	585.48547	-340.24194	-406.23938	1
214	O	75.81806	61.05136	73.34772	-419.15649	-173.04408	-511.94141	1
215	H	74.85975	60.96953	73.12959	-1071.84350	1559.71507	-1960.13012	1
216	C	76.25719	68.74428	75.49734	291.41878	-183.13091	710.72246	1
217	O	75.36722	69.30351	76.09693	379.87695	523.47396	-222.23622	1
218	N	77.37556	69.27021	75.01392	564.30591	373.09380	277.24371	1
219	H	78.05277	68.66930	74.54901	-120.59931	-2436.07824	-1214.35098	1
220	C	77.54468	70.69390	75.05255	404.07514	-299.37480	608.84009	1
221	H	76.56383	71.07988	74.64412	-1071.07882	-841.69025	2359.66467	1
222	C	77.69123	71.11260	76.56880	-683.12807	68.71770	-390.13096	1
223	H	76.88782	70.62167	77.16700	2068.88918	1596.58590	770.89603	1
224	H	78.64928	70.75172	77.00715	1379.86429	2342.49779	-179.85638	1
225	C	77.56209	72.66721	76.65065	-176.39967	537.49466	550.97268	1
226	H	78.48619	73.18435	76.30863	-396.28051	1942.22168	1869.33314	1
227	H	76.75143	73.02915	75.96769	-94.44700	586.00678	-2659.20016	1
228	C	77.23322	73.00213	78.17610	-291.69381	-718.18079	-150.72929	1
229	H	76.29250	72.54290	78.57457	-2303.38776	1089.76242	964.62032	1
230	H	78.05172	72.76925	78.90364	884.16729	2568.80533	-207.74283	1
231	N	77.04945	74.38507	78.17242	-594.49522	-252.81478	342.29276	1
232	H	77.18591	74.85787	77.26957	-1735.17426	2084.05705	-263.71605	1
233	C	76.72019	75.04164	79.21211	595.23177	-271.52487	442.22352	1
234	N	76.54134	74.34170	80.40592	585.53813	-424.79750	-105.81303	1
235	H	76.64409	73.34425	80.59384	959.88797	1327.56823	-2177.11905	1
236	H	76.28626	74.76267	81.30089	1578.48647	16.27378	-2220.76233	1
237	N	76.60328	76.39894	78.89424	-452.17763	-390.33541	-421.51853	1
238	H	76.72131	76.85536	77.98863	470.26107	1974.25629	-1817.92087	1
239	H	76.34696	77.12802	79.56196	1856.67307	-1573.97321	-1224.35416	1
240	C	78.81869	71.01049	74.08508	-531.47271	-581.45780	-55.06206	1
241	O	78.78567	70.67981	72.92110	-243.00837	192.73507	609.52485	1
242	N	79.76503	71.69286	74.72477	343.49288	-644.25607	38.09164	1
243	H	79.66553	71.88952	75.71836	-1691.16043	-1535.97525	-1484.73099	1
244	C	81.02797	71.85477	74.09005	542.66492	350.14337	454.42563	1
245	H	80.93050	71.25994	73.15201	1209.57979	-2396.95920	463.86744	1
246	C	81.20974	73.40961	73.81762	-737.14309	145.93010	242.71942	1
247	H	81.22141	73.98111	74.77092	-1050.18303	159.36419	-2509.06125	1
248	C	82.54158	73.60389	73.01706	-706.77696	-252.88343	-245.16230	1
249	H	82.77819	74.68379	72.86696	-1624.64039	-1665.49085	1417.86935	1
250	H	83.42240	73.13173	73.54796	2566.10521	598.51109	693.22305	1

251	H	82.48071	73.13429	72.00690	-1972.69758	107.10018	-1876.34312	1
252	C	80.02020	73.90001	72.92209	412.85148	672.58832	-27.69222	1
253	H	80.10750	74.98335	72.67223	1447.02277	1762.76533	-1490.78944	1
254	H	79.97323	73.33555	71.96133	1320.77379	-145.20455	2378.68491	1
255	H	79.04102	73.75238	73.43662	-1512.10848	1470.52031	1724.75147	1
256	C	82.11334	71.23372	75.15962	-607.11113	499.56689	73.73769	1
257	O	82.18401	70.03115	75.26567	357.97126	460.81534	356.68785	1
258	N	82.71541	72.17476	75.87572	536.55407	-368.62270	332.76306	1
259	H	82.49694	73.14641	75.66017	524.38866	2297.69985	1367.20941	1
260	C	83.94346	71.88786	76.54214	46.50277	-774.29190	-147.97904	1
261	H	84.14539	72.82114	77.11253	1676.51875	1883.29066	1032.55549	1
262	C	83.74659	70.60515	77.50167	-559.41456	-34.19198	-556.30433	1
263	H	83.51447	69.70731	76.86907	-64.66664	395.18769	2695.05373	1
264	H	84.68241	70.36381	78.05987	-2703.44278	-60.40056	333.79418	1
265	C	82.61480	70.87860	78.45424	-519.76435	377.31045	459.42366	1
266	H	81.76342	71.29270	77.86736	-1746.74323	1667.50644	-1261.73691	1
267	C	82.15604	69.58714	79.12066	570.95554	16.46261	-545.27700	1
268	H	81.29958	69.76361	79.82110	2391.58273	28.05277	-1305.07271	1
269	H	81.81811	68.83132	78.36530	175.75588	917.63458	2559.43867	1
270	H	82.97958	69.11591	79.71649	-1063.97851	-2155.34650	1283.00462	1
271	C	83.01655	71.88891	79.52066	193.76014	2.62946	-765.53141	1
272	H	82.17738	72.09231	80.23458	507.39394	-846.55087	2539.60089	1
273	H	83.88533	71.52425	80.12691	1337.57841	1818.19054	1526.01994	1
274	H	83.31442	72.87095	79.07202	1100.88635	-1172.91350	-2199.08909	1
275	C	85.05648	71.65320	75.41421	-549.21115	475.64486	-309.38218	1
276	O	84.98742	72.16607	74.32059	556.06106	-390.37755	-78.24250	1
277	O	86.22309	70.95145	75.79182	-572.27940	-310.19032	-209.75862	1
278	H	85.97118	70.72135	76.72669	-1380.08193	2212.14486	790.85944	1

Listing 107: C00107.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.7945	3178
		0.2500	300.00	0.00	0.00	0.00	-1293.4053	0.0000	300.0000
3	H	73.71269	86.56676	77.05086	-2043.14101	-1757.64893	399.89339		1
4	N	74.17203	87.13851	77.77890	426.75047	490.45733	-334.42467		1
5	H	74.49890	86.46919	78.49537	442.25559	-1110.30854	-2448.52907		1
6	C	75.22354	87.97304	77.35375	415.32972	-666.39213	83.73172		1
7	H	75.17555	88.07182	76.24761	879.32219	2491.00447	667.35213		1
8	C	75.12021	89.38181	78.13417	31.35357	477.41777	628.23362		1
9	H	75.10777	89.18567	79.23299	1168.38489	2240.25337	-1019.71136		1
10	H	76.02953	90.00087	77.94192	-360.43770	2534.90498	931.67112		1
11	C	73.87387	90.11931	77.72018	463.18208	512.70242	-382.34388		1
12	H	73.00872	89.42463	77.81503	1725.29117	1863.52247	-987.07854		1
13	C	73.64193	91.31437	78.63665	710.42801	-144.27427	-313.15367		1
14	H	72.70781	91.87047	78.36519	364.20195	-1033.13725	2494.72524		1
15	H	73.54342	91.00229	79.70848	2567.61904	335.80679	847.48802		1
16	H	74.48981	92.04509	78.58212	-2587.99029	680.92867	-512.16411		1
17	C	73.96787	90.59431	76.27664	268.17616	741.64379	-40.42634		1
18	H	73.06496	91.18656	75.97701	1283.54314	-1945.37420	-1411.27812		1
19	H	74.86257	91.25017	76.11741	-1258.57796	1317.15249	-2026.02085		1
20	H	74.05327	89.73560	75.56217	-2502.84526	909.80597	575.92391		1
21	C	76.52784	87.19185	77.93080	619.36578	-458.64843	-172.09273		1
22	O	76.37697	86.32202	78.78829	-81.40433	433.87611	522.34594		1
23	N	77.60955	87.71209	77.39844	175.23996	-622.20190	341.55523		1
24	H	77.42905	88.43579	76.70187	-876.57256	-303.22879	-2561.90213		1
25	C	78.96069	87.45381	77.76419	-571.88214	-534.10783	-106.15033		1
26	H	79.45676	88.37486	77.38477	-2713.20841	-16.25800	-248.80809		1
27	C	79.08637	87.34695	79.35487	166.60354	288.16399	-716.09568		1
28	H	78.43886	86.50536	79.72980	-2097.85574	1636.78449	-586.18044		1
29	O	78.63040	88.50005	80.09185	-317.80580	-363.38227	484.43082		1
30	H	77.83704	88.13136	80.52881	1863.74748	-1451.84923	1357.29467		1

31	C	80.60836	86.99242	79.52513	503.80731	517.99032	318.51606	1
32	H	80.85134	86.73452	80.58197	640.61020	-2157.10410	-1536.29104	1
33	H	80.91380	86.12809	78.89021	1687.88455	465.60692	2087.56452	1
34	H	81.25690	87.85299	79.23987	-1293.07895	-1899.88581	-1463.57452	1
35	C	79.52010	86.27153	76.79171	-153.07550	-733.68902	248.70981	1
36	O	79.94285	86.67247	75.71423	186.15459	-480.78787	-449.34387	1
37	N	79.48202	85.02042	77.24587	-487.53139	543.18517	42.03850	1
38	C	80.05466	83.93910	76.48929	-699.35871	69.34393	360.10701	1
39	H	81.04948	84.29512	76.13640	2.81126	-221.99807	-2715.58072	1
40	C	80.04267	82.73585	77.52036	-507.46439	-592.59194	122.07761	1
41	H	80.08616	81.74237	77.01862	-1975.08116	525.87560	-1801.71556	1
42	H	80.89685	82.78250	78.23276	1588.27743	-1913.22100	1113.83566	1
43	C	78.67906	83.00568	78.23114	-613.62442	-457.55993	-194.14490	1
44	H	77.83145	82.73179	77.56258	1707.54637	-721.27992	1996.92523	1
45	H	78.54376	82.44162	79.18108	758.23357	2100.81767	1560.55011	1
46	C	78.77616	84.57746	78.43946	-352.41524	704.96076	49.21465	1
47	H	77.78865	85.14202	78.47258	1714.76886	-2070.42778	443.35792	1
48	H	79.40612	84.87199	79.31131	1224.15040	1801.50881	1636.97633	1
49	C	79.03744	83.53203	75.26524	566.85117	537.05831	117.62814	1
50	O	78.55288	82.42832	75.27465	-550.26779	-406.08867	4.21666	1
51	N	78.99845	84.49981	74.36441	566.34832	-425.77725	180.18749	1
52	H	79.52135	85.38355	74.57075	644.44502	2646.80550	-52.73430	1
53	C	77.96803	84.56035	73.38184	612.34801	-281.48662	411.56221	1
54	H	78.35039	85.30078	72.64508	1667.23498	-1490.75142	1556.16753	1
55	C	77.78744	83.10695	72.75134	-714.45746	-175.43074	286.98927	1
56	H	77.33488	82.44033	73.54197	-787.09484	1763.03619	-1922.46060	1
57	O	79.02959	82.48080	72.34194	-429.46514	516.51932	-128.40526	1
58	H	79.21814	81.95338	73.14556	1981.82785	436.16847	-1818.18182	1
59	C	76.74752	83.26887	71.58515	630.79189	-468.94448	76.03230	1
60	H	76.56828	82.29652	71.07037	-1775.71861	2062.30353	131.89849	1
61	H	75.75672	83.63329	71.94319	-1855.14608	88.94118	1993.53760	1
62	H	77.11076	83.98486	70.81174	-1504.82350	-780.94249	-2132.90992	1
63	C	76.63190	85.11731	74.13474	288.57638	618.62814	-397.00270	1
64	O	76.49913	85.12415	75.34476	321.70495	-185.26452	574.37218	1
65	N	75.75311	85.48438	73.22128	-447.05792	-446.53431	367.76425	1
66	H	76.01610	85.44861	72.24004	350.31316	1975.63644	-1843.31522	1
67	C	74.44908	85.92461	73.63675	-511.23061	374.03917	-471.51480	1
68	H	74.58487	86.96741	73.99727	2234.79579	-898.70890	-1273.45190	1
69	C	73.51330	85.79436	72.35411	529.53781	-159.34528	563.72604	1
70	H	72.51495	86.21346	72.64500	654.59388	2347.94251	1217.51488	1
71	H	73.91733	86.45568	71.54181	-1526.55661	2103.42026	817.87394	1
72	O	73.37739	84.45364	71.79140	-554.84278	14.12789	399.58769	1
73	H	72.84861	84.02961	72.49458	1297.06236	2061.84854	1220.68812	1
74	C	73.85350	84.94467	74.78713	-662.15484	-412.13544	123.62687	1
75	O	73.18559	85.41198	75.70445	-540.01537	-317.05804	274.91456	1
76	N	74.06505	83.68267	74.45140	-202.76299	-690.00100	-131.49145	1
77	H	74.63285	83.63171	73.60223	-702.62132	-2617.37191	281.70413	1
78	C	73.89275	82.51273	75.28707	-491.73914	576.34187	222.73509	1
79	H	74.84459	81.94192	75.16487	1977.17978	-1823.58850	-434.68928	1
80	C	73.62660	82.91033	76.72709	-649.50797	-328.66843	306.11224	1
81	H	72.84359	83.71619	76.72800	2075.07803	1452.16490	-1004.45904	1
82	C	73.11103	81.74379	77.54931	-615.18735	-489.99689	-70.96352	1
83	H	72.89920	82.04468	78.61200	-1226.32661	-1724.38906	-1716.47170	1
84	H	72.15655	81.32756	77.12276	2381.64273	-969.84735	900.46860	1
85	H	73.85308	80.89939	77.58383	2122.74991	1702.23946	-141.36228	1
86	C	74.88182	83.47574	77.36312	-501.86074	-479.61276	-376.42482	1
87	H	74.66923	83.97370	78.34854	993.79261	-2246.95401	-1177.81305	1
88	H	75.64285	82.67046	77.55262	42.71279	-626.15391	-2651.37258	1
89	H	75.37998	84.25131	76.68064	-2026.39012	-1590.33709	-887.82922	1
90	C	72.62285	81.68042	74.56332	-672.89153	382.57394	-156.34072	1
91	O	71.70847	82.21856	73.98240	410.04627	221.86223	500.35950	1
92	N	72.87497	80.39311	74.71811	-378.11782	-443.79414	-441.10984	1

93	H	73.68625	80.25905	75.31519	2404.15973	-568.14894	1149.30085	1
94	C	71.89527	79.35188	74.54295	-544.54484	466.16019	331.29119	1
95	H	71.47479	79.20434	75.56162	-1409.80988	-170.17955	2325.32679	1
96	C	70.80587	79.83806	73.50715	-184.48284	116.78282	-758.89137	1
97	H	70.11425	80.57998	73.97305	1893.78641	1861.14652	611.04528	1
98	H	71.29003	80.39531	72.66971	-2170.79665	-974.19311	1327.50117	1
99	C	70.03783	78.57410	73.00194	389.51668	672.81878	-138.49152	1
100	H	70.75550	77.75501	72.77376	510.64577	1933.03327	1851.02484	1
101	H	69.40603	78.15403	73.81488	-2302.30869	-1105.72939	-948.89774	1
102	C	69.16374	78.85107	71.72227	-559.93427	-126.34590	542.30857	1
103	O	68.59990	77.93683	71.17710	-670.36003	-111.83166	76.36448	1
104	N	69.13561	80.14745	71.34295	-216.06729	-537.07037	446.51379	1
105	H	69.56180	80.97121	71.78361	-1251.96487	1074.12894	-2168.52500	1
106	H	68.59566	80.49755	70.54437	-2451.83023	-720.73851	944.84612	1
107	C	72.78310	78.05481	74.14905	546.24052	-563.88337	-85.11809	1
108	O	73.06817	77.31993	75.08589	71.70702	-307.40463	606.69673	1
109	N	73.17215	77.97739	72.88275	479.90863	-504.50129	222.86849	1
110	C	73.72051	76.76709	72.31947	75.51268	-600.91904	506.73700	1
111	H	73.09191	75.93127	72.70692	-2033.61562	1795.30103	254.89480	1
112	C	73.65417	77.05185	70.75449	523.79067	517.99274	284.45581	1
113	H	74.38421	76.43454	70.18225	1599.61665	-1127.00911	1895.98173	1
114	H	72.64490	76.84158	70.33499	-1881.83093	1275.82488	-1501.55016	1
115	C	73.98371	78.57596	70.71947	-600.05639	-404.05026	316.64485	1
116	H	75.07057	78.75193	70.88487	-2597.05260	496.36221	657.73249	1
117	H	73.72092	79.06985	69.75693	-1666.24518	1294.38985	-1723.90591	1
118	C	73.11320	79.09129	71.94655	493.57570	-129.95376	-602.56394	1
119	H	73.49232	80.00273	72.46726	-1469.08415	-637.84797	2204.22581	1
120	H	72.03441	79.22702	71.69381	-1038.97840	1068.88701	-2280.71789	1
121	C	75.28909	76.61497	72.67808	188.88100	241.05089	-727.87821	1
122	O	76.09095	76.46346	71.77764	531.88613	-49.19943	427.07960	1
123	N	75.50027	76.63462	73.98857	708.14833	26.93417	-179.73509	1
124	H	74.66567	76.73650	74.61519	-2232.69501	-1179.09831	1023.94816	1
125	C	76.84207	77.01011	74.47860	-738.32412	259.92548	104.42456	1
126	H	77.20933	77.65411	73.64569	2028.89123	1260.02983	1311.33324	1
127	C	76.71362	77.72210	75.80687	-258.65678	-345.52513	661.28459	1
128	H	76.22850	77.01951	76.52200	-1826.06090	-1801.46097	-918.64554	1
129	C	78.06689	78.11495	76.37278	-541.23400	531.92970	-218.41428	1
130	H	77.96768	78.63086	77.36729	1311.73218	-2219.18200	882.19023	1
131	H	78.72676	77.21415	76.52700	-1048.71298	1223.58118	-2196.97971	1
132	H	78.61463	78.81855	75.68671	419.06414	1903.92898	1903.44670	1
133	C	75.83848	78.95958	75.70652	-423.86431	152.66566	-648.55262	1
134	H	75.69213	79.45171	76.70718	105.68386	-2342.50080	1387.51238	1
135	H	76.28512	79.72939	75.01843	-1695.63603	-1484.73621	-1531.02793	1
136	H	74.81939	78.70395	75.30346	-1853.57121	-487.39031	1936.59343	1
137	C	77.70942	75.60247	74.58322	539.71428	-510.58232	267.58633	1
138	O	78.16153	75.23326	75.63622	-15.93758	-278.34085	-624.49402	1
139	N	77.88829	75.12122	73.36846	-676.81886	12.05292	276.17960	1
140	H	77.43047	75.61611	72.56919	-1694.44250	-373.84189	-2100.66098	1
141	C	78.30340	73.77116	73.16211	412.33078	-664.70360	108.35451	1
142	H	78.68631	73.79794	72.11752	1765.77476	1294.44366	1621.76594	1
143	C	79.37682	73.36309	74.24724	-179.66635	-721.95667	-264.73915	1
144	H	80.14992	74.15732	74.35543	-607.34922	2587.87032	-598.10018	1
145	H	78.90559	73.25549	75.25626	-359.69332	-1479.13954	-2259.74260	1
146	C	80.00406	72.00710	73.77509	-240.01076	616.02425	431.85322	1
147	H	79.25042	71.18483	73.82243	-1359.17131	782.54425	2227.99181	1
148	H	80.32879	72.06753	72.71235	-820.36667	85.81767	-2596.78715	1
149	C	81.23660	71.69379	74.71384	-513.07015	236.18570	-551.87280	1
150	H	82.01903	72.48279	74.62947	1816.11944	-1183.11722	-1650.94321	1
151	H	80.92960	71.68004	75.78506	-1800.04429	-1361.53473	1526.34643	1
152	C	81.78167	70.31267	74.27954	726.08972	-253.19732	-179.64713	1
153	H	81.11347	69.45989	74.52380	1224.27271	-456.51798	-2390.90304	1
154	H	82.09824	70.25528	73.21882	1206.40339	-1150.93514	-2154.90344	1

155	N	83.08987	70.04111	75.09262	329.70796	-633.68968	-155.67358	1
156	H	83.58768	69.13175	74.86765	1348.31305	1938.76845	1359.00643	1
157	H	83.88009	70.74237	74.98832	2096.92035	1446.54551	-966.48890	1
158	H	82.99496	69.97081	76.14742	-1197.07217	-2303.53719	827.28733	1
159	C	77.01132	72.77327	73.31333	-378.01186	-556.17301	-413.96481	1
160	O	76.54930	72.40691	74.38561	-409.44433	-307.55053	-453.30833	1
161	N	76.60358	72.45299	72.10220	-429.02477	524.70884	274.08502	1
162	H	77.11806	72.80845	71.29912	1706.34263	-1425.96036	1574.38926	1
163	C	75.66009	71.37764	72.01453	-45.25864	-626.22952	478.93267	1
164	H	74.95807	71.61536	72.84714	1988.63164	570.90773	1772.87287	1
165	C	75.03544	71.36466	70.56540	551.77128	-20.49526	-564.54996	1
166	H	74.57062	72.34571	70.31752	1434.61535	-1753.10253	1513.99471	1
167	H	75.82387	71.19882	69.79690	-714.67738	1819.09770	1898.36494	1
168	C	73.97899	70.20845	70.53933	446.99263	-555.77305	338.97221	1
169	H	74.45157	69.24185	70.83248	1953.68466	1892.25957	-161.67766	1
170	H	73.17234	70.39850	71.28191	-403.03785	2688.07032	-188.43591	1
171	C	73.38917	70.11522	69.07655	567.86262	335.74681	434.04421	1
172	H	73.17508	71.12796	68.66370	-1080.02275	1568.26081	-1948.78900	1
173	H	74.13102	69.64793	68.37717	-919.54108	2111.34692	1456.13463	1
174	C	72.09528	69.26987	69.14343	195.81897	173.33862	-745.11536	1
175	H	72.22372	68.27117	69.60551	1405.67949	-2301.21089	-390.08113	1
176	H	71.22237	69.78312	69.59403	-940.37328	-1118.32446	2299.72133	1
177	N	71.68580	68.97579	67.66120	319.26422	656.36007	-42.02424	1
178	H	70.88734	68.29322	67.50676	1961.03633	619.91968	1787.09422	1
179	H	71.37255	69.80337	67.07600	854.14343	-2156.80752	1429.08711	1
180	H	72.44616	68.56071	67.04808	1237.02905	-1378.50857	-1998.28500	1
181	C	76.47397	69.97772	72.29352	532.53319	-268.57236	517.55729	1
182	O	76.82129	69.24953	71.39705	266.16714	-290.73804	-558.88002	1
183	N	76.67141	69.84618	73.60220	-226.25352	640.49678	-270.32839	1
184	H	76.37023	70.59679	74.25669	2007.69063	-1035.27229	1523.50231	1
185	C	77.11157	68.55582	74.03013	-540.76542	-573.33303	49.50000	1
186	H	77.75217	68.18853	73.19559	-2374.20950	-1036.76023	843.75774	1
187	C	77.85190	68.74274	75.43316	-77.09082	666.87422	-415.84136	1
188	H	77.14166	69.25231	76.14037	-985.81834	617.19825	2463.91927	1
189	O	79.04042	69.55951	75.41314	293.29899	-391.65602	-477.80926	1
190	H	78.75743	70.31027	75.97264	2528.72714	-681.76262	-751.27122	1
191	C	78.05715	67.25020	75.88371	252.47363	-605.14473	440.05134	1
192	H	78.47065	67.18819	76.91665	-2052.65063	1456.49051	-1043.51830	1
193	H	77.09874	66.67984	75.87439	-2152.98800	-1661.97574	-161.70652	1
194	H	78.76578	66.71593	75.20960	-473.12726	-1584.27339	2165.61725	1
195	C	75.78097	67.62721	74.25950	360.36307	488.46713	505.10056	1
196	O	74.91423	67.91359	75.07753	-200.08817	-528.03552	-385.82850	1
197	N	75.92145	66.53461	73.54039	-597.54095	-226.44775	355.20479	1
198	H	76.74394	66.49988	72.94130	2179.23655	-1300.70981	-991.33835	1
199	C	74.75794	65.76710	73.20702	-687.68921	297.39807	-249.45179	1
200	H	73.95806	66.52920	73.07845	-349.16256	-2467.37713	-1101.72831	1
201	C	75.08340	64.87462	71.92582	672.47345	361.54328	-201.62880	1
202	H	76.05318	64.34506	72.06991	1541.41502	582.18425	2169.97026	1
203	H	74.29872	64.09016	71.81408	-2534.67717	60.25153	997.72295	1
204	C	75.13368	65.77011	70.67706	574.26774	-389.43119	-377.02542	1
205	C	73.93636	65.99076	69.93386	688.82679	-287.33580	-257.96133	1
206	H	72.98300	65.52926	70.24862	331.14182	1470.38163	2269.80013	1
207	C	76.35760	66.37485	70.26279	-383.52382	-675.04808	144.24917	1
208	H	77.28844	66.21238	70.83503	4.09847	1517.59662	2262.86397	1
209	C	73.99709	66.79442	68.79386	-134.76730	428.45285	-649.50303	1
210	H	73.07318	66.94568	68.21046	-903.23433	1600.49020	2011.53387	1
211	C	76.36075	67.18745	69.12427	-335.53281	-615.00040	-364.39058	1
212	H	77.31263	67.66063	68.82550	1596.45398	-1369.33862	1732.02659	1
213	C	75.19118	67.42996	68.34936	585.48547	-340.24194	-406.23938	1
214	O	75.18445	68.26026	67.18800	-419.15649	-173.04408	-511.94141	1
215	H	76.13863	68.50364	67.16050	-1071.84350	1559.71507	-1960.13012	1
216	C	74.42827	64.71736	74.39651	291.41878	-183.13091	710.72246	1

217	O	74.41059	63.53206	74.16719	379.87695	523.47396	-222.23622	1
218	N	74.10037	65.35337	75.53363	564.30591	373.09380	277.24371	1
219	H	74.21994	66.39747	75.58544	-120.59931	-2436.07824	-1214.35098	1
220	C	74.20183	64.52791	76.71014	404.07514	-299.37480	608.84009	1
221	H	73.85489	63.53407	76.34170	-1071.07882	-841.69025	2359.66467	1
222	C	75.72428	64.45854	77.14735	-683.12807	68.71770	-390.13096	1
223	H	76.37213	64.18662	76.28359	2068.88918	1596.58590	770.89603	1
224	H	76.08798	65.44858	77.50285	1379.86429	2342.49779	-179.85638	1
225	C	75.79890	63.38647	78.27838	-176.39967	537.49466	550.97268	1
226	H	75.19143	63.72447	79.15962	-396.28051	1942.22168	1869.33314	1
227	H	75.32927	62.43576	77.93908	-94.44700	586.00678	-2659.20016	1
228	C	77.31444	63.12751	78.70827	-291.69381	-718.18079	-150.72929	1
229	H	77.95686	62.59863	77.95855	-2303.38776	1089.76242	964.62032	1
230	H	77.87867	64.01056	79.10301	884.16729	2568.80533	-207.74283	1
231	N	77.04687	62.25181	79.77743	-594.49522	-252.81478	342.29276	1
232	H	76.07757	62.02605	79.94676	-1735.17426	2084.05705	-263.71605	1
233	C	77.92411	61.73274	80.53896	595.23177	-271.52487	442.22352	1
234	N	79.26530	62.04437	80.30049	585.53813	-424.79750	-105.81303	1
235	H	79.66836	62.64389	79.58138	959.88797	1327.56823	-2177.11905	1
236	H	80.05577	61.69094	80.84088	1578.48647	16.27378	-2220.76233	1
237	N	77.31579	60.91651	81.50243	-452.17763	-390.33541	-421.51853	1
238	H	76.33285	60.70900	81.67320	470.26107	1974.25629	-1817.92087	1
239	H	77.83440	60.41267	82.22243	1856.67307	-1573.97321	-1224.35416	1
240	C	73.27803	65.14586	77.89213	-531.47271	-581.45780	-55.06206	1
241	O	73.50773	64.89487	79.05873	-243.00837	192.73507	609.52485	1
242	N	72.27212	65.86264	77.39645	343.49288	-644.25607	38.09164	1
243	H	72.19830	65.95271	76.38344	-1691.16043	-1535.97525	-1484.73099	1
244	C	71.19372	66.16756	78.27337	542.66492	350.14337	454.42563	1
245	H	71.45569	65.70956	79.25697	1209.57979	-2396.95920	463.86744	1
246	C	71.08550	67.75654	78.32145	-737.14309	145.93010	242.71942	1
247	H	71.22319	68.19163	77.30819	-1050.18303	159.36419	-2509.06125	1
248	C	69.70292	68.16527	78.93179	-706.77696	-252.88343	-245.16230	1
249	H	69.62135	69.26978	79.06489	-1624.64039	-1665.49085	1417.86935	1
250	H	68.85913	67.84607	78.27449	2566.10521	598.51109	693.22305	1
251	H	69.53857	67.69407	79.92988	-1972.69758	107.10018	-1876.34312	1
252	C	72.20692	68.24103	79.30178	412.85148	672.58832	-27.69222	1
253	H	72.25259	69.35348	79.36458	1447.02277	1762.76533	-1490.78944	1
254	H	72.04007	67.85426	80.33491	1320.77379	-145.20455	2378.68491	1
255	H	73.21074	67.88022	78.97345	-1512.10848	1470.52031	1724.75147	1
256	C	69.82232	65.58213	77.59041	-607.11113	499.56689	73.73769	1
257	O	69.44040	65.91573	76.48808	357.97126	460.81534	356.68785	1
258	N	69.25922	64.76063	78.46275	536.55407	-368.62270	332.76306	1
259	H	69.69600	64.61053	79.37271	524.38866	2297.69985	1367.20941	1
260	C	67.90316	64.39244	78.27114	46.50277	-774.29190	-147.97904	1
261	H	67.55233	65.04141	77.43552	1676.51875	1883.29066	1032.55549	1
262	C	67.80811	62.81677	77.91742	-559.41456	-34.19198	-556.30433	1
263	H	68.15741	62.22034	78.79298	-64.66664	395.18769	2695.05373	1
264	H	66.74418	62.52305	77.75610	-2703.44278	-60.40056	333.79418	1
265	C	68.63471	62.49074	76.70454	-519.76435	377.31045	459.42366	1
266	H	69.70055	62.71937	76.93498	-1746.74323	1667.50644	-1261.73691	1
267	C	68.51289	61.00965	76.36468	570.95554	16.46261	-545.27700	1
268	H	69.14166	60.73579	75.47881	2391.58273	28.05277	-1305.07271	1
269	H	68.83886	60.36048	77.21739	175.75588	917.63458	2559.43867	1
270	H	67.45642	60.72913	76.11969	-1063.97851	-2155.34650	1283.00462	1
271	C	68.22161	63.32616	75.50258	193.76014	2.62946	-765.53141	1
272	H	68.71066	62.96782	74.56014	507.39394	-846.55087	2539.60089	1
273	H	67.11412	63.29844	75.33420	1337.57841	1818.19054	1526.01994	1
274	H	68.52665	64.41517	75.64696	1100.88635	-1172.91350	-2199.08909	1
275	C	67.16994	64.62532	79.68657	-549.21115	475.64486	-309.38218	1
276	O	67.73810	65.04626	80.66073	556.06106	-390.37755	-78.24250	1
277	O	65.79406	64.29643	79.74314	-572.27940	-310.19032	-209.75862	1
278	H	65.66448	64.01489	78.79645	-1380.08193	2212.14486	790.85944	1

Listing 108: C00108.xmolout

1	276								
2	150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.9140	3656	
	0.2500	300.00	0.00	0.00	0.00	-1293.4041	0.0000	300.0000	
3	H	63.95723	67.35718	74.02234	-2043.14101	-1757.64893	399.89339	1	
4	N	64.64856	67.60708	74.72660	426.75047	490.45733	-334.42467	1	
5	H	64.99886	66.69235	75.00538	442.25559	-1110.30854	-2448.52907	1	
6	C	65.64527	68.49083	74.25474	415.32972	-666.39213	83.73172	1	
7	H	65.07140	69.22189	73.64747	879.32219	2491.00447	667.35213	1	
8	C	66.38859	69.15710	75.51658	31.35357	477.41777	628.23362	1	
9	H	66.82630	68.35506	76.15900	1168.38489	2240.25337	-1019.71136	1	
10	H	67.24748	69.78252	75.17066	-360.43770	2534.90498	931.67112	1	
11	C	65.41784	69.98225	76.32374	463.18208	512.70242	-382.34388	1	
12	H	64.53578	69.34593	76.56208	1725.29117	1863.52247	-987.07854	1	
13	C	66.06952	70.42310	77.62867	710.42801	-144.27427	-313.15367	1	
14	H	65.36003	71.00835	78.26882	364.20195	-1033.13725	2494.72524	1	
15	H	66.41978	69.54772	78.23446	2567.61904	335.80679	847.48802	1	
16	H	66.96161	71.07531	77.44258	-2587.99029	680.92867	-512.16411	1	
17	C	64.94139	71.20679	75.55562	268.17616	741.64379	-40.42634	1	
18	H	64.26113	71.84471	76.17753	1283.54314	-1945.37420	-1411.27812	1	
19	H	65.79953	71.85244	75.23483	-1258.57796	1317.15249	-2026.02085	1	
20	H	64.37442	70.92396	74.63154	-2502.84526	909.80597	575.92391	1	
21	C	66.65017	67.59654	73.33121	619.36578	-458.64843	-172.09273	1	
22	O	66.36448	67.29553	72.18664	-81.40433	433.87611	522.34594	1	
23	N	67.73293	67.24805	74.01045	175.23996	-622.20190	341.55523	1	
24	H	67.85477	67.51451	74.98506	-876.57256	-303.22879	-2561.90213	1	
25	C	68.77247	66.60461	73.27096	-571.88214	-534.10783	-106.15033	1	
26	H	68.62840	66.97909	72.23257	-2713.20841	-16.25800	-248.80809	1	
27	C	70.16529	66.96319	73.96627	166.60354	288.16399	-716.09568	1	
28	H	70.22020	66.41402	74.94871	-2097.85574	1636.78449	-586.18044	1	
29	O	70.37781	68.35413	74.28007	-317.80580	-363.38227	484.43082	1	
30	H	70.64037	68.28442	75.22161	1863.74748	-1451.84923	1357.29467	1	
31	C	71.18757	66.30589	72.96679	503.80731	517.99032	318.51606	1	
32	H	72.20965	66.26097	73.41589	640.61020	-2157.10410	-1536.29104	1	
33	H	70.89716	65.26348	72.69836	1687.88455	465.60692	2087.56452	1	
34	H	71.26071	66.88425	72.01688	-1293.07895	-1899.88581	-1463.57452	1	
35	C	68.54495	64.99277	73.44874	-153.07550	-733.68902	248.70981	1	
36	O	68.70838	64.48987	74.53824	186.15459	-480.78787	-449.34387	1	
37	N	68.26500	64.41061	72.27796	-487.53139	543.18517	42.03850	1	
38	C	67.79144	63.05993	72.18824	-699.35871	69.34393	360.10701	1	
39	H	67.10837	62.92198	73.05709	2.81126	-221.99807	-2715.58072	1	
40	C	67.09508	63.00828	70.76706	-507.46439	-592.59194	122.07761	1	
41	H	67.09566	61.98359	70.32979	-1975.08116	525.87560	-1801.71556	1	
42	H	66.03139	63.33184	70.82095	1588.27743	-1913.22100	1113.83566	1	
43	C	67.95250	64.02479	69.94777	-613.62442	-457.55993	-194.14490	1	
44	H	68.90964	63.56161	69.61755	1707.54637	-721.27992	1996.92523	1	
45	H	67.44629	64.39941	69.02953	758.23357	2100.81767	1560.55011	1	
46	C	68.20630	65.15901	71.02884	-352.41524	704.96076	49.21465	1	
47	H	69.16385	65.71847	70.90585	1714.76886	-2070.42778	443.35792	1	
48	H	67.35460	65.89198	71.17647	1224.15040	1801.50881	1636.97633	1	
49	C	69.03938	62.00184	72.23250	566.85117	537.05831	117.62814	1	
50	O	68.94241	60.92503	71.69577	-550.26779	-406.08867	4.21666	1	
51	N	70.03734	62.48963	72.96395	566.34832	-425.77725	180.18749	1	
52	H	69.89443	63.40090	73.42520	644.44502	2646.80550	-52.73430	1	
53	C	71.19328	61.69387	73.14619	612.34801	-281.48662	411.56221	1	
54	H	70.90833	60.67293	72.79988	1667.23498	-1490.75142	1556.16753	1	
55	C	72.39502	62.34623	72.30569	-714.45746	-175.43074	286.98927	1	
56	H	72.57877	63.38975	72.68450	-787.09484	1763.03619	-1922.46060	1	
57	O	72.19468	62.48137	70.89119	-429.46514	516.51932	-128.40526	1	

58	H	72.24276	63.45373	70.78265	1981.82785	436.16847	-1818.18182	1
59	C	73.57746	61.41397	72.75948	630.79189	-468.94448	76.03230	1
60	H	74.56070	61.79055	72.39324	-1775.71861	2062.30353	131.89849	1
61	H	73.63951	61.34344	73.87450	-1855.14608	88.94118	1993.53760	1
62	H	73.45139	60.37743	72.36824	-1504.82350	-780.94249	-2132.90992	1
63	C	71.65494	61.82098	74.72160	288.57638	618.62814	-397.00270	1
64	O	71.96557	60.83463	75.34651	321.70495	-185.26452	574.37218	1
65	N	71.72995	63.09272	75.07642	-447.05792	-446.53431	367.76425	1
66	H	71.49091	63.82367	74.41034	350.31316	1975.63644	-1843.31522	1
67	C	72.22336	63.43943	76.36954	-511.23061	374.03917	-471.51480	1
68	H	71.64540	62.81605	77.08698	2234.79579	-898.70890	-1273.45190	1
69	C	73.76585	63.00662	76.39010	529.53781	-159.34528	563.72604	1
70	H	74.13383	63.19638	77.43256	654.59388	2347.94251	1217.51488	1
71	H	73.78809	61.89045	76.22756	-1526.55661	2103.42026	817.87394	1
72	O	74.64270	63.58246	75.38862	-554.84278	14.12789	399.58769	1
73	H	74.82329	64.44766	75.80138	1297.06236	2061.84854	1220.68812	1
74	C	71.98445	65.04243	76.51296	-662.15484	-412.13544	123.62687	1
75	O	72.30922	65.83268	75.65952	-540.01537	-317.05804	274.91456	1
76	N	71.44312	65.28517	77.71096	-202.76299	-690.00100	-131.49145	1
77	H	71.27173	64.47259	78.30354	-702.62132	-2617.37191	281.70413	1
78	C	70.94795	66.61328	78.06859	-491.73914	576.34187	222.73509	1
79	H	70.43353	66.99974	77.15863	1977.17978	-1823.58850	-434.68928	1
80	C	70.04858	66.45425	79.27573	-649.50797	-328.66843	306.11224	1
81	H	70.61792	65.89180	80.04964	2075.07803	1452.16490	-1004.45904	1
82	C	69.65201	67.79616	79.86545	-615.18735	-489.99689	-70.96352	1
83	H	69.03262	67.67425	80.79624	-1226.32661	-1724.38906	-1716.47170	1
84	H	70.55454	68.40871	80.14178	2381.64273	-969.84735	900.46860	1
85	H	69.04634	68.40534	79.13950	2122.74991	1702.23946	-141.36228	1
86	C	68.79913	65.65500	78.94854	-501.86074	-479.61276	-376.42482	1
87	H	68.17087	65.47124	79.86308	993.79261	-2246.95401	-1177.81305	1
88	H	68.15102	66.19023	78.20129	42.71279	-626.15391	-2651.37258	1
89	H	69.05045	64.65214	78.50612	-2026.39012	-1590.33709	-887.82922	1
90	C	72.28916	67.52924	78.46198	-672.89153	382.57394	-156.34072	1
91	O	73.21561	67.06764	79.08910	410.04627	221.86223	500.35950	1
92	N	72.05691	68.78162	78.11557	-378.11782	-443.79414	-441.10984	1
93	H	71.13862	68.92283	77.70144	2404.15973	-568.14894	1149.30085	1
94	C	73.03029	69.81357	78.20336	-544.54484	466.16019	331.29119	1
95	H	72.42459	70.74722	78.19145	-1409.80988	-170.17955	2325.32679	1
96	C	73.90015	69.56893	79.50846	-184.48284	116.78282	-758.89137	1
97	H	73.24106	69.34108	80.37761	1893.78641	1861.14652	611.04528	1
98	H	74.55701	68.66903	79.36913	-2170.79665	-974.19311	1327.50117	1
99	C	74.77039	70.83909	79.77050	389.51668	672.81878	-138.49152	1
100	H	75.48834	70.97681	78.92831	510.64577	1933.03327	1851.02484	1
101	H	74.14094	71.75544	79.74910	-2302.30869	-1105.72939	-948.89774	1
102	C	75.55323	70.77156	81.13607	-559.93427	-126.34590	542.30857	1
103	O	76.19280	71.72507	81.49968	-670.36003	-111.83166	76.36448	1
104	N	75.42087	69.59823	81.79226	-216.06729	-537.07037	446.51379	1
105	H	74.92984	68.74063	81.51307	-1251.96487	1074.12894	-2168.52500	1
106	H	75.89538	69.37969	82.67472	-2451.83023	-720.73851	944.84612	1
107	C	74.09859	69.72552	76.96953	546.24052	-563.88337	-85.11809	1
108	O	75.23577	69.44637	77.24894	71.70702	-307.40463	606.69673	1
109	N	73.57373	70.06511	75.78244	479.90863	-504.50129	222.86849	1
110	C	74.26173	69.77791	74.56526	75.51268	-600.91904	506.73700	1
111	H	74.90329	68.88697	74.75544	-2033.61562	1795.30103	254.89480	1
112	C	73.03839	69.55723	73.57729	523.79067	517.99274	284.45581	1
113	H	73.32439	69.63949	72.50454	1599.61665	-1127.00911	1895.98173	1
114	H	72.58246	68.54906	73.71433	-1881.83093	1275.82488	-1501.55016	1
115	C	72.04639	70.66691	74.04564	-600.05639	-404.05026	316.64485	1
116	H	72.33478	71.66731	73.65083	-2597.05260	496.36221	657.73249	1
117	H	70.99733	70.47946	73.71667	-1666.24518	1294.38985	-1723.90591	1
118	C	72.21819	70.58049	75.62196	493.57570	-129.95376	-602.56394	1
119	H	72.14344	71.55255	76.16396	-1469.08415	-637.84797	2204.22581	1

120	H	71.55360	69.83812	76.11648	-1038.97840	1068.88701	-2280.71789	1
121	C	75.13383	71.06714	74.03857	188.88100	241.05089	-727.87821	1
122	O	76.01107	70.89385	73.22781	531.88613	-49.19943	427.07960	1
123	N	74.68088	72.21173	74.53188	708.14833	26.93417	-179.73509	1
124	H	73.91388	72.12031	75.19736	-2232.69501	-1179.09831	1023.94816	1
125	C	75.12548	73.52866	74.09674	-738.32412	259.92548	104.42456	1
126	H	76.23340	73.46438	73.98175	2028.89123	1260.02983	1311.33324	1
127	C	74.42107	73.91951	72.80676	-258.65678	-345.52513	661.28459	1
128	H	73.32576	73.82444	72.97819	-1826.06090	-1801.46097	-918.64554	1
129	C	74.72030	75.36004	72.43232	-541.23400	531.92970	-218.41428	1
130	H	74.19053	75.66831	71.48897	1311.73218	-2219.18200	882.19023	1
131	H	74.40247	76.07508	73.24140	-1048.71298	1223.58118	-2196.97971	1
132	H	75.81982	75.52759	72.26101	419.06414	1903.92898	1903.44670	1
133	C	74.78415	73.00731	71.64998	-423.86431	152.66566	-648.55262	1
134	H	74.26642	73.30943	70.69797	105.68386	-2342.50080	1387.51238	1
135	H	75.89122	73.01957	71.44849	-1695.63603	-1484.73621	-1531.02793	1
136	H	74.50264	71.93770	71.86323	-1853.57121	-487.39031	1936.59343	1
137	C	74.57933	74.52507	75.31205	539.71428	-510.58232	267.58633	1
138	O	73.52888	74.31915	75.87237	-15.93758	-278.34085	-624.49402	1
139	N	75.39703	75.55998	75.44031	-676.81886	12.05292	276.17960	1
140	H	76.24573	75.54910	74.87682	-1694.44250	-373.84189	-2100.66098	1
141	C	75.12391	76.47942	76.49560	412.33078	-664.70360	108.35451	1
142	H	74.01748	76.42133	76.62790	1765.77476	1294.44366	1621.76594	1
143	C	75.90136	75.93570	77.76789	-179.66635	-721.95667	-264.73915	1
144	H	75.60471	74.88687	77.99386	-607.34922	2587.87032	-598.10018	1
145	H	76.99535	75.90037	77.56818	-359.69332	-1479.13954	-2259.74260	1
146	C	75.58415	76.88464	78.96843	-240.01076	616.02425	431.85322	1
147	H	75.80048	77.94512	78.69691	-1359.17131	782.54425	2227.99181	1
148	H	74.50312	76.85082	79.23224	-820.36667	85.81767	-2596.78715	1
149	C	76.48334	76.41467	80.18246	-513.07015	236.18570	-551.87280	1
150	H	76.23064	75.37150	80.48328	1816.11944	-1183.11722	-1650.94321	1
151	H	77.55888	76.39207	79.89219	-1800.04429	-1361.53473	1526.34643	1
152	C	76.25753	77.39604	81.35548	726.08972	-253.19732	-179.64713	1
153	H	76.61017	78.43009	81.16822	1224.27271	-456.51798	-2390.90304	1
154	H	75.22213	77.41453	81.75019	1206.40339	-1150.93514	-2154.90344	1
155	N	77.12950	76.88559	82.55210	329.70796	-633.68968	-155.67358	1
156	H	77.08132	77.44952	83.45023	1348.31305	1938.76845	1359.00643	1
157	H	76.91044	75.90977	82.90517	2096.92035	1446.54551	-966.48890	1
158	H	78.17759	76.82777	82.39547	-1197.07217	-2303.53719	827.28733	1
159	C	75.70914	77.96976	76.15645	-378.01186	-556.17301	-413.96481	1
160	O	75.22684	78.92787	76.71439	-409.44433	-307.55053	-453.30833	1
161	N	76.79190	77.93232	75.38383	-429.02477	524.70884	274.08502	1
162	H	77.07844	77.03442	74.99525	1706.34263	-1425.96036	1574.38926	1
163	C	77.18626	79.14388	74.73956	-45.25864	-626.22952	478.93267	1
164	H	76.55950	79.96091	75.17030	1988.63164	570.90773	1772.87287	1
165	C	78.74301	79.28693	75.02041	551.77128	-20.49526	-564.54996	1
166	H	78.92173	79.39953	76.11277	1434.61535	-1753.10253	1513.99471	1
167	H	79.27813	78.35661	74.72742	-714.67738	1819.09770	1898.36494	1
168	C	79.31165	80.51574	74.23935	446.99263	-555.77305	338.97221	1
169	H	79.31258	80.33086	73.14185	1953.68466	1892.25957	-161.67766	1
170	H	78.68266	81.42102	74.39270	-403.03785	2688.07032	-188.43591	1
171	C	80.77680	80.72810	74.79531	567.86262	335.74681	434.04421	1
172	H	80.74943	80.89788	75.89606	-1080.02275	1568.26081	-1948.78900	1
173	H	81.38616	79.80718	74.64990	-919.54108	2111.34692	1456.13463	1
174	C	81.44208	81.93269	74.08423	195.81897	173.33862	-745.11536	1
175	H	81.73550	81.75896	73.02889	1405.67949	-2301.21089	-390.08113	1
176	H	80.87487	82.88199	74.16458	-940.37328	-1118.32446	2299.72133	1
177	N	82.75678	82.23601	74.85498	319.26422	656.36007	-42.02424	1
178	H	83.08031	83.28721	74.84925	1961.03633	619.91968	1787.09422	1
179	H	82.73930	82.00188	75.89154	854.14343	-2156.80752	1429.08711	1
180	H	83.61998	81.69779	74.55115	1237.02905	-1378.50857	-1998.28500	1
181	C	77.02214	78.90701	73.13393	532.53319	-268.57236	517.55729	1

182	O	77.32613	77.84476	72.59083	266.16714	-290.73804	-558.88002	1
183	N	76.59225	80.02246	72.59356	-226.25352	640.49678	-270.32839	1
184	H	76.37956	80.79936	73.21742	2007.69063	-1035.27229	1523.50231	1
185	C	76.84510	80.27203	71.20673	-540.76542	-573.33303	49.50000	1
186	H	77.85279	79.83683	71.02623	-2374.20950	-1036.76023	843.75774	1
187	C	75.71804	79.52659	70.37697	-77.09082	666.87422	-415.84136	1
188	H	74.69690	79.90412	70.67695	-985.81834	617.19825	2463.91927	1
189	O	75.57124	78.10608	70.58107	293.29899	-391.65602	-477.80926	1
190	H	76.25623	77.96051	71.32475	2528.72714	-681.76262	-751.27122	1
191	C	76.04141	80.00692	68.91923	252.47363	-605.14473	440.05134	1
192	H	75.28318	79.63795	68.18956	-2052.65063	1456.49051	-1043.51830	1
193	H	76.05390	81.12048	68.85496	-2152.98800	-1661.97574	-161.70652	1
194	H	77.03800	79.64260	68.57620	-473.12726	-1584.27339	2165.61725	1
195	C	76.75304	81.90662	71.02493	360.36307	488.46713	505.10056	1
196	O	75.68467	82.42711	70.80952	-200.08817	-528.03552	-385.82850	1
197	N	77.96629	82.43074	71.10785	-597.54095	-226.44775	355.20479	1
198	H	78.73763	81.78158	71.26369	2179.23655	-1300.70981	-991.33835	1
199	C	78.21199	83.82089	71.18506	-687.68921	297.39807	-249.45179	1
200	H	79.30949	83.87860	71.01467	-349.16256	-2467.37713	-1101.72831	1
201	C	77.33209	84.62501	70.12394	672.47345	361.54328	-201.62880	1
202	H	76.25200	84.53554	70.39865	1541.41502	582.18425	2169.97026	1
203	H	77.59055	85.70841	70.17150	-2534.67717	60.25153	997.72295	1
204	C	77.56954	84.06993	68.71013	574.26774	-389.43119	-377.02542	1
205	C	78.80021	84.28212	68.01983	688.82679	-287.33580	-257.96133	1
206	H	79.60992	84.87902	68.47746	331.14182	1470.38163	2269.80013	1
207	C	76.52679	83.30712	68.10482	-383.52382	-675.04808	144.24917	1
208	H	75.57210	83.14686	68.64247	4.09847	1517.59662	2262.86397	1
209	C	78.96083	83.71223	66.75621	-134.76730	428.45285	-649.50303	1
210	H	79.91238	83.87426	66.22036	-903.23433	1600.49020	2011.53387	1
211	C	76.73624	82.75128	66.84039	-335.53281	-615.00040	-364.39058	1
212	H	75.92474	82.15319	66.39004	1596.45398	-1369.33862	1732.02659	1
213	C	77.95408	82.92808	66.12145	585.48547	-340.24194	-406.23938	1
214	O	78.18123	82.36431	64.83849	-419.15649	-173.04408	-511.94141	1
215	H	77.31288	81.91928	64.69576	-1071.84350	1559.71507	-1960.13012	1
216	C	77.78763	84.35137	72.68115	291.41878	-183.13091	710.72246	1
217	O	76.75105	84.93045	72.91028	379.87695	523.47396	-222.23622	1
218	N	78.73939	83.99667	73.54760	564.30591	373.09380	277.24371	1
219	H	79.57966	83.57653	73.15313	-120.59931	-2436.07824	-1214.35098	1
220	C	78.72244	84.65599	74.81455	404.07514	-299.37480	608.84009	1
221	H	77.64225	84.84836	75.01474	-1071.07882	-841.69025	2359.66467	1
222	C	79.44933	83.69582	75.84203	-683.12807	68.71770	-390.13096	1
223	H	79.08353	82.65378	75.71207	2068.88918	1596.58590	770.89603	1
224	H	80.54420	83.66033	75.63265	1379.86429	2342.49779	-179.85638	1
225	C	79.20747	84.15893	77.31128	-176.39967	537.49466	550.97268	1
226	H	79.63038	85.17058	77.50343	-396.28051	1942.22168	1869.33314	1
227	H	78.12201	84.22457	77.54776	-94.44700	586.00678	-2659.20016	1
228	C	79.93809	83.03929	78.18718	-291.69381	-718.18079	-150.72929	1
229	H	79.57364	81.99256	78.02605	-2303.38776	1089.76242	964.62032	1
230	H	81.05464	83.02190	78.10720	884.16729	2568.80533	-207.74283	1
231	N	79.60018	83.39654	79.49864	-594.49522	-252.81478	342.29276	1
232	H	79.03223	84.22152	79.61408	-1735.17426	2084.05705	-263.71605	1
233	C	79.95393	82.74529	80.53203	595.23177	-271.52487	442.22352	1
234	N	80.74625	81.60828	80.33941	585.53813	-424.79750	-105.81303	1
235	H	81.09291	81.20165	79.47135	959.88797	1327.56823	-2177.11905	1
236	H	81.09327	81.00428	81.08501	1578.48647	16.27378	-2220.76233	1
237	N	79.45631	83.34394	81.69788	-452.17763	-390.33541	-421.51853	1
238	H	78.86470	84.16285	81.83076	470.26107	1974.25629	-1817.92087	1
239	H	79.61724	82.96396	82.63142	1856.67307	-1573.97321	-1224.35416	1
240	C	79.61331	86.02682	74.70033	-531.47271	-581.45780	-55.06206	1
241	O	80.51000	86.19175	73.90860	-243.00837	192.73507	609.52485	1
242	N	79.23486	86.83005	75.69755	343.49288	-644.25607	38.09164	1
243	H	78.46918	86.47736	76.27014	-1691.16043	-1535.97525	-1484.73099	1

244	C	79.80891	88.16189	75.88493	542.66492	350.14337	454.42563	1
245	H	80.09867	88.46997	74.85146	1209.57979	-2396.95920	463.86744	1
246	C	78.75138	89.04228	76.52840	-737.14309	145.93010	242.71942	1
247	H	78.52056	88.61274	77.52922	-1050.18303	159.36419	-2509.06125	1
248	C	79.23952	90.46445	76.72862	-706.77696	-252.88343	-245.16230	1
249	H	78.49056	91.08822	77.29000	-1624.64039	-1665.49085	1417.86935	1
250	H	80.21005	90.48656	77.31487	2566.10521	598.51109	693.22305	1
251	H	79.43148	90.97912	75.74728	-1972.69758	107.10018	-1876.34312	1
252	C	77.46210	89.05682	75.72567	412.85148	672.58832	-27.69222	1
253	H	76.65049	89.63195	76.24945	1447.02277	1762.76533	-1490.78944	1
254	H	77.61066	89.53294	74.71820	1320.77379	-145.20455	2378.68491	1
255	H	77.07371	88.01785	75.54251	-1512.10848	1470.52031	1724.75147	1
256	C	81.13846	87.99164	76.86046	-607.11113	499.56689	73.73769	1
257	O	81.51762	88.92062	77.54241	357.97126	460.81534	356.68785	1
258	N	81.67719	86.79175	76.74607	536.55407	-368.62270	332.76306	1
259	H	81.24296	86.15532	76.07527	524.38866	2297.69985	1367.20941	1
260	C	82.95605	86.57322	77.33267	46.50277	-774.29190	-147.97904	1
261	H	83.37702	87.59236	77.49411	1676.51875	1883.29066	1032.55549	1
262	C	82.78266	85.74845	78.71634	-559.41456	-34.19198	-556.30433	1
263	H	82.28674	84.77370	78.49748	-64.66664	395.18769	2695.05373	1
264	H	83.78730	85.49426	79.13060	-2703.44278	-60.40056	333.79418	1
265	C	81.97898	86.52265	79.72298	-519.76435	377.31045	459.42366	1
266	H	80.99780	86.78128	79.26372	-1746.74323	1667.50644	-1261.73691	1
267	C	81.73395	85.66500	80.95960	570.95554	16.46261	-545.27700	1
268	H	81.09763	86.19432	81.71440	2391.58273	28.05277	-1305.07271	1
269	H	81.21384	84.70757	80.70003	175.75588	917.63458	2559.43867	1
270	H	82.69375	85.39083	81.46836	-1063.97851	-2155.34650	1283.00462	1
271	C	82.67507	87.81342	80.13098	193.76014	2.62946	-765.53141	1
272	H	82.14698	88.31643	80.98186	507.39394	-846.55087	2539.60089	1
273	H	83.73188	87.63190	80.45730	1337.57841	1818.19054	1526.01994	1
274	H	82.70106	88.54937	79.27809	1100.88635	-1172.91350	-2199.08909	1
275	C	83.80305	85.61419	76.37134	-549.21115	475.64486	-309.38218	1
276	O	83.29934	84.67695	75.76765	556.06106	-390.37755	-78.24250	1
277	O	85.19159	85.75831	76.40781	-572.27940	-310.19032	-209.75862	1
278	H	85.24377	86.58056	76.99091	-1380.08193	2212.14486	790.85944	1

Listing 109: C00109.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.4020	0.0000	300.0000
3	H	68.85742	84.37051	78.01415	-2043.14101	-1757.64893	399.89339		1
4	N	69.86759	84.25051	77.94731	426.75047	490.45733	-334.42467		1
5	H	69.91794	83.41010	77.37085	442.25559	-1110.30854	-2448.52907		1
6	C	70.52627	85.37002	77.38477	415.32972	-666.39213	83.73172		1
7	H	69.74958	85.97820	76.87411	879.32219	2491.00447	667.35213		1
8	C	71.27161	86.17107	78.56652	31.35357	477.41777	628.23362		1
9	H	71.90174	85.44894	79.13879	1168.38489	2240.25337	-1019.71136		1
10	H	71.97098	86.92435	78.12977	-360.43770	2534.90498	931.67112		1
11	C	70.30962	86.85626	79.50520	463.18208	512.70242	-382.34388		1
12	H	69.48638	86.15058	79.75450	1725.29117	1863.52247	-987.07854		1
13	C	71.03823	87.23044	80.79028	710.42801	-144.27427	-313.15367		1
14	H	70.36347	87.75619	81.51380	364.20195	-1033.13725	2494.72524		1
15	H	71.44720	86.32681	81.31233	2567.61904	335.80679	847.48802		1
16	H	71.90382	87.91318	80.58745	-2587.99029	680.92867	-512.16411		1
17	C	69.72222	88.10490	78.86331	268.17616	741.64379	-40.42634		1
18	H	69.03506	88.64692	79.56354	1283.54314	-1945.37420	-1411.27812		1
19	H	70.52526	88.82719	78.56229	-1258.57796	1317.15249	-2026.02085		1
20	H	69.13486	87.86101	77.94057	-2502.84526	909.80597	575.92391		1
21	C	71.68729	84.81295	76.37627	619.36578	-458.64843	-172.09273		1
22	O	71.98756	85.41435	75.36548	-81.40433	433.87611	522.34594		1
23	N	72.30378	83.77865	76.94994	175.23996	-622.20190	341.55523		1

24	H	71.86837	83.43850	77.80491	-876.57256	-303.22879	-2561.90213	1
25	C	73.33693	83.02320	76.29734	-571.88214	-534.10783	-106.15033	1
26	H	73.46818	82.15117	76.97810	-2713.20841	-16.25800	-248.80809	1
27	C	72.72630	82.56733	74.92880	166.60354	288.16399	-716.09568	1
28	H	72.25223	83.41459	74.38322	-2097.85574	1636.78449	-586.18044	1
29	O	71.46605	81.59542	75.17373	-317.80580	-363.38227	484.43082	1
30	H	70.81619	82.14324	74.74780	1863.74748	-1451.84923	1357.29467	1
31	C	73.82696	81.88808	74.08580	503.80731	517.99032	318.51606	1
32	H	73.40122	81.21189	73.29947	640.61020	-2157.10410	-1536.29104	1
33	H	74.47841	82.63135	73.54795	1687.88455	465.60692	2087.56452	1
34	H	74.50110	81.26914	74.73987	-1293.07895	-1899.88581	-1463.57452	1
35	C	74.75498	83.83511	76.14511	-153.07550	-733.68902	248.70981	1
36	O	75.48601	83.42022	75.27698	186.15459	-480.78787	-449.34387	1
37	N	75.03727	84.78064	77.05344	-487.53139	543.18517	42.03850	1
38	C	76.23581	85.55286	76.92170	-699.35871	69.34393	360.10701	1
39	H	76.45945	85.61571	75.83188	2.81126	-221.99807	-2715.58072	1
40	C	75.83496	86.91561	77.63247	-507.46439	-592.59194	122.07761	1
41	H	76.71885	87.50340	77.96718	-1975.08116	525.87560	-1801.71556	1
42	H	75.25308	87.57276	76.94839	1588.27743	-1913.22100	1113.83566	1
43	C	74.94905	86.41167	78.81321	-613.62442	-457.55993	-194.14490	1
44	H	75.57507	86.00150	79.64744	1707.54637	-721.27992	1996.92523	1
45	H	74.30198	87.20099	79.25889	758.23357	2100.81767	1560.55011	1
46	C	74.12203	85.27203	78.07449	-352.41524	704.96076	49.21465	1
47	H	73.79106	84.41560	78.70849	1714.76886	-2070.42778	443.35792	1
48	H	73.26487	85.64989	77.47164	1224.15040	1801.50881	1636.97633	1
49	C	77.46068	84.85748	77.76021	566.85117	537.05831	117.62814	1
50	O	78.60420	85.09625	77.44328	-550.26779	-406.08867	4.21666	1
51	N	77.03070	84.09027	78.75886	566.34832	-425.77725	180.18749	1
52	H	76.02038	84.02213	78.86371	644.44502	2646.80550	-52.73430	1
53	C	77.95291	83.77921	79.81203	612.34801	-281.48662	411.56221	1
54	H	78.76115	84.53119	79.65325	1667.23498	-1490.75142	1556.16753	1
55	C	77.18461	83.95300	81.19515	-714.45746	-175.43074	286.98927	1
56	H	76.40433	83.15165	81.28922	-787.09484	1763.03619	-1922.46060	1
57	O	76.46254	85.20515	81.35201	-429.46514	516.51932	-128.40526	1
58	H	75.57722	84.87070	81.58624	1981.82785	436.16847	-1818.18182	1
59	C	78.31083	83.70777	82.26022	630.79189	-468.94448	76.03230	1
60	H	77.90972	83.77433	83.29883	-1775.71861	2062.30353	131.89849	1
61	H	78.77952	82.69159	82.14768	-1855.14608	88.94118	1993.53760	1
62	H	79.12658	84.46342	82.17342	-1504.82350	-780.94249	-2132.90992	1
63	C	78.49141	82.26821	79.54762	288.57638	618.62814	-397.00270	1
64	O	78.73959	81.51146	80.49713	321.70495	-185.26452	574.37218	1
65	N	78.65733	82.06074	78.26610	-447.05792	-446.53431	367.76425	1
66	H	78.43572	82.88600	77.70666	350.31316	1975.63644	-1843.31522	1
67	C	78.95015	80.81385	77.65284	-511.23061	374.03917	-471.51480	1
68	H	78.99015	81.08861	76.57415	2234.79579	-898.70890	-1273.45190	1
69	C	80.37174	80.31849	78.19893	529.53781	-159.34528	563.72604	1
70	H	80.80497	79.56651	77.48322	654.59388	2347.94251	1217.51488	1
71	H	81.04456	81.21679	78.14664	-1526.55661	2103.42026	817.87394	1
72	O	80.42883	79.73686	79.50688	-554.84278	14.12789	399.58769	1
73	H	79.78699	80.37596	80.00093	1297.06236	2061.84854	1220.68812	1
74	C	77.78678	79.72401	77.95190	-662.15484	-412.13544	123.62687	1
75	O	77.96800	78.55236	77.67789	-540.01537	-317.05804	274.91456	1
76	N	76.64672	80.28488	78.35176	-202.76299	-690.00100	-131.49145	1
77	H	76.72501	81.28823	78.51355	-702.62132	-2617.37191	281.70413	1
78	C	75.54865	79.46702	78.88056	-491.73914	576.34187	222.73509	1
79	H	76.06818	78.61256	79.37786	1977.17978	-1823.58850	-434.68928	1
80	C	74.74575	80.32218	79.84093	-649.50797	-328.66843	306.11224	1
81	H	74.49095	81.27371	79.32292	2075.07803	1452.16490	-1004.45904	1
82	C	73.45173	79.65164	80.26501	-615.18735	-489.99689	-70.96352	1
83	H	72.88369	80.27047	81.01294	-1226.32661	-1724.38906	-1716.47170	1
84	H	72.76599	79.47526	79.38882	2381.64273	-969.84735	900.46860	1
85	H	73.64339	78.64877	80.73804	2122.74991	1702.23946	-141.36228	1

86	C	75.55965	80.66750	81.07623	-501.86074	-479.61276	-376.42482	1
87	H	75.04145	81.43049	81.71969	993.79261	-2246.95401	-1177.81305	1
88	H	75.73681	79.76024	81.71688	42.71279	-626.15391	-2651.37258	1
89	H	76.57530	81.07661	80.80495	-2026.39012	-1590.33709	-887.82922	1
90	C	74.64303	78.92189	77.61029	-672.89153	382.57394	-156.34072	1
91	O	73.73931	78.14233	77.80697	410.04627	221.86223	500.35950	1
92	N	74.97786	79.47992	76.43856	-378.11782	-443.79414	-441.10984	1
93	H	75.82964	80.03267	76.51227	2404.15973	-568.14894	1149.30085	1
94	C	74.69307	78.62603	75.29837	-544.54484	466.16019	331.29119	1
95	H	74.87879	77.59793	75.68280	-1409.80988	-170.17955	2325.32679	1
96	C	73.15902	78.86705	75.01688	-184.48284	116.78282	-758.89137	1
97	H	72.54966	78.37531	75.81310	1893.78641	1861.14652	611.04528	1
98	H	72.90363	79.95233	75.08457	-2170.79665	-974.19311	1327.50117	1
99	C	72.82522	78.28890	73.60580	389.51668	672.81878	-138.49152	1
100	H	73.41355	78.83677	72.83263	510.64577	1933.03327	1851.02484	1
101	H	73.17198	77.23575	73.52343	-2302.30869	-1105.72939	-948.89774	1
102	C	71.27812	78.36150	73.27791	-559.93427	-126.34590	542.30857	1
103	O	70.80257	77.61751	72.45716	-670.36003	-111.83166	76.36448	1
104	N	70.62626	79.32185	73.95729	-216.06729	-537.07037	446.51379	1
105	H	71.01891	80.07465	74.60024	-1251.96487	1074.12894	-2168.52500	1
106	H	69.62454	79.49734	73.80031	-2451.83023	-720.73851	944.84612	1
107	C	75.69511	79.05189	74.09542	546.24052	-563.88337	-85.11809	1
108	O	75.36979	79.91476	73.31846	71.70702	-307.40463	606.69673	1
109	N	76.82561	78.33790	74.14211	479.90863	-504.50129	222.86849	1
110	C	77.88063	78.53799	73.18927	75.51268	-600.91904	506.73700	1
111	H	78.00475	79.63431	73.03027	-2033.61562	1795.30103	254.89480	1
112	C	79.09816	77.79278	73.89828	523.79067	517.99274	284.45581	1
113	H	79.90908	77.51672	73.18798	1599.61665	-1127.00911	1895.98173	1
114	H	79.56308	78.42272	74.68908	-1881.83093	1275.82488	-1501.55016	1
115	C	78.36973	76.55939	74.51097	-600.05639	-404.05026	316.64485	1
116	H	78.12180	75.80880	73.72661	-2597.05260	496.36221	657.73249	1
117	H	78.96454	76.03085	75.28939	-1666.24518	1294.38985	-1723.90591	1
118	C	77.06133	77.25688	75.08650	493.57570	-129.95376	-602.56394	1
119	H	76.14973	76.61316	75.13352	-1469.08415	-637.84797	2204.22581	1
120	H	77.22108	77.76636	76.08574	-1038.97840	1068.88701	-2280.71789	1
121	C	77.49670	77.73066	71.83210	188.88100	241.05089	-727.87821	1
122	O	76.63711	76.85551	71.79827	531.88613	-49.19943	427.07960	1
123	N	78.30413	78.12812	70.87113	708.14833	26.93417	-179.73509	1
124	H	78.98992	78.82659	71.14938	-2232.69501	-1179.09831	1023.94816	1
125	C	78.24443	77.56547	69.52478	-738.32412	259.92548	104.42456	1
126	H	77.14360	77.50715	69.34864	2028.89123	1260.02983	1311.33324	1
127	C	79.00266	78.46979	68.56692	-258.65678	-345.52513	661.28459	1
128	H	80.06396	78.50293	68.90151	-1826.06090	-1801.46097	-918.64554	1
129	C	78.97507	77.91539	67.15429	-541.23400	531.92970	-218.41428	1
130	H	79.56532	78.55549	66.44241	1311.73218	-2219.18200	882.19023	1
131	H	79.41301	76.87667	67.11653	-1048.71298	1223.58118	-2196.97971	1
132	H	77.92573	77.85083	66.75446	419.06414	1903.92898	1903.44670	1
133	C	78.47292	79.89184	68.57691	-423.86431	152.66566	-648.55262	1
134	H	79.06523	80.56234	67.89529	105.68386	-2342.50080	1387.51238	1
135	H	77.40136	79.93502	68.23860	-1695.63603	-1484.73621	-1531.02793	1
136	H	78.51086	80.34260	69.60643	-1853.57121	-487.39031	1936.59343	1
137	C	78.92755	76.05082	69.61038	539.71428	-510.58232	267.58633	1
138	O	79.96821	75.80664	69.05725	-15.93758	-278.34085	-624.49402	1
139	N	78.15014	75.24651	70.31046	-676.81886	12.05292	276.17960	1
140	H	77.28326	75.59857	70.78138	-1694.44250	-373.84189	-2100.66098	1
141	C	78.59399	73.89146	70.44819	412.33078	-664.70360	108.35451	1
142	H	79.07573	73.73808	69.45444	1765.77476	1294.44366	1621.76594	1
143	C	79.67834	73.82888	71.59856	-179.66635	-721.95667	-264.73915	1
144	H	80.45982	74.60895	71.45644	-607.34922	2587.87032	-598.10018	1
145	H	79.23403	74.03374	72.59799	-359.69332	-1479.13954	-2259.74260	1
146	C	80.28449	72.38684	71.50643	-240.01076	616.02425	431.85322	1
147	H	79.47414	71.63045	71.39991	-1359.17131	782.54425	2227.99181	1

148	H	80.91614	72.28498	70.59558	-820.36667	85.81767	-2596.78715	1
149	C	81.12093	72.09787	72.80998	-513.07015	236.18570	-551.87280	1
150	H	81.93546	72.84585	72.94261	1816.11944	-1183.11722	-1650.94321	1
151	H	80.48103	72.17450	73.71861	-1800.04429	-1361.53473	1526.34643	1
152	C	81.69344	70.65736	72.65583	726.08972	-253.19732	-179.64713	1
153	H	80.93715	69.89419	72.37184	1224.27271	-456.51798	-2390.90304	1
154	H	82.58179	70.57724	71.99447	1206.40339	-1150.93514	-2154.90344	1
155	N	82.14099	70.21134	74.04748	329.70796	-633.68968	-155.67358	1
156	H	82.60403	69.26636	74.08320	1348.31305	1938.76845	1359.00643	1
157	H	82.85355	70.79894	74.55248	2096.92035	1446.54551	-966.48890	1
158	H	81.22861	70.10323	74.79379	-1197.07217	-2303.53719	827.28733	1
159	C	77.25206	72.98006	70.69363	-378.01186	-556.17301	-413.96481	1
160	O	76.51462	72.82390	69.74822	-409.44433	-307.55053	-453.30833	1
161	N	77.20653	72.39570	71.90067	-429.02477	524.70884	274.08502	1
162	H	77.93700	72.77440	72.50593	1706.34263	-1425.96036	1574.38926	1
163	C	75.93079	72.13480	72.53262	-45.25864	-626.22952	478.93267	1
164	H	75.79883	73.01565	73.19780	1988.63164	570.90773	1772.87287	1
165	C	74.77885	72.04417	71.46398	551.77128	-20.49526	-564.54996	1
166	H	74.61837	73.04779	71.00268	1434.61535	-1753.10253	1513.99471	1
167	H	75.08426	71.37639	70.62242	-714.67738	1819.09770	1898.36494	1
168	C	73.44354	71.52154	72.09462	446.99263	-555.77305	338.97221	1
169	H	73.52125	70.42790	72.30868	1953.68466	1892.25957	-161.67766	1
170	H	73.22677	72.01433	73.06910	-403.03785	2688.07032	-188.43591	1
171	C	72.30141	71.81132	71.03797	567.86262	335.74681	434.04421	1
172	H	72.05903	72.89814	70.98652	-1080.02275	1568.26081	-1948.78900	1
173	H	72.62410	71.51857	70.01208	-919.54108	2111.34692	1456.13463	1
174	C	71.07954	70.97412	71.47745	195.81897	173.33862	-745.11536	1
175	H	71.24413	69.87610	71.39968	1405.67949	-2301.21089	-390.08113	1
176	H	70.68368	71.23907	72.47820	-940.37328	-1118.32446	2299.72133	1
177	N	69.88104	71.24100	70.50582	319.26422	656.36007	-42.02424	1
178	H	68.98828	70.70854	70.72465	1961.03633	619.91968	1787.09422	1
179	H	69.52008	72.23669	70.44208	854.14343	-2156.80752	1429.08711	1
180	H	70.02627	70.99202	69.48483	1237.02905	-1378.50857	-1998.28500	1
181	C	76.03657	70.79160	73.42668	532.53319	-268.57236	517.55729	1
182	O	75.05016	70.39567	74.00642	266.16714	-290.73804	-558.88002	1
183	N	77.30402	70.31541	73.56989	-226.25352	640.49678	-270.32839	1
184	H	77.89317	70.92072	72.98997	2007.69063	-1035.27229	1523.50231	1
185	C	77.57144	68.89405	73.35809	-540.76542	-573.33303	49.50000	1
186	H	78.04775	68.91399	72.35308	-2374.20950	-1036.76023	843.75774	1
187	C	78.57209	68.48414	74.44855	-77.09082	666.87422	-415.84136	1
188	H	78.13473	68.55686	75.46777	-985.81834	617.19825	2463.91927	1
189	O	79.90541	69.46806	74.83150	293.29899	-391.65602	-477.80926	1
190	H	79.59977	69.74605	75.69445	2528.72714	-681.76262	-751.27122	1
191	C	79.06921	67.06870	74.09418	252.47363	-605.14473	440.05134	1
192	H	79.65064	66.61953	74.93745	-2052.65063	1456.49051	-1043.51830	1
193	H	78.22081	66.38178	73.85755	-2152.98800	-1661.97574	-161.70652	1
194	H	79.73805	67.08918	73.19836	-473.12726	-1584.27339	2165.61725	1
195	C	76.23929	67.92248	73.39026	360.36307	488.46713	505.10056	1
196	O	75.85238	67.40167	74.41599	-200.08817	-528.03552	-385.82850	1
197	N	75.81742	67.75698	72.15108	-597.54095	-226.44775	355.20479	1
198	H	76.30381	68.28313	71.42650	2179.23655	-1300.70981	-991.33835	1
199	C	74.67680	66.98363	71.82604	-687.68921	297.39807	-249.45179	1
200	H	74.81955	66.80098	70.73896	-349.16256	-2467.37713	-1101.72831	1
201	C	74.59904	65.64875	72.69913	672.47345	361.54328	-201.62880	1
202	H	74.50639	65.89301	73.78831	1541.41502	582.18425	2169.97026	1
203	H	73.68127	65.08261	72.41664	-2534.67717	60.25153	997.72295	1
204	C	75.84817	64.77910	72.48491	574.26774	-389.43119	-377.02542	1
205	C	76.09945	64.08746	71.26262	688.82679	-287.33580	-257.96133	1
206	H	75.40134	64.16981	70.40986	331.14182	1470.38163	2269.80013	1
207	C	76.75276	64.66927	73.58235	-383.52382	-675.04808	144.24917	1
208	H	76.55128	65.22301	74.52048	4.09847	1517.59662	2262.86397	1
209	C	77.24682	63.29872	71.17483	-134.76730	428.45285	-649.50303	1

210	H	77.44398	62.75659	70.23354	-903.23433	1600.49020	2011.53387	1
211	C	77.88860	63.86711	73.44522	-335.53281	-615.00040	-364.39058	1
212	H	78.58221	63.78845	74.30062	1596.45398	-1369.33862	1732.02659	1
213	C	78.17646	63.15345	72.24540	585.48547	-340.24194	-406.23938	1
214	O	79.32626	62.33510	72.09046	-419.15649	-173.04408	-511.94141	1
215	H	79.71702	62.42446	72.99124	-1071.84350	1559.71507	-1960.13012	1
216	C	73.33949	67.90036	72.08153	291.41878	-183.13091	710.72246	1
217	O	72.91094	68.55308	71.15379	379.87695	523.47396	-222.23622	1
218	N	72.84339	67.78092	73.30305	564.30591	373.09380	277.24371	1
219	H	73.37731	67.27139	74.00423	-120.59931	-2436.07824	-1214.35098	1
220	C	71.65464	68.52791	73.61658	404.07514	-299.37480	608.84009	1
221	H	71.89378	69.57489	73.33075	-1071.07882	-841.69025	2359.66467	1
222	C	70.49933	67.90195	72.73244	-683.12807	68.71770	-390.13096	1
223	H	70.79802	67.88091	71.65899	2068.88918	1596.58590	770.89603	1
224	H	70.32333	66.83795	73.00774	1379.86429	2342.49779	-179.85638	1
225	C	69.20227	68.74511	72.93228	-176.39967	537.49466	550.97268	1
226	H	68.78216	68.60617	73.95348	-396.28051	1942.22168	1869.33314	1
227	H	69.40702	69.83310	72.84335	-94.44700	586.00678	-2659.20016	1
228	C	68.18570	68.26055	71.79917	-291.69381	-718.18079	-150.72929	1
229	H	68.57397	68.32539	70.75050	-2303.38776	1089.76242	964.62032	1
230	H	67.74933	67.23903	71.93886	884.16729	2568.80533	-207.74283	1
231	N	67.15331	69.20204	71.91942	-594.49522	-252.81478	342.29276	1
232	H	67.29306	69.95001	72.58097	-1735.17426	2084.05705	-263.71605	1
233	C	66.06934	69.17117	71.25569	595.23177	-271.52487	442.22352	1
234	N	65.89570	68.12668	70.34100	585.53813	-424.79750	-105.81303	1
235	H	66.52108	67.35404	70.11573	959.88797	1327.56823	-2177.11905	1
236	H	65.06980	67.99106	69.75724	1578.48647	16.27378	-2220.76233	1
237	N	65.23990	70.24844	71.59786	-452.17763	-390.33541	-421.51853	1
238	H	65.36383	70.99939	72.27527	470.26107	1974.25629	-1817.92087	1
239	H	64.31716	70.39391	71.18641	1856.67307	-1573.97321	-1224.35416	1
240	C	71.26332	68.35267	75.18408	-531.47271	-581.45780	-55.06206	1
241	O	70.90883	69.30410	75.83762	-243.00837	192.73507	609.52485	1
242	N	71.21567	67.05572	75.53330	343.49288	-644.25607	38.09164	1
243	H	71.59968	66.41290	74.84010	-1691.16043	-1535.97525	-1484.73099	1
244	C	71.10484	66.71009	76.94678	542.66492	350.14337	454.42563	1
245	H	70.82452	67.67374	77.43939	1209.57979	-2396.95920	463.86744	1
246	C	70.06779	65.60657	77.07380	-737.14309	145.93010	242.71942	1
247	H	70.38401	64.76443	76.41890	-1050.18303	159.36419	-2509.06125	1
248	C	69.97546	65.09230	78.49794	-706.77696	-252.88343	-245.16230	1
249	H	69.21672	64.26696	78.59479	-1624.64039	-1665.49085	1417.86935	1
250	H	70.96260	64.68491	78.85464	2566.10521	598.51109	693.22305	1
251	H	69.67581	65.90701	79.21413	-1972.69758	107.10018	-1876.34312	1
252	C	68.70584	66.07637	76.59584	412.85148	672.58832	-27.69222	1
253	H	67.94304	65.25009	76.62010	1447.02277	1762.76533	-1490.78944	1
254	H	68.31162	66.91389	77.23538	1320.77379	-145.20455	2378.68491	1
255	H	68.75312	66.46338	75.54016	-1512.10848	1470.52031	1724.75147	1
256	C	72.61853	66.14584	77.36626	-607.11113	499.56689	73.73769	1
257	O	73.11114	65.18079	76.83782	357.97126	460.81534	356.68785	1
258	N	73.09988	66.90660	78.33385	536.55407	-368.62270	332.76306	1
259	H	72.54058	67.68804	78.67255	524.38866	2297.69985	1367.20941	1
260	C	74.34628	66.57213	78.92435	46.50277	-774.29190	-147.97904	1
261	H	74.64609	65.59153	78.48191	1676.51875	1883.29066	1032.55549	1
262	C	75.35188	67.77303	78.61733	-559.41456	-34.19198	-556.30433	1
263	H	74.86932	68.74089	78.87621	-64.66664	395.18769	2695.05373	1
264	H	76.26575	67.70678	79.24793	-2703.44278	-60.40056	333.79418	1
265	C	75.72621	67.73718	77.09978	-519.76435	377.31045	459.42366	1
266	H	74.85512	67.43592	76.47137	-1746.74323	1667.50644	-1261.73691	1
267	C	76.17457	69.19333	76.71053	570.95554	16.46261	-545.27700	1
268	H	76.27489	69.30860	75.60083	2391.58273	28.05277	-1305.07271	1
269	H	75.42665	69.95219	77.03855	175.75588	917.63458	2559.43867	1
270	H	77.15092	69.46539	77.17520	-1063.97851	-2155.34650	1283.00462	1
271	C	76.90128	66.70154	76.95326	193.76014	2.62946	-765.53141	1

272	H	77.30166	66.68018	75.91194	507.39394	-846.55087	2539.60089	1
273	H	77.75296	66.94089	77.63105	1337.57841	1818.19054	1526.01994	1
274	H	76.56337	65.66651	77.19335	1100.88635	-1172.91350	-2199.08909	1
275	C	74.14041	66.58534	80.53807	-549.21115	475.64486	-309.38218	1
276	O	73.23854	67.16318	81.08400	556.06106	-390.37755	-78.24250	1
277	O	75.17340	65.98292	81.28900	-572.27940	-310.19032	-209.75862	1
278	H	75.72451	65.63039	80.53281	-1380.08193	2212.14486	790.85944	1

Listing 110: C00110.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.4019	0.0000	300.0000
3	H	78.54615	64.31219	79.81565	-2043.14101	-1757.64893	399.89339		1
4	N	78.26460	65.29048	79.78473	426.75047	490.45733	-334.42467		1
5	H	77.43313	65.25726	79.19856	442.25559	-1110.30854	-2448.52907		1
6	C	79.25782	66.19042	79.34363	415.32972	-666.39213	83.73172		1
7	H	80.17129	65.85260	79.87675	879.32219	2491.00447	667.35213		1
8	C	79.38506	66.13986	77.74338	31.35357	477.41777	628.23362		1
9	H	78.44619	66.55075	77.29904	1168.38489	2240.25337	-1019.71136		1
10	H	80.19969	66.82947	77.41499	-360.43770	2534.90498	931.67112		1
11	C	79.63668	64.74150	77.23256	463.18208	512.70242	-382.34388		1
12	H	78.82086	64.07725	77.59484	1725.29117	1863.52247	-987.07854		1
13	C	79.62092	64.73389	75.70915	710.42801	-144.27427	-313.15367		1
14	H	79.78205	63.70399	75.29782	364.20195	-1033.13725	2494.72524		1
15	H	78.64491	65.10574	75.30274	2567.61904	335.80679	847.48802		1
16	H	80.42635	65.38859	75.28642	-2587.99029	680.92867	-512.16411		1
17	C	80.96571	64.19341	77.73180	268.17616	741.64379	-40.42634		1
18	H	81.17201	63.17178	77.31910	1283.54314	-1945.37420	-1411.27812		1
19	H	81.82173	64.85116	77.43051	-1258.57796	1317.15249	-2026.02085		1
20	H	80.98784	64.10992	78.84902	-2502.84526	909.80597	575.92391		1
21	C	78.74930	67.69937	79.75656	619.36578	-458.64843	-172.09273		1
22	O	78.27008	68.44550	78.93419	-81.40433	433.87611	522.34594		1
23	N	78.99659	67.89547	81.04574	175.23996	-622.20190	341.55523		1
24	H	79.45734	67.12325	81.52750	-876.57256	-303.22879	-2561.90213		1
25	C	78.43888	68.96519	81.79367	-571.88214	-534.10783	-106.15033		1
26	H	78.88939	68.81243	82.79953	-2713.20841	-16.25800	-248.80809		1
27	C	78.87659	70.34178	81.11085	166.60354	288.16399	-716.09568		1
28	H	78.36553	70.40014	80.10877	-2097.85574	1636.78449	-586.18044		1
29	O	80.28862	70.49208	80.87253	-317.80580	-363.38227	484.43082		1
30	H	80.31425	70.46583	79.89511	1863.74748	-1451.84923	1357.29467		1
31	C	78.26235	71.40198	82.09846	503.80731	517.99032	318.51606		1
32	H	78.41769	72.44015	81.72498	640.61020	-2157.10410	-1536.29104		1
33	H	77.16407	71.26285	82.24820	1687.88455	465.60692	2087.56452		1
34	H	78.73913	71.34190	83.10451	-1293.07895	-1899.88581	-1463.57452		1
35	C	76.80835	68.81375	81.81515	-153.07550	-733.68902	248.70981		1
36	O	76.12534	69.57632	81.18194	186.15459	-480.78787	-449.34387		1
37	N	76.43140	67.79167	82.59589	-487.53139	543.18517	42.03850		1
38	C	75.11686	67.74001	83.16669	-699.35871	69.34393	360.10701		1
39	H	74.43788	68.11211	82.35769	2.81126	-221.99807	-2715.58072		1
40	C	74.96038	66.19460	83.51244	-507.46439	-592.59194	122.07761		1
41	H	74.19812	65.99002	84.29611	-1975.08116	525.87560	-1801.71556		1
42	H	74.65707	65.60933	82.61608	1588.27743	-1913.22100	1113.83566		1
43	C	76.40805	65.82845	83.95923	-613.62442	-457.55993	-194.14490		1
44	H	76.60136	66.17710	84.99859	1707.54637	-721.27992	1996.92523		1
45	H	76.61607	64.73470	83.94830	758.23357	2100.81767	1560.55011		1
46	C	77.26967	66.64141	82.89743	-352.41524	704.96076	49.21465		1
47	H	78.25523	67.00071	83.27306	1714.76886	-2070.42778	443.35792		1
48	H	77.41815	66.12526	81.91825	1224.15040	1801.50881	1636.97633		1
49	C	75.11506	68.72371	84.46495	566.85117	537.05831	117.62814		1
50	O	75.95390	69.61489	84.58424	-550.26779	-406.08867	4.21666		1
51	N	74.07607	68.45199	85.22256	566.34832	-425.77725	180.18749		1

52	H	73.49734	67.68425	84.88739	644.44502	2646.80550	-52.73430	1
53	C	73.94336	68.90817	86.55993	612.34801	-281.48662	411.56221	1
54	H	73.14138	68.26164	86.97912	1667.23498	-1490.75142	1556.16753	1
55	C	75.34563	68.73536	87.31088	-714.45746	-175.43074	286.98927	1
56	H	76.12605	69.36258	86.79283	-787.09484	1763.03619	-1922.46060	1
57	O	75.88564	67.40159	87.33935	-429.46514	516.51932	-128.40526	1
58	H	76.72615	67.53260	86.85385	1981.82785	436.16847	-1818.18182	1
59	C	75.02064	69.38140	88.70736	630.79189	-468.94448	76.03230	1
60	H	75.93151	69.44724	89.34665	-1775.71861	2062.30353	131.89849	1
61	H	74.61423	70.41500	88.60196	-1855.14608	88.94118	1993.53760	1
62	H	74.26556	68.78250	89.26731	-1504.82350	-780.94249	-2132.90992	1
63	C	73.50562	70.48884	86.53400	288.57638	618.62814	-397.00270	1
64	O	72.44116	70.80820	87.00295	321.70495	-185.26452	574.37218	1
65	N	74.46629	71.25486	86.03292	-447.05792	-446.53431	367.76425	1
66	H	75.33684	70.84287	85.60618	350.31316	1975.63644	-1843.31522	1
67	C	74.15156	72.61878	85.79850	-511.23061	374.03917	-471.51480	1
68	H	73.11094	72.73533	86.18831	2234.79579	-898.70890	-1273.45190	1
69	C	75.25006	73.49491	86.55680	529.53781	-159.34528	563.72604	1
70	H	74.89275	74.55769	86.50350	654.59388	2347.94251	1217.51488	1
71	H	75.25220	73.22581	87.64530	-1526.55661	2103.42026	817.87394	1
72	O	76.59496	73.40859	86.03642	-554.84278	14.12789	399.58769	1
73	H	76.40454	73.57016	85.07093	1297.06236	2061.84854	1220.68812	1
74	C	74.31831	72.83625	84.18243	-662.15484	-412.13544	123.62687	1
75	O	75.21877	73.47897	83.68002	-540.01537	-317.05804	274.91456	1
76	N	73.25701	72.26136	83.55571	-202.76299	-690.00100	-131.49145	1
77	H	72.81269	71.73776	84.32176	-702.62132	-2617.37191	281.70413	1
78	C	73.47835	71.59070	82.24875	-491.73914	576.34187	222.73509	1
79	H	74.39795	70.97280	82.37304	1977.17978	-1823.58850	-434.68928	1
80	C	72.22019	70.80395	81.97656	-649.50797	-328.66843	306.11224	1
81	H	71.36308	71.39069	82.37895	2075.07803	1452.16490	-1004.45904	1
82	C	71.99348	70.61105	80.48722	-615.18735	-489.99689	-70.96352	1
83	H	71.05008	70.03637	80.27682	-1226.32661	-1724.38906	-1716.47170	1
84	H	71.90743	71.60709	79.96367	2381.64273	-969.84735	900.46860	1
85	H	72.84301	70.05044	80.00763	2122.74991	1702.23946	-141.36228	1
86	C	72.23185	69.45487	82.67179	-501.86074	-479.61276	-376.42482	1
87	H	71.24887	68.91884	82.56241	993.79261	-2246.95401	-1177.81305	1
88	H	73.03132	68.78477	82.23546	42.71279	-626.15391	-2651.37258	1
89	H	72.44201	69.55512	83.77332	-2026.39012	-1590.33709	-887.82922	1
90	C	73.62692	72.77413	81.11623	-672.89153	382.57394	-156.34072	1
91	O	72.71447	73.53523	80.89150	410.04627	221.86223	500.35950	1
92	N	74.75533	72.62825	80.42162	-378.11782	-443.79414	-441.10984	1
93	H	75.40973	71.91295	80.74167	2404.15973	-568.14894	1149.30085	1
94	C	75.20151	73.80260	79.72567	-544.54484	466.16019	331.29119	1
95	H	74.25504	74.37760	79.58217	-1409.80988	-170.17955	2325.32679	1
96	C	76.19507	74.51227	80.73784	-184.48284	116.78282	-758.89137	1
97	H	75.73319	74.56804	81.75401	1893.78641	1861.14652	611.04528	1
98	H	77.12623	73.91529	80.86081	-2170.79665	-974.19311	1327.50117	1
99	C	76.52019	75.92976	80.17525	389.51668	672.81878	-138.49152	1
100	H	76.97126	75.83759	79.15955	510.64577	1933.03327	1851.02484	1
101	H	75.58012	76.50070	80.00731	-2302.30869	-1105.72939	-948.89774	1
102	C	77.48326	76.76143	81.10525	-559.93427	-126.34590	542.30857	1
103	O	77.91539	77.81463	80.71379	-670.36003	-111.83166	76.36448	1
104	N	77.71966	76.19592	82.30848	-216.06729	-537.07037	446.51379	1
105	H	77.35098	75.32659	82.71219	-1251.96487	1074.12894	-2168.52500	1
106	H	78.29227	76.62909	83.04123	-2451.83023	-720.73851	944.84612	1
107	C	75.92868	73.38642	78.32949	546.24052	-563.88337	-85.11809	1
108	O	77.02677	73.81773	78.09363	71.70702	-307.40463	606.69673	1
109	N	75.12908	72.64661	77.53972	479.90863	-504.50129	222.86849	1
110	C	75.61623	72.03199	76.35004	75.51268	-600.91904	506.73700	1
111	H	76.71807	71.92971	76.47704	-2033.61562	1795.30103	254.89480	1
112	C	74.76924	70.68937	76.34508	523.79067	517.99274	284.45581	1
113	H	74.74377	70.19770	75.34724	1599.61665	-1127.00911	1895.98173	1

114	H	75.18588	69.94605	77.06125	-1881.83093	1275.82488	-1501.55016	1
115	C	73.37038	71.19950	76.81349	-600.05639	-404.05026	316.64485	1
116	H	72.83105	71.71346	75.98284	-2597.05260	496.36221	657.73249	1
117	H	72.69674	70.39291	77.18197	-1666.24518	1294.38985	-1723.90591	1
118	C	73.79321	72.22673	77.94756	493.57570	-129.95376	-602.56394	1
119	H	73.15091	73.13508	78.03518	-1469.08415	-637.84797	2204.22581	1
120	H	73.93235	71.77658	78.96041	-1038.97840	1068.88701	-2280.71789	1
121	C	75.18648	72.93527	75.04518	188.88100	241.05089	-727.87821	1
122	O	74.07874	72.88146	74.57025	531.88613	-49.19943	427.07960	1
123	N	76.27224	73.60303	74.52565	708.14833	26.93417	-179.73509	1
124	H	76.94573	73.51351	75.29870	-2232.69501	-1179.09831	1023.94816	1
125	C	76.01911	74.95388	73.96010	-738.32412	259.92548	104.42456	1
126	H	75.48091	75.49389	74.77170	2028.89123	1260.02983	1311.33324	1
127	C	77.36389	75.54679	73.63021	-258.65678	-345.52513	661.28459	1
128	H	77.97097	74.75374	73.13716	-1826.06090	-1801.46097	-918.64554	1
129	C	77.25183	76.71576	72.66593	-541.23400	531.92970	-218.41428	1
130	H	78.26231	77.11830	72.38055	1311.73218	-2219.18200	882.19023	1
131	H	76.73092	76.41778	71.71314	-1048.71298	1223.58118	-2196.97971	1
132	H	76.66663	77.56675	73.10981	419.06414	1903.92898	1903.44670	1
133	C	78.11727	75.99105	74.87308	-423.86431	152.66566	-648.55262	1
134	H	79.15082	76.35721	74.62341	105.68386	-2342.50080	1387.51238	1
135	H	77.58655	76.83005	75.40066	-1695.63603	-1484.73621	-1531.02793	1
136	H	78.23032	75.15406	75.61554	-1853.57121	-487.39031	1936.59343	1
137	C	75.09278	74.80989	72.60873	539.71428	-510.58232	267.58633	1
138	O	74.15812	75.61568	72.43372	-15.93758	-278.34085	-624.49402	1
139	N	75.55236	73.91187	71.77069	-676.81886	12.05292	276.17960	1
140	H	76.35902	73.48446	72.23420	-1694.44250	-373.84189	-2100.66098	1
141	C	74.72955	73.19062	70.85955	412.33078	-664.70360	108.35451	1
142	H	75.45168	72.45880	70.43613	1765.77476	1294.44366	1621.76594	1
143	C	73.62018	72.48019	71.73072	-179.66635	-721.95667	-264.73915	1
144	H	74.08952	71.85540	72.52616	-607.34922	2587.87032	-598.10018	1
145	H	72.99595	73.21598	72.28697	-359.69332	-1479.13954	-2259.74260	1
146	C	72.76867	71.61342	70.74321	-240.01076	616.02425	431.85322	1
147	H	72.11111	72.26075	70.12083	-1359.17131	782.54425	2227.99181	1
148	H	73.43031	71.07808	70.02634	-820.36667	85.81767	-2596.78715	1
149	C	71.91481	70.57286	71.57180	-513.07015	236.18570	-551.87280	1
150	H	72.57341	69.90549	72.17408	1816.11944	-1183.11722	-1650.94321	1
151	H	71.25138	71.08746	72.30437	-1800.04429	-1361.53473	1526.34643	1
152	C	71.09236	69.75973	70.54419	726.08972	-253.19732	-179.64713	1
153	H	70.30594	70.33982	70.02150	1224.27271	-456.51798	-2390.90304	1
154	H	71.70164	69.20090	69.80600	1206.40339	-1150.93514	-2154.90344	1
155	N	70.31565	68.64625	71.32337	329.70796	-633.68968	-155.67358	1
156	H	69.69853	68.02037	70.72927	1348.31305	1938.76845	1359.00643	1
157	H	70.89748	67.92739	71.84451	2096.92035	1446.54551	-966.48890	1
158	H	69.63314	68.96224	72.07227	-1197.07217	-2303.53719	827.28733	1
159	C	74.11572	74.17219	69.68917	-378.01186	-556.17301	-413.96481	1
160	O	74.78161	74.35617	68.69780	-409.44433	-307.55053	-453.30833	1
161	N	72.89294	74.60674	69.95639	-429.02477	524.70884	274.08502	1
162	H	72.49761	74.39688	70.87107	1706.34263	-1425.96036	1574.38926	1
163	C	72.20869	75.42416	69.01717	-45.25864	-626.22952	478.93267	1
164	H	72.88057	75.46051	68.12553	1988.63164	570.90773	1772.87287	1
165	C	70.81204	74.71045	68.75191	551.77128	-20.49526	-564.54996	1
166	H	70.95473	73.63543	68.50436	1434.61535	-1753.10253	1513.99471	1
167	H	70.21157	74.71945	69.68827	-714.67738	1819.09770	1898.36494	1
168	C	70.04486	75.44557	67.60714	446.99263	-555.77305	338.97221	1
169	H	70.18151	76.55817	67.70255	1953.68466	1892.25957	-161.67766	1
170	H	70.44007	75.17056	66.60289	-403.03785	2688.07032	-188.43591	1
171	C	68.50975	75.08724	67.74700	567.86262	335.74681	434.04421	1
172	H	68.29577	74.06052	67.37120	-1080.02275	1568.26081	-1948.78900	1
173	H	68.19854	75.09101	68.81675	-919.54108	2111.34692	1456.13463	1
174	C	67.71932	76.16045	66.96298	195.81897	173.33862	-745.11536	1
175	H	67.86386	77.19682	67.33315	1405.67949	-2301.21089	-390.08113	1

176	H	67.85506	76.13280	65.86306	-940.37328	-1118.32446	2299.72133	1
177	N	66.19437	75.88937	67.18545	319.26422	656.36007	-42.02424	1
178	H	65.54983	76.58061	66.70432	1961.03633	619.91968	1787.09422	1
179	H	65.80601	74.96460	66.83850	854.14343	-2156.80752	1429.08711	1
180	H	65.83147	75.92440	68.18252	1237.02905	-1378.50857	-1998.28500	1
181	C	71.88695	76.88663	69.66334	532.53319	-268.57236	517.55729	1
182	O	71.10255	77.63093	69.11429	266.16714	-290.73804	-558.88002	1
183	N	72.55252	77.10546	70.78673	-226.25352	640.49678	-270.32839	1
184	H	73.23484	76.41277	71.17814	2007.69063	-1035.27229	1523.50231	1
185	C	72.40072	78.42551	71.34123	-540.76542	-573.33303	49.50000	1
186	H	71.30687	78.62440	71.38280	-2374.20950	-1036.76023	843.75774	1
187	C	73.15224	78.37976	72.74613	-77.09082	666.87422	-415.84136	1
188	H	74.20473	78.02193	72.54327	-985.81834	617.19825	2463.91927	1
189	O	72.65521	77.42144	73.68682	293.29899	-391.65602	-477.80926	1
190	H	73.22403	76.61929	73.43367	2528.72714	-681.76262	-751.27122	1
191	C	73.16724	79.88715	73.18614	252.47363	-605.14473	440.05134	1
192	H	73.75573	80.03401	74.12132	-2052.65063	1456.49051	-1043.51830	1
193	H	73.61558	80.54455	72.40360	-2152.98800	-1661.97574	-161.70652	1
194	H	72.13595	80.26302	73.38147	-473.12726	-1584.27339	2165.61725	1
195	C	73.19402	79.46183	70.36527	360.36307	488.46713	505.10056	1
196	O	74.37888	79.27781	70.10183	-200.08817	-528.03552	-385.82850	1
197	N	72.42887	80.49808	70.10500	-597.54095	-226.44775	355.20479	1
198	H	71.46615	80.46067	70.43516	2179.23655	-1300.70981	-991.33835	1
199	C	72.79347	81.37966	69.03689	-687.68921	297.39807	-249.45179	1
200	H	73.16349	80.69489	68.24222	-349.16256	-2467.37713	-1101.72831	1
201	C	71.54084	82.28587	68.65531	672.47345	361.54328	-201.62880	1
202	H	71.18137	82.83442	69.55645	1541.41502	582.18425	2169.97026	1
203	H	71.85875	83.05802	67.91653	-2534.67717	60.25153	997.72295	1
204	C	70.41374	81.41954	68.06927	574.26774	-389.43119	-377.02542	1
205	C	70.54484	80.90942	66.74348	688.82679	-287.33580	-257.96133	1
206	H	71.45588	81.10737	66.14980	331.14182	1470.38163	2269.80013	1
207	C	69.24290	81.14939	68.83914	-383.52382	-675.04808	144.24917	1
208	H	69.14483	81.53394	69.87058	4.09847	1517.59662	2262.86397	1
209	C	69.49223	80.16384	66.21085	-134.76730	428.45285	-649.50303	1
210	H	69.58829	79.77518	65.18235	-903.23433	1600.49020	2011.53387	1
211	C	68.21518	80.40039	68.25897	-335.53281	-615.00040	-364.39058	1
212	H	67.30876	80.20478	68.85824	1596.45398	-1369.33862	1732.02659	1
213	C	68.29436	79.88845	66.93140	585.48547	-340.24194	-406.23938	1
214	O	67.24934	79.13340	66.33183	-419.15649	-173.04408	-511.94141	1
215	H	66.57997	79.17734	67.05509	-1071.84350	1559.71507	-1960.13012	1
216	C	73.94414	82.39866	69.56643	291.41878	-183.13091	710.72246	1
217	O	73.71075	83.57255	69.72517	379.87695	523.47396	-222.23622	1
218	N	75.10226	81.74690	69.71065	564.30591	373.09380	277.24371	1
219	H	75.16009	80.70101	69.57307	-120.59931	-2436.07824	-1214.35098	1
220	C	76.09065	82.42391	70.50056	404.07514	-299.37480	608.84009	1
221	H	75.55161	83.26170	71.00409	-1071.07882	-841.69025	2359.66467	1
222	C	76.70607	81.35216	71.49454	-683.12807	68.71770	-390.13096	1
223	H	75.90627	80.83089	72.06750	2068.88918	1596.58590	770.89603	1
224	H	77.23650	80.55268	70.92942	1379.86429	2342.49779	-179.85638	1
225	C	77.68071	82.11462	72.44282	-176.39967	537.49466	550.97268	1
226	H	78.42765	82.69491	71.84972	-396.28051	1942.22168	1869.33314	1
227	H	77.13894	82.86763	73.05781	-94.44700	586.00678	-2659.20016	1
228	C	78.38152	81.01263	73.36443	-291.69381	-718.18079	-150.72929	1
229	H	77.70177	80.42235	74.03013	-2303.38776	1089.76242	964.62032	1
230	H	79.03881	80.29198	72.81410	884.16729	2568.80533	-207.74283	1
231	N	79.20365	81.80926	74.17491	-594.49522	-252.81478	342.29276	1
232	H	79.33858	82.76432	73.88021	-1735.17426	2084.05705	-263.71605	1
233	C	79.79443	81.41075	75.22786	595.23177	-271.52487	442.22352	1
234	N	79.61127	80.07945	75.61609	585.53813	-424.79750	-105.81303	1
235	H	79.05986	79.34211	75.17881	959.88797	1327.56823	-2177.11905	1
236	H	80.02407	79.65492	76.44746	1578.48647	16.27378	-2220.76233	1
237	N	80.54543	82.44703	75.80015	-452.17763	-390.33541	-421.51853	1

238	H	80.67293	83.41730	75.51616	470.26107	1974.25629	-1817.92087	1
239	H	81.08951	82.33344	76.65626	1856.67307	-1573.97321	-1224.35416	1
240	C	77.26664	82.96739	69.51436	-531.47271	-581.45780	-55.06206	1
241	O	77.99450	83.84524	69.92179	-243.00837	192.73507	609.52485	1
242	N	77.33917	82.28967	68.37448	343.49288	-644.25607	38.09164	1
243	H	76.73095	81.46685	68.20182	-1691.16043	-1535.97525	-1484.73099	1
244	C	77.88018	82.99560	67.24506	542.66492	350.14337	454.42563	1
245	H	77.63880	84.05607	67.47915	1209.57979	-2396.95920	463.86744	1
246	C	79.45508	82.76981	67.28896	-737.14309	145.93010	242.71942	1
247	H	79.69847	81.91366	67.95426	-1050.18303	159.36419	-2509.06125	1
248	C	80.08212	82.56737	65.86749	-706.77696	-252.88343	-245.16230	1
249	H	81.19715	82.59685	65.89788	-1624.64039	-1665.49085	1417.86935	1
250	H	79.78531	81.58293	65.42889	2566.10521	598.51109	693.22305	1
251	H	79.74311	83.35943	65.15579	-1972.69758	107.10018	-1876.34312	1
252	C	80.05997	84.10381	67.84492	412.85148	672.58832	-27.69222	1
253	H	81.16159	84.02851	68.00260	1447.02277	1762.76533	-1490.78944	1
254	H	79.88209	84.95720	67.14825	1320.77379	-145.20455	2378.68491	1
255	H	79.58710	84.37270	68.83554	-1512.10848	1470.52031	1724.75147	1
256	C	77.12553	82.44221	65.92142	-607.11113	499.56689	73.73769	1
257	O	77.71027	82.35514	64.86384	357.97126	460.81534	356.68785	1
258	N	75.80576	82.30750	66.14506	536.55407	-368.62270	332.76306	1
259	H	75.54956	82.48497	67.11918	524.38866	2297.69985	1367.20941	1
260	C	75.13251	81.19995	65.51114	46.50277	-774.29190	-147.97904	1
261	H	74.05914	81.42774	65.68756	1676.51875	1883.29066	1032.55549	1
262	C	75.49847	81.10196	63.94598	-559.41456	-34.19198	-556.30433	1
263	H	76.55770	80.75695	63.83806	-64.66664	395.18769	2695.05373	1
264	H	74.87490	80.33244	63.43023	-2703.44278	-60.40056	333.79418	1
265	C	75.32473	82.45566	63.30728	-519.76435	377.31045	459.42366	1
266	H	75.76765	83.21023	63.99400	-1746.74323	1667.50644	-1261.73691	1
267	C	76.06839	82.52350	61.97962	570.95554	16.46261	-545.27700	1
268	H	75.96799	83.53119	61.50003	2391.58273	28.05277	-1305.07271	1
269	H	77.16403	82.32868	62.11577	175.75588	917.63458	2559.43867	1
270	H	75.68318	81.76719	61.24845	-1063.97851	-2155.34650	1283.00462	1
271	C	73.85351	82.78587	63.09934	193.76014	2.62946	-765.53141	1
272	H	73.71847	83.80458	62.65272	507.39394	-846.55087	2539.60089	1
273	H	73.36074	82.05381	62.40893	1337.57841	1818.19054	1526.01994	1
274	H	73.28497	82.76776	64.06451	1100.88635	-1172.91350	-2199.08909	1
275	C	75.57382	79.88765	66.28854	-549.21115	475.64486	-309.38218	1
276	O	76.16095	79.92377	67.35229	556.06106	-390.37755	-78.24250	1
277	O	75.17855	78.65213	65.73368	-572.27940	-310.19032	-209.75862	1
278	H	74.69719	78.98904	64.92735	-1380.08193	2212.14486	790.85944	1

Listing 111: C00111.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.3991	0.0000	300.0000
3	H	71.45839	78.32557	88.18066	-2043.14101	-1757.64893	399.89339		1
4	N	72.08738	78.01669	87.44287	426.75047	490.45733	-334.42467		1
5	H	72.32469	77.07469	87.74562	442.25559	-1110.30854	-2448.52907		1
6	C	73.18235	78.86575	87.18421	415.32972	-666.39213	83.73172		1
7	H	72.73789	79.88364	87.20217	879.32219	2491.00447	667.35213		1
8	C	74.33493	78.68110	88.29404	31.35357	477.41777	628.23362		1
9	H	74.67417	77.61756	88.30418	1168.38489	2240.25337	-1019.71136		1
10	H	75.22667	79.27990	87.98779	-360.43770	2534.90498	931.67112		1
11	C	73.86522	79.09575	89.66445	463.18208	512.70242	-382.34388		1
12	H	72.99400	78.46491	89.94981	1725.29117	1863.52247	-987.07854		1
13	C	74.97962	78.87587	90.68086	710.42801	-144.27427	-313.15367		1
14	H	74.65613	79.15176	91.71750	364.20195	-1033.13725	2494.72524		1
15	H	75.31129	77.80592	90.70834	2567.61904	335.80679	847.48802		1
16	H	75.88204	79.49542	90.44033	-2587.99029	680.92867	-512.16411		1
17	C	73.43785	80.55666	89.69600	268.17616	741.64379	-40.42634		1

18	H	73.16379	80.88423	90.73213	1283.54314	-1945.37420	-1411.27812	1
19	H	74.25784	81.23296	89.34062	-1258.57796	1317.15249	-2026.02085	1
20	H	72.54608	80.74495	89.04456	-2502.84526	909.80597	575.92391	1
21	C	73.84953	78.48050	85.75948	619.36578	-458.64843	-172.09273	1
22	O	75.03711	78.70506	85.57713	-81.40433	433.87611	522.34594	1
23	N	72.96507	77.96377	84.92022	175.23996	-622.20190	341.55523	1
24	H	72.00722	77.90398	85.26355	-876.57256	-303.22879	-2561.90213	1
25	C	73.32052	77.71264	83.56290	-571.88214	-534.10783	-106.15033	1
26	H	74.37906	77.37411	83.58714	-2713.20841	-16.25800	-248.80809	1
27	C	72.27382	76.64040	83.00797	166.60354	288.16399	-716.09568	1
28	H	71.23808	77.06297	83.12537	-2097.85574	1636.78449	-586.18044	1
29	O	72.26272	75.37040	83.68561	-317.80580	-363.38227	484.43082	1
30	H	71.36082	75.36283	84.06369	1863.74748	-1451.84923	1357.29467	1
31	C	72.64851	76.60360	81.48070	503.80731	517.99032	318.51606	1
32	H	71.95498	75.94495	80.90807	640.61020	-2157.10410	-1536.29104	1
33	H	72.60143	77.61741	81.01646	1687.88455	465.60692	2087.56452	1
34	H	73.68054	76.21358	81.32260	-1293.07895	-1899.88581	-1463.57452	1
35	C	73.10887	79.11913	82.75782	-153.07550	-733.68902	248.70981	1
36	O	71.99660	79.56797	82.66902	186.15459	-480.78787	-449.34387	1
37	N	74.26118	79.59490	82.24882	-487.53139	543.18517	42.03850	1
38	C	74.24904	80.81550	81.51084	-699.35871	69.34393	360.10701	1
39	H	73.33127	81.34438	81.85791	2.81126	-221.99807	-2715.58072	1
40	C	75.62803	81.46817	81.94553	-507.46439	-592.59194	122.07761	1
41	H	76.02513	82.17519	81.18314	-1975.08116	525.87560	-1801.71556	1
42	H	75.50325	82.05812	82.88086	1588.27743	-1913.22100	1113.83566	1
43	C	76.57668	80.25139	82.19285	-613.62442	-457.55993	-194.14490	1
44	H	77.12404	79.96477	81.26628	1707.54637	-721.27992	1996.92523	1
45	H	77.36351	80.46391	82.95131	758.23357	2100.81767	1560.55011	1
46	C	75.57350	79.11613	82.66056	-352.41524	704.96076	49.21465	1
47	H	75.73550	78.12349	82.17686	1714.76886	-2070.42778	443.35792	1
48	H	75.49594	78.97987	83.79132	1224.15040	1801.50881	1636.97633	1
49	C	74.17471	80.51762	79.89543	566.85117	537.05831	117.62814	1
50	O	73.24967	80.98716	79.27063	-550.26779	-406.08867	4.21666	1
51	N	75.16931	79.75518	79.45104	566.34832	-425.77725	180.18749	1
52	H	75.85090	79.47785	80.15440	644.44502	2646.80550	-52.73430	1
53	C	75.54034	79.92007	78.07187	612.34801	-281.48662	411.56221	1
54	H	75.40303	81.00178	77.85322	1667.23498	-1490.75142	1556.16753	1
55	C	77.03308	79.39696	77.90096	-714.45746	-175.43074	286.98927	1
56	H	77.12330	78.37754	78.36647	-787.09484	1763.03619	-1922.46060	1
57	O	78.05227	80.20929	78.51416	-429.46514	516.51932	-128.40526	1
58	H	78.50498	79.55746	79.08402	1981.82785	436.16847	-1818.18182	1
59	C	77.07607	79.25142	76.33407	630.79189	-468.94448	76.03230	1
60	H	78.02044	78.77105	75.98784	-1775.71861	2062.30353	131.89849	1
61	H	76.22169	78.62563	75.96844	-1855.14608	88.94118	1993.53760	1
62	H	77.00124	80.24200	75.82780	-1504.82350	-780.94249	-2132.90992	1
63	C	74.53339	78.97642	77.18811	288.57638	618.62814	-397.00270	1
64	O	74.53130	77.76993	77.24760	321.70495	-185.26452	574.37218	1
65	N	73.87903	79.77960	76.35080	-447.05792	-446.53431	367.76425	1
66	H	73.98386	80.78842	76.45922	350.31316	1975.63644	-1843.31522	1
67	C	72.67767	79.29064	75.73248	-511.23061	374.03917	-471.51480	1
68	H	73.06102	78.42335	75.14854	2234.79579	-898.70890	-1273.45190	1
69	C	71.69459	78.81393	76.90072	529.53781	-159.34528	563.72604	1
70	H	70.94786	78.10696	76.44758	654.59388	2347.94251	1217.51488	1
71	H	72.32013	78.21031	77.61296	-1526.55661	2103.42026	817.87394	1
72	O	70.96866	79.86276	77.58328	-554.84278	14.12789	399.58769	1
73	H	71.67990	80.20077	78.17569	1297.06236	2061.84854	1220.68812	1
74	C	72.14677	80.51907	74.83326	-662.15484	-412.13544	123.62687	1
75	O	72.91981	81.25101	74.25570	-540.01537	-317.05804	274.91456	1
76	N	70.80576	80.49220	74.73427	-202.76299	-690.00100	-131.49145	1
77	H	70.34138	79.86355	75.39275	-702.62132	-2617.37191	281.70413	1
78	C	70.05504	81.49597	73.99122	-491.73914	576.34187	222.73509	1
79	H	68.99549	81.31112	74.28656	1977.17978	-1823.58850	-434.68928	1

80	C	70.54167	82.85730	74.45022	-649.50797	-328.66843	306.11224	1
81	H	71.65289	82.88800	74.30270	2075.07803	1452.16490	-1004.45904	1
82	C	69.92780	83.99357	73.65548	-615.18735	-489.99689	-70.96352	1
83	H	70.27057	84.99769	74.03062	-1226.32661	-1724.38906	-1716.47170	1
84	H	70.20294	83.92808	72.56422	2381.64273	-969.84735	900.46860	1
85	H	68.80454	83.98040	73.71333	2122.74991	1702.23946	-141.36228	1
86	C	70.26984	83.05535	75.93153	-501.86074	-479.61276	-376.42482	1
87	H	70.70061	84.02077	76.31392	993.79261	-2246.95401	-1177.81305	1
88	H	69.16703	83.07268	76.15041	42.71279	-626.15391	-2651.37258	1
89	H	70.71385	82.22116	76.54422	-2026.39012	-1590.33709	-887.82922	1
90	C	70.25868	81.23274	72.35406	-672.89153	382.57394	-156.34072	1
91	O	69.67282	81.93930	71.56886	410.04627	221.86223	500.35950	1
92	N	71.06309	80.22302	72.10331	-378.11782	-443.79414	-441.10984	1
93	H	71.51429	79.81749	72.92121	2404.15973	-568.14894	1149.30085	1
94	C	71.25756	79.67812	70.79080	-544.54484	466.16019	331.29119	1
95	H	70.25282	79.42132	70.38931	-1409.80988	-170.17955	2325.32679	1
96	C	71.93168	80.85175	69.96712	-184.48284	116.78282	-758.89137	1
97	H	71.22782	81.71631	69.90810	1893.78641	1861.14652	611.04528	1
98	H	72.83164	81.22855	70.50442	-2170.79665	-974.19311	1327.50117	1
99	C	72.31113	80.33163	68.54556	389.51668	672.81878	-138.49152	1
100	H	72.99277	79.45373	68.61945	510.64577	1933.03327	1851.02484	1
101	H	71.41340	79.93029	68.02609	-2302.30869	-1105.72939	-948.89774	1
102	C	72.97673	81.45102	67.65761	-559.93427	-126.34590	542.30857	1
103	O	73.40616	81.17312	66.56759	-670.36003	-111.83166	76.36448	1
104	N	72.98356	82.67579	68.22775	-216.06729	-537.07037	446.51379	1
105	H	72.60917	82.98240	69.13308	-1251.96487	1074.12894	-2168.52500	1
106	H	73.33280	83.52085	67.76324	-2451.83023	-720.73851	944.84612	1
107	C	72.27094	78.43004	70.99689	546.24052	-563.88337	-85.11809	1
108	O	73.23983	78.56506	71.70457	71.70702	-307.40463	606.69673	1
109	N	71.91771	77.36601	70.25822	479.90863	-504.50129	222.86849	1
110	C	72.83117	76.27704	70.10837	75.51268	-600.91904	506.73700	1
111	H	73.35459	76.15475	71.08539	-2033.61562	1795.30103	254.89480	1
112	C	71.87844	75.09158	69.67293	523.79067	517.99274	284.45581	1
113	H	72.42800	74.27075	69.15959	1599.61665	-1127.00911	1895.98173	1
114	H	71.36507	74.63482	70.54914	-1881.83093	1275.82488	-1501.55016	1
115	C	70.87764	75.85252	68.74628	-600.05639	-404.05026	316.64485	1
116	H	71.34210	76.03901	67.74877	-2597.05260	496.36221	657.73249	1
117	H	69.93140	75.29668	68.55960	-1666.24518	1294.38985	-1723.90591	1
118	C	70.66174	77.21300	69.53812	493.57570	-129.95376	-602.56394	1
119	H	70.51373	78.11113	68.89481	-1469.08415	-637.84797	2204.22581	1
120	H	69.86361	77.18099	70.31681	-1038.97840	1068.88701	-2280.71789	1
121	C	73.84413	76.73968	68.88133	188.88100	241.05089	-727.87821	1
122	O	73.49391	76.76932	67.72809	531.88613	-49.19943	427.07960	1
123	N	74.97675	77.12522	69.44695	708.14833	26.93417	-179.73509	1
124	H	74.98664	77.15875	70.46510	-2232.69501	-1179.09831	1023.94816	1
125	C	76.18128	77.23216	68.68736	-738.32412	259.92548	104.42456	1
126	H	75.79122	77.67392	67.74251	2028.89123	1260.02983	1311.33324	1
127	C	77.12215	78.19090	69.52645	-258.65678	-345.52513	661.28459	1
128	H	77.38223	77.71408	70.52708	-1826.06090	-1801.46097	-918.64554	1
129	C	78.40191	78.56795	68.70508	-541.23400	531.92970	-218.41428	1
130	H	79.01658	79.33286	69.23532	1311.73218	-2219.18200	882.19023	1
131	H	79.05831	77.68243	68.52409	-1048.71298	1223.58118	-2196.97971	1
132	H	78.13534	78.99125	67.70823	419.06414	1903.92898	1903.44670	1
133	C	76.32940	79.52612	69.75007	-423.86431	152.66566	-648.55262	1
134	H	76.92281	80.26671	70.33525	105.68386	-2342.50080	1387.51238	1
135	H	76.05703	80.00687	68.78103	-1695.63603	-1484.73621	-1531.02793	1
136	H	75.37765	79.34742	70.30575	-1853.57121	-487.39031	1936.59343	1
137	C	76.73809	75.72549	68.39038	539.71428	-510.58232	267.58633	1
138	O	76.00578	74.93841	67.82628	-15.93758	-278.34085	-624.49402	1
139	N	77.99812	75.51413	68.75276	-676.81886	12.05292	276.17960	1
140	H	78.51947	76.24060	69.24160	-1694.44250	-373.84189	-2100.66098	1
141	C	78.62188	74.36804	68.15978	412.33078	-664.70360	108.35451	1

142	H	78.04761	74.18449	67.22199	1765.77476	1294.44366	1621.76594	1
143	C	80.15187	74.69292	67.94506	-179.66635	-721.95667	-264.73915	1
144	H	80.28210	75.56637	67.26735	-607.34922	2587.87032	-598.10018	1
145	H	80.63677	74.98502	68.90309	-359.69332	-1479.13954	-2259.74260	1
146	C	80.82766	73.41183	67.34871	-240.01076	616.02425	431.85322	1
147	H	80.68855	72.54718	68.03619	-1359.17131	782.54425	2227.99181	1
148	H	80.34588	73.11777	66.38963	-820.36667	85.81767	-2596.78715	1
149	C	82.36567	73.70988	67.13437	-513.07015	236.18570	-551.87280	1
150	H	82.51173	74.52671	66.39074	1816.11944	-1183.11722	-1650.94321	1
151	H	82.83325	74.07293	68.07820	-1800.04429	-1361.53473	1526.34643	1
152	C	83.04479	72.40454	66.65817	726.08972	-253.19732	-179.64713	1
153	H	83.03156	71.58095	67.39969	1224.27271	-456.51798	-2390.90304	1
154	H	82.69405	72.03261	65.67490	1206.40339	-1150.93514	-2154.90344	1
155	N	84.56538	72.71227	66.44147	329.70796	-633.68968	-155.67358	1
156	H	85.15901	71.89092	66.12775	1348.31305	1938.76845	1359.00643	1
157	H	84.81107	73.43765	65.70657	2096.92035	1446.54551	-966.48890	1
158	H	85.11522	73.05679	67.28150	-1197.07217	-2303.53719	827.28733	1
159	C	78.47263	73.08157	69.17534	-378.01186	-556.17301	-413.96481	1
160	O	77.98874	72.05088	68.76655	-409.44433	-307.55053	-453.30833	1
161	N	79.01528	73.33137	70.36023	-429.02477	524.70884	274.08502	1
162	H	79.34713	74.28053	70.52747	1706.34263	-1425.96036	1574.38926	1
163	C	78.86118	72.36827	71.39650	-45.25864	-626.22952	478.93267	1
164	H	78.48319	71.46377	70.86322	1988.63164	570.90773	1772.87287	1
165	C	80.29044	72.16577	72.04998	551.77128	-20.49526	-564.54996	1
166	H	81.05695	71.98374	71.26357	1434.61535	-1753.10253	1513.99471	1
167	H	80.61935	73.08621	72.58192	-714.67738	1819.09770	1898.36494	1
168	C	80.19058	70.95207	73.03101	446.99263	-555.77305	338.97221	1
169	H	79.44452	71.16986	73.83610	1953.68466	1892.25957	-161.67766	1
170	H	79.81760	70.04501	72.50421	-403.03785	2688.07032	-188.43591	1
171	C	81.62394	70.68902	73.64525	567.86262	335.74681	434.04421	1
172	H	82.33507	70.33596	72.86321	-1080.02275	1568.26081	-1948.78900	1
173	H	82.06299	71.62837	74.05304	-919.54108	2111.34692	1456.13463	1
174	C	81.45074	69.63373	74.76247	195.81897	173.33862	-745.11536	1
175	H	80.88238	69.98789	75.64582	1405.67949	-2301.21089	-390.08113	1
176	H	81.04800	68.65964	74.42030	-940.37328	-1118.32446	2299.72133	1
177	N	82.87605	69.29694	75.31532	319.26422	656.36007	-42.02424	1
178	H	82.89900	68.60278	76.11696	1961.03633	619.91968	1787.09422	1
179	H	83.56655	68.85743	74.63927	854.14343	-2156.80752	1429.08711	1
180	H	83.44191	70.09948	75.71824	1237.02905	-1378.50857	-1998.28500	1
181	C	77.80655	72.92361	72.52280	532.53319	-268.57236	517.55729	1
182	O	77.76174	72.42820	73.63010	266.16714	-290.73804	-558.88002	1
183	N	77.00418	73.83840	72.00840	-226.25352	640.49678	-270.32839	1
184	H	77.17968	74.11164	71.04246	2007.69063	-1035.27229	1523.50231	1
185	C	76.05876	74.52079	72.83968	-540.76542	-573.33303	49.50000	1
186	H	76.40316	74.32570	73.88424	-2374.20950	-1036.76023	843.75774	1
187	C	76.10809	76.01273	72.39299	-77.09082	666.87422	-415.84136	1
188	H	75.97168	76.07366	71.27409	-985.81834	617.19825	2463.91927	1
189	O	77.52258	76.78913	72.17597	293.29899	-391.65602	-477.80926	1
190	H	77.51943	77.25661	72.99464	2528.72714	-681.76262	-751.27122	1
191	C	75.09944	76.83946	73.22211	252.47363	-605.14473	440.05134	1
192	H	74.90832	77.85094	72.76271	-2052.65063	1456.49051	-1043.51830	1
193	H	74.09795	76.31892	73.29898	-2152.98800	-1661.97574	-161.70652	1
194	H	75.46351	77.00727	74.26712	-473.12726	-1584.27339	2165.61725	1
195	C	74.57921	73.84809	72.53481	360.36307	488.46713	505.10056	1
196	O	73.56520	74.50521	72.65363	-200.08817	-528.03552	-385.82850	1
197	N	74.69093	72.56516	72.22548	-597.54095	-226.44775	355.20479	1
198	H	75.64279	72.20372	72.19286	2179.23655	-1300.70981	-991.33835	1
199	C	73.52024	71.82289	71.96390	-687.68921	297.39807	-249.45179	1
200	H	72.70095	72.57350	71.87439	-349.16256	-2467.37713	-1101.72831	1
201	C	73.74995	70.89906	70.67407	672.47345	361.54328	-201.62880	1
202	H	74.76441	70.44137	70.70683	1541.41502	582.18425	2169.97026	1
203	H	73.00999	70.06594	70.69499	-2534.67717	60.25153	997.72295	1

204	C	73.56144	71.70751	69.38493	574.26774	-389.43119	-377.02542	1
205	C	72.23542	71.91188	68.89352	688.82679	-287.33580	-257.96133	1
206	H	71.36047	71.55289	69.46444	331.14182	1470.38163	2269.80013	1
207	C	74.68872	72.19745	68.65769	-383.52382	-675.04808	144.24917	1
208	H	75.71949	72.05986	69.04113	4.09847	1517.59662	2262.86397	1
209	C	72.06755	72.56109	67.67090	-134.76730	428.45285	-649.50303	1
210	H	71.04343	72.71518	67.28895	-903.23433	1600.49020	2011.53387	1
211	C	74.46633	72.83695	67.43411	-335.53281	-615.00040	-364.39058	1
212	H	75.34873	73.18736	66.85782	1596.45398	-1369.33862	1732.02659	1
213	C	73.16185	73.04180	66.89305	585.48547	-340.24194	-406.23938	1
214	O	72.92987	73.67451	65.64362	-419.15649	-173.04408	-511.94141	1
215	H	73.83543	74.02287	65.46216	-1071.84350	1559.71507	-1960.13012	1
216	C	73.22368	70.68453	73.10404	291.41878	-183.13091	710.72246	1
217	O	72.09309	70.25532	73.20376	379.87695	523.47396	-222.23622	1
218	N	74.31132	70.26157	73.73899	564.30591	373.09380	277.24371	1
219	H	75.20387	70.70239	73.52444	-120.59931	-2436.07824	-1214.35098	1
220	C	74.14752	69.14574	74.61470	404.07514	-299.37480	608.84009	1
221	H	73.03921	69.09533	74.75277	-1071.07882	-841.69025	2359.66467	1
222	C	74.71763	67.86839	73.86544	-683.12807	68.71770	-390.13096	1
223	H	74.17387	67.70295	72.90835	2068.88918	1596.58590	770.89603	1
224	H	75.78156	68.00902	73.57198	1379.86429	2342.49779	-179.85638	1
225	C	74.55151	66.64625	74.82071	-176.39967	537.49466	550.97268	1
226	H	75.03695	66.83332	75.80782	-396.28051	1942.22168	1869.33314	1
227	H	73.47900	66.46438	75.05641	-94.44700	586.00678	-2659.20016	1
228	C	75.20162	65.38445	74.08754	-291.69381	-718.18079	-150.72929	1
229	H	74.70291	65.05924	73.13904	-2303.38776	1089.76242	964.62032	1
230	H	76.30078	65.46076	73.88670	884.16729	2568.80533	-207.74283	1
231	N	75.01367	64.37417	75.04238	-594.49522	-252.81478	342.29276	1
232	H	74.63143	64.65722	75.93238	-1735.17426	2084.05705	-263.71605	1
233	C	75.29737	63.14826	74.86290	595.23177	-271.52487	442.22352	1
234	N	75.83371	62.77324	73.62615	585.53813	-424.79750	-105.81303	1
235	H	76.04911	63.34819	72.81266	959.88797	1327.56823	-2177.11905	1
236	H	76.10452	61.82347	73.36897	1578.48647	16.27378	-2220.76233	1
237	N	74.99745	62.39090	76.00354	-452.17763	-390.33541	-421.51853	1
238	H	74.61118	62.67323	76.90348	470.26107	1974.25629	-1817.92087	1
239	H	75.15347	61.38422	76.06774	1856.67307	-1573.97321	-1224.35416	1
240	C	74.95364	69.44946	76.00832	-531.47271	-581.45780	-55.06206	1
241	O	74.31022	69.88939	76.95942	-243.00837	192.73507	609.52485	1
242	N	76.23073	69.16418	75.93731	343.49288	-644.25607	38.09164	1
243	H	76.51654	68.80849	75.02660	-1691.16043	-1535.97525	-1484.73099	1
244	C	77.22739	69.50375	76.93534	542.66492	350.14337	454.42563	1
245	H	78.19893	69.33865	76.40947	1209.57979	-2396.95920	463.86744	1
246	C	77.00488	70.95188	77.35931	-737.14309	145.93010	242.71942	1
247	H	75.94135	71.04830	77.69073	-1050.18303	159.36419	-2509.06125	1
248	C	77.89788	71.33649	78.52182	-706.77696	-252.88343	-245.16230	1
249	H	77.71741	72.39670	78.85304	-1624.64039	-1665.49085	1417.86935	1
250	H	77.72358	70.67138	79.41364	2566.10521	598.51109	693.22305	1
251	H	78.98721	71.24929	78.25353	-1972.69758	107.10018	-1876.34312	1
252	C	77.20306	71.90216	76.19254	412.85148	672.58832	-27.69222	1
253	H	77.00232	72.97096	76.48048	1447.02277	1762.76533	-1490.78944	1
254	H	78.25427	71.85768	75.78852	1320.77379	-145.20455	2378.68491	1
255	H	76.51371	71.65118	75.33541	-1512.10848	1470.52031	1724.75147	1
256	C	77.08991	68.49482	78.25830	-607.11113	499.56689	73.73769	1
257	O	78.09503	68.02184	78.72170	357.97126	460.81534	356.68785	1
258	N	75.85039	68.42498	78.70752	536.55407	-368.62270	332.76306	1
259	H	75.07957	68.93259	78.21717	524.38866	2297.69985	1367.20941	1
260	C	75.59147	67.42692	79.68212	46.50277	-774.29190	-147.97904	1
261	H	76.59913	67.03511	79.95740	1676.51875	1883.29066	1032.55549	1
262	C	74.81072	68.11169	80.92150	-559.41456	-34.19198	-556.30433	1
263	H	73.82713	68.50888	80.57436	-64.66664	395.18769	2695.05373	1
264	H	74.57493	67.35075	81.70277	-2703.44278	-60.40056	333.79418	1
265	C	75.65155	69.22115	81.48980	-519.76435	377.31045	459.42366	1

266	H	75.86457	69.94621	80.67168	-1746.74323	1667.50644	-1261.73691	1
267	C	74.90852	69.95080	82.60245	570.95554	16.46261	-545.27700	1
268	H	75.51637	70.79374	83.02194	2391.58273	28.05277	-1305.07271	1
269	H	73.94247	70.38769	82.24025	175.75588	917.63458	2559.43867	1
270	H	74.66387	69.26556	83.45442	-1063.97851	-2155.34650	1283.00462	1
271	C	76.97790	68.70249	82.03025	193.76014	2.62946	-765.53141	1
272	H	77.57624	69.51876	82.51105	507.39394	-846.55087	2539.60089	1
273	H	76.82617	67.90445	82.80204	1337.57841	1818.19054	1526.01994	1
274	H	77.61339	68.26549	81.21663	1100.88635	-1172.91350	-2199.08909	1
275	C	74.64279	66.30365	79.01317	-549.21115	475.64486	-309.38218	1
276	O	74.10621	66.41428	77.94218	556.06106	-390.37755	-78.24250	1
277	O	74.44390	65.14016	79.79606	-572.27940	-310.19032	-209.75862	1
278	H	75.04143	65.37029	80.56118	-1380.08193	2212.14486	790.85944	1

Listing 112: C00112.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.3914	0.0000	300.0000
3	H	64.63594	72.37309	66.81011	-2043.14101	-1757.64893	399.89339		1
4	N	64.84861	72.80134	65.90970	426.75047	490.45733	-334.42467		1
5	H	64.01408	73.36882	65.71179	442.25559	-1110.30854	-2448.52907		1
6	C	66.00704	73.60648	65.91379	415.32972	-666.39213	83.73172		1
7	H	66.68574	73.24469	66.71575	879.32219	2491.00447	667.35213		1
8	C	66.65893	73.53436	64.44160	31.35357	477.41777	628.23362		1
9	H	65.90814	73.88280	63.69230	1168.38489	2240.25337	-1019.71136		1
10	H	67.52884	74.22961	64.35666	-360.43770	2534.90498	931.67112		1
11	C	67.06514	72.11056	64.15782	463.18208	512.70242	-382.34388		1
12	H	66.23591	71.44426	64.48793	1725.29117	1863.52247	-987.07854		1
13	C	67.28183	71.90228	62.66454	710.42801	-144.27427	-313.15367		1
14	H	67.56532	70.84335	62.43154	364.20195	-1033.13725	2494.72524		1
15	H	66.35747	72.13590	62.07541	2567.61904	335.80679	847.48802		1
16	H	68.10050	72.55875	62.27143	-2587.99029	680.92867	-512.16411		1
17	C	68.32979	71.73270	64.91635	268.17616	741.64379	-40.42634		1
18	H	68.62826	70.67083	64.71764	1283.54314	-1945.37420	-1411.27812		1
19	H	69.19545	72.38053	64.62163	-1258.57796	1317.15249	-2026.02085		1
20	H	68.19737	71.83838	66.02377	-2502.84526	909.80597	575.92391		1
21	C	65.40060	75.10542	66.14881	619.36578	-458.64843	-172.09273		1
22	O	64.25307	75.35249	65.82911	-81.40433	433.87611	522.34594		1
23	N	66.34864	75.88733	66.63784	175.23996	-622.20190	341.55523		1
24	H	67.26005	75.44743	66.76771	-876.57256	-303.22879	-2561.90213		1
25	C	66.20984	77.27893	66.86827	-571.88214	-534.10783	-106.15033		1
26	H	67.26273	77.60517	67.01102	-2713.20841	-16.25800	-248.80809		1
27	C	65.50723	77.94116	65.59020	166.60354	288.16399	-716.09568		1
28	H	64.47340	77.49890	65.49697	-2097.85574	1636.78449	-586.18044		1
29	O	66.17458	77.72628	64.33450	-317.80580	-363.38227	484.43082		1
30	H	65.52166	77.15883	63.87504	1863.74748	-1451.84923	1357.29467		1
31	C	65.39076	79.44159	66.04548	503.80731	517.99032	318.51606		1
32	H	64.84700	80.05538	65.28992	640.61020	-2157.10410	-1536.29104		1
33	H	64.83315	79.53840	67.01318	1687.88455	465.60692	2087.56452		1
34	H	66.39391	79.90638	66.18846	-1293.07895	-1899.88581	-1463.57452		1
35	C	65.28699	77.50960	68.20017	-153.07550	-733.68902	248.70981		1
36	O	64.09679	77.64980	68.06566	186.15459	-480.78787	-449.34387		1
37	N	66.01665	77.57003	69.32269	-487.53139	543.18517	42.03850		1
38	C	65.37952	77.48408	70.60265	-699.35871	69.34393	360.10701		1
39	H	64.57952	76.71668	70.49494	2.81126	-221.99807	-2715.58072		1
40	C	66.57501	77.07327	71.55788	-507.46439	-592.59194	122.07761		1
41	H	66.40764	77.40170	72.62930	-1975.08116	525.87560	-1801.71556		1
42	H	66.71231	75.96842	71.58040	1588.27743	-1913.22100	1113.83566		1
43	C	67.80087	77.77520	70.89420	-613.62442	-457.55993	-194.14490		1
44	H	67.84529	78.85063	71.17851	1707.54637	-721.27992	1996.92523		1
45	H	68.77802	77.33231	71.19039	758.23357	2100.81767	1560.55011		1

46	C	67.47250	77.58876	69.35060	-352.41524	704.96076	49.21465	1
47	H	67.82855	78.41321	68.68923	1714.76886	-2070.42778	443.35792	1
48	H	67.79387	76.60978	68.92307	1224.15040	1801.50881	1636.97633	1
49	C	64.72321	78.92093	71.04102	566.85117	537.05831	117.62814	1
50	O	63.79274	78.89607	71.85340	-550.26779	-406.08867	4.21666	1
51	N	65.36753	79.95572	70.54102	566.34832	-425.77725	180.18749	1
52	H	66.11340	79.58978	69.94792	644.44502	2646.80550	-52.73430	1
53	C	64.83015	81.24909	70.31919	612.34801	-281.48662	411.56221	1
54	H	65.54939	81.72202	69.61541	1667.23498	-1490.75142	1556.16753	1
55	C	63.39131	81.02651	69.66117	-714.45746	-175.43074	286.98927	1
56	H	62.85451	80.25076	70.27567	-787.09484	1763.03619	-1922.46060	1
57	O	63.41292	80.53061	68.30618	-429.46514	516.51932	-128.40526	1
58	H	63.25792	79.57128	68.44668	1981.82785	436.16847	-1818.18182	1
59	C	62.71845	82.42994	69.85838	630.79189	-468.94448	76.03230	1
60	H	61.64220	82.41582	69.56725	-1775.71861	2062.30353	131.89849	1
61	H	62.78071	82.76910	70.92334	-1855.14608	88.94118	1993.53760	1
62	H	63.21981	83.20900	69.23722	-1504.82350	-780.94249	-2132.90992	1
63	C	64.66981	82.13690	71.68660	288.57638	618.62814	-397.00270	1
64	O	64.87902	83.32650	71.63682	321.70495	-185.26452	574.37218	1
65	N	64.16817	81.42677	72.68456	-447.05792	-446.53431	367.76425	1
66	H	63.96446	80.39846	72.56730	350.31316	1975.63644	-1843.31522	1
67	C	63.99256	82.08195	73.93434	-511.23061	374.03917	-471.51480	1
68	H	63.81177	83.14902	73.66608	2234.79579	-898.70890	-1273.45190	1
69	C	62.75632	81.28874	74.57631	529.53781	-159.34528	563.72604	1
70	H	62.47244	81.80274	75.53291	654.59388	2347.94251	1217.51488	1
71	H	61.89366	81.42108	73.87084	-1526.55661	2103.42026	817.87394	1
72	O	62.97295	79.88162	74.85292	-554.84278	14.12789	399.58769	1
73	H	62.99417	79.53464	73.93677	1297.06236	2061.84854	1220.68812	1
74	C	65.35416	81.92566	74.82019	-662.15484	-412.13544	123.62687	1
75	O	65.81473	82.91649	75.32899	-540.01537	-317.05804	274.91456	1
76	N	65.75680	80.66454	74.95933	-202.76299	-690.00100	-131.49145	1
77	H	65.22054	79.92156	74.49459	-702.62132	-2617.37191	281.70413	1
78	C	67.10017	80.34634	75.46286	-491.73914	576.34187	222.73509	1
79	H	67.76262	81.15603	75.07544	1977.17978	-1823.58850	-434.68928	1
80	C	67.05587	80.31696	76.98076	-649.50797	-328.66843	306.11224	1
81	H	66.39099	79.47752	77.28496	2075.07803	1452.16490	-1004.45904	1
82	C	68.42743	80.08377	77.58194	-615.18735	-489.99689	-70.96352	1
83	H	68.40242	80.14168	78.70491	-1226.32661	-1724.38906	-1716.47170	1
84	H	68.84036	79.04870	77.30952	2381.64273	-969.84735	900.46860	1
85	H	69.17180	80.84909	77.22775	2122.74991	1702.23946	-141.36228	1
86	C	66.46825	81.59224	77.56284	-501.86074	-479.61276	-376.42482	1
87	H	66.48604	81.59083	78.68739	993.79261	-2246.95401	-1177.81305	1
88	H	67.03636	82.50157	77.21613	42.71279	-626.15391	-2651.37258	1
89	H	65.39821	81.73469	77.24121	-2026.39012	-1590.33709	-887.82922	1
90	C	67.36856	78.85852	74.80330	-672.89153	382.57394	-156.34072	1
91	O	66.44441	78.17127	74.40184	410.04627	221.86223	500.35950	1
92	N	68.65965	78.58077	74.76386	-378.11782	-443.79414	-441.10984	1
93	H	69.26379	79.27393	75.20032	2404.15973	-568.14894	1149.30085	1
94	C	69.04225	77.20763	74.62882	-544.54484	466.16019	331.29119	1
95	H	68.21115	76.74322	74.04919	-1409.80988	-170.17955	2325.32679	1
96	C	70.45212	77.23250	73.89489	-184.48284	116.78282	-758.89137	1
97	H	70.33655	77.70781	72.89553	1893.78641	1861.14652	611.04528	1
98	H	71.16182	77.88243	74.45378	-2170.79665	-974.19311	1327.50117	1
99	C	71.04460	75.79800	73.74785	389.51668	672.81878	-138.49152	1
100	H	71.25295	75.34955	74.76527	510.64577	1933.03327	1851.02484	1
101	H	70.28919	75.11665	73.29445	-2302.30869	-1105.72939	-948.89774	1
102	C	72.35500	75.75245	72.87069	-559.93427	-126.34590	542.30857	1
103	O	72.91747	74.70394	72.68285	-670.36003	-111.83166	76.36448	1
104	N	72.71900	76.95273	72.37053	-216.06729	-537.07037	446.51379	1
105	H	72.29623	77.87729	72.51270	-1251.96487	1074.12894	-2168.52500	1
106	H	73.54575	77.10398	71.78307	-2451.83023	-720.73851	944.84612	1
107	C	69.22946	76.57909	76.11470	546.24052	-563.88337	-85.11809	1

108	O	69.54126	77.28345	77.04884	71.70702	-307.40463	606.69673	1
109	N	69.02853	75.26055	76.09090	479.90863	-504.50129	222.86849	1
110	C	69.31578	74.45093	77.24636	75.51268	-600.91904	506.73700	1
111	H	68.90067	75.00491	78.12024	-2033.61562	1795.30103	254.89480	1
112	C	68.57628	73.08424	76.91121	523.79067	517.99274	284.45581	1
113	H	69.05001	72.20606	77.40464	1599.61665	-1127.00911	1895.98173	1
114	H	67.51672	73.10275	77.25038	-1881.83093	1275.82488	-1501.55016	1
115	C	68.66925	73.03684	75.35570	-600.05639	-404.05026	316.64485	1
116	H	69.68919	72.73787	75.02421	-2597.05260	496.36221	657.73249	1
117	H	67.95504	72.32412	74.88526	-1666.24518	1294.38985	-1723.90591	1
118	C	68.36555	74.55799	75.00259	493.57570	-129.95376	-602.56394	1
119	H	68.77426	74.90741	74.02584	-1469.08415	-637.84797	2204.22581	1
120	H	67.28863	74.84374	75.07213	-1038.97840	1068.88701	-2280.71789	1
121	C	70.91529	74.22687	77.38409	188.88100	241.05089	-727.87821	1
122	O	71.72754	74.53620	76.51702	531.88613	-49.19943	427.07960	1
123	N	71.16090	73.55811	78.52337	708.14833	26.93417	-179.73509	1
124	H	70.25773	73.52678	78.99847	-2232.69501	-1179.09831	1023.94816	1
125	C	72.44010	73.74778	79.23926	-738.32412	259.92548	104.42456	1
126	H	72.69356	74.80935	79.01067	2028.89123	1260.02983	1311.33324	1
127	C	72.21684	73.46536	80.70405	-258.65678	-345.52513	661.28459	1
128	H	71.77312	72.44769	80.79063	-1826.06090	-1801.46097	-918.64554	1
129	C	73.51802	73.48121	81.48863	-541.23400	531.92970	-218.41428	1
130	H	73.34882	73.26441	82.57893	1311.73218	-2219.18200	882.19023	1
131	H	74.24250	72.70939	81.10289	-1048.71298	1223.58118	-2196.97971	1
132	H	74.02992	74.48013	81.42226	419.06414	1903.92898	1903.44670	1
133	C	71.24751	74.45141	81.33548	-423.86431	152.66566	-648.55262	1
134	H	71.05939	74.21423	82.41801	105.68386	-2342.50080	1387.51238	1
135	H	71.64297	75.50274	81.28963	-1695.63603	-1484.73621	-1531.02793	1
136	H	70.25099	74.45211	80.81666	-1853.57121	-487.39031	1936.59343	1
137	C	73.50476	72.69621	78.53633	539.71428	-510.58232	267.58633	1
138	O	73.88670	71.70193	79.09832	-15.93758	-278.34085	-624.49402	1
139	N	73.82596	73.14349	77.33380	-676.81886	12.05292	276.17960	1
140	H	73.34801	73.97740	76.92242	-1694.44250	-373.84189	-2100.66098	1
141	C	74.77000	72.37747	76.58037	412.33078	-664.70360	108.35451	1
142	H	74.59482	71.31961	76.88867	1765.77476	1294.44366	1621.76594	1
143	C	74.42222	72.71315	75.07153	-179.66635	-721.95667	-264.73915	1
144	H	73.33080	72.58475	74.89158	-607.34922	2587.87032	-598.10018	1
145	H	74.62326	73.78707	74.85660	-359.69332	-1479.13954	-2259.74260	1
146	C	75.24830	71.79849	74.10973	-240.01076	616.02425	431.85322	1
147	H	76.34073	71.96516	74.24404	-1359.17131	782.54425	2227.99181	1
148	H	75.06762	70.72131	74.32493	-820.36667	85.81767	-2596.78715	1
149	C	74.81361	72.16192	72.63293	-513.07015	236.18570	-551.87280	1
150	H	73.73038	71.95654	72.47097	1816.11944	-1183.11722	-1650.94321	1
151	H	74.93788	73.25269	72.43619	-1800.04429	-1361.53473	1526.34643	1
152	C	75.69346	71.31529	71.68354	726.08972	-253.19732	-179.64713	1
153	H	76.78258	71.50130	71.77272	1224.27271	-456.51798	-2390.90304	1
154	H	75.49303	70.22566	71.71644	1206.40339	-1150.93514	-2154.90344	1
155	N	75.33999	71.74513	70.22097	329.70796	-633.68968	-155.67358	1
156	H	75.86871	71.24070	69.45187	1348.31305	1938.76845	1359.00643	1
157	H	74.33427	71.61137	69.90960	2096.92035	1446.54551	-966.48890	1
158	H	75.51276	72.76049	69.96460	-1197.07217	-2303.53719	827.28733	1
159	C	76.27601	72.87876	76.95611	-378.01186	-556.17301	-413.96481	1
160	O	76.52109	73.96050	77.48603	-409.44433	-307.55053	-453.30833	1
161	N	77.16373	72.02732	76.40567	-429.02477	524.70884	274.08502	1
162	H	76.55553	71.26963	76.06795	1706.34263	-1425.96036	1574.38926	1
163	C	78.31299	71.61472	77.18671	-45.25864	-626.22952	478.93267	1
164	H	77.90162	71.05168	78.05213	1988.63164	570.90773	1772.87287	1
165	C	79.12742	70.72277	76.18293	551.77128	-20.49526	-564.54996	1
166	H	78.52516	69.85620	75.82829	1434.61535	-1753.10253	1513.99471	1
167	H	79.35007	71.31798	75.26847	-714.67738	1819.09770	1898.36494	1
168	C	80.46323	70.24357	76.84966	446.99263	-555.77305	338.97221	1
169	H	80.88605	71.03079	77.51493	1953.68466	1892.25957	-161.67766	1

170	H	80.29963	69.35505	77.49942	-403.03785	2688.07032	-188.43591	1
171	C	81.46221	69.92840	75.66750	567.86262	335.74681	434.04421	1
172	H	81.11135	69.05695	75.06863	-1080.02275	1568.26081	-1948.78900	1
173	H	81.52005	70.78320	74.95375	-919.54108	2111.34692	1456.13463	1
174	C	82.85290	69.65610	76.29439	195.81897	173.33862	-745.11536	1
175	H	83.35529	70.55664	76.71849	1405.67949	-2301.21089	-390.08113	1
176	H	82.87977	68.82783	77.03234	-940.37328	-1118.32446	2299.72133	1
177	N	83.79383	69.18192	75.15449	319.26422	656.36007	-42.02424	1
178	H	84.84421	69.07929	75.48146	1961.03633	619.91968	1787.09422	1
179	H	83.56509	68.23110	74.74237	854.14343	-2156.80752	1429.08711	1
180	H	83.84373	69.77227	74.27452	1237.02905	-1378.50857	-1998.28500	1
181	C	79.26797	72.85089	77.64081	532.53319	-268.57236	517.55729	1
182	O	79.88923	72.72941	78.67552	266.16714	-290.73804	-558.88002	1
183	N	79.40637	73.77239	76.68135	-226.25352	640.49678	-270.32839	1
184	H	78.73570	73.64924	75.92193	2007.69063	-1035.27229	1523.50231	1
185	C	80.02227	75.02902	76.92391	-540.76542	-573.33303	49.50000	1
186	H	79.75373	75.64273	76.03635	-2374.20950	-1036.76023	843.75774	1
187	C	79.32614	75.61882	78.23847	-77.09082	666.87422	-415.84136	1
188	H	79.13813	74.77300	78.96597	-985.81834	617.19825	2463.91927	1
189	O	78.01069	76.13129	77.99925	293.29899	-391.65602	-477.80926	1
190	H	77.48598	75.25522	77.88134	2528.72714	-681.76262	-751.27122	1
191	C	80.40627	76.58910	78.82824	252.47363	-605.14473	440.05134	1
192	H	80.00204	77.18073	79.68372	-2052.65063	1456.49051	-1043.51830	1
193	H	81.29860	76.03042	79.20463	-2152.98800	-1661.97574	-161.70652	1
194	H	80.77316	77.31024	78.05673	-473.12726	-1584.27339	2165.61725	1
195	C	81.64382	74.86477	77.03615	360.36307	488.46713	505.10056	1
196	O	82.30533	75.87172	77.15896	-200.08817	-528.03552	-385.82850	1
197	N	82.04078	73.60048	76.96005	-597.54095	-226.44775	355.20479	1
198	H	81.28787	72.91488	76.88775	2179.23655	-1300.70981	-991.33835	1
199	C	83.38261	73.23805	76.68463	-687.68921	297.39807	-249.45179	1
200	H	83.30382	72.13419	76.53213	-349.16256	-2467.37713	-1101.72831	1
201	C	83.84188	74.01305	75.36312	672.47345	361.54328	-201.62880	1
202	H	83.62265	75.10387	75.45516	1541.41502	582.18425	2169.97026	1
203	H	84.93894	73.89456	75.20574	-2534.67717	60.25153	997.72295	1
204	C	83.06942	73.39561	74.18820	574.26774	-389.43119	-377.02542	1
205	C	83.54535	72.17088	73.63296	688.82679	-287.33580	-257.96133	1
206	H	84.45727	71.69076	74.03199	331.14182	1470.38163	2269.80013	1
207	C	81.89108	74.01750	73.67701	-383.52382	-675.04808	144.24917	1
208	H	81.51871	74.96185	74.11397	4.09847	1517.59662	2262.86397	1
209	C	82.83524	71.59746	72.57862	-134.76730	428.45285	-649.50303	1
210	H	83.20209	70.65046	72.14611	-903.23433	1600.49020	2011.53387	1
211	C	81.22081	73.40892	72.61294	-335.53281	-615.00040	-364.39058	1
212	H	80.31706	73.90210	72.21455	1596.45398	-1369.33862	1732.02659	1
213	C	81.66001	72.18555	72.02766	585.48547	-340.24194	-406.23938	1
214	O	80.97825	71.55576	70.95325	-419.15649	-173.04408	-511.94141	1
215	H	80.28598	72.23521	70.77504	-1071.84350	1559.71507	-1960.13012	1
216	C	84.29484	73.60025	77.99286	291.41878	-183.13091	710.72246	1
217	O	84.14682	72.96825	79.01483	379.87695	523.47396	-222.23622	1
218	N	85.22153	74.51434	77.71033	564.30591	373.09380	277.24371	1
219	H	85.14772	74.94913	76.79122	-120.59931	-2436.07824	-1214.35098	1
220	C	85.87045	75.25558	78.73834	404.07514	-299.37480	608.84009	1
221	H	86.11939	76.22307	78.24863	-1071.07882	-841.69025	2359.66467	1
222	C	84.86793	75.41143	79.95336	-683.12807	68.71770	-390.13096	1
223	H	83.85372	75.70422	79.59590	2068.88918	1596.58590	770.89603	1
224	H	84.73393	74.43344	80.47931	1379.86429	2342.49779	-179.85638	1
225	C	85.47503	76.48480	80.91066	-176.39967	537.49466	550.97268	1
226	H	86.52916	76.22739	81.16645	-396.28051	1942.22168	1869.33314	1
227	H	85.52282	77.47962	80.41411	-94.44700	586.00678	-2659.20016	1
228	C	84.57646	76.54247	82.22884	-291.69381	-718.18079	-150.72929	1
229	H	83.53270	76.92697	82.10007	-2303.38776	1089.76242	964.62032	1
230	H	84.52813	75.59257	82.82043	884.16729	2568.80533	-207.74283	1
231	N	85.31018	77.47875	82.97589	-594.49522	-252.81478	342.29276	1

232	H	86.18543	77.78812	82.58125	-1735.17426	2084.05705	-263.71605	1
233	C	84.95892	77.94748	84.10464	595.23177	-271.52487	442.22352	1
234	N	83.74703	77.50507	84.64447	585.53813	-424.79750	-105.81303	1
235	H	83.07980	76.83278	84.26799	959.88797	1327.56823	-2177.11905	1
236	H	83.36384	77.80179	85.54257	1578.48647	16.27378	-2220.76233	1
237	N	85.91498	78.85245	84.58651	-452.17763	-390.33541	-421.51853	1
238	H	86.79985	79.16287	84.18783	470.26107	1974.25629	-1817.92087	1
239	H	85.82739	79.33766	85.48006	1856.67307	-1573.97321	-1224.35416	1
240	C	87.21462	74.49644	79.28927	-531.47271	-581.45780	-55.06206	1
241	O	88.04885	75.11879	79.90829	-243.00837	192.73507	609.52485	1
242	N	87.18225	73.13941	79.10931	343.49288	-644.25607	38.09164	1
243	H	86.36615	73.03344	78.49416	-1691.16043	-1535.97525	-1484.73099	1
244	C	88.45280	72.57001	78.69091	542.66492	350.14337	454.42563	1
245	H	88.80809	73.24561	77.88330	1209.57979	-2396.95920	463.86744	1
246	C	89.41069	72.63529	79.95090	-737.14309	145.93010	242.71942	1
247	H	88.84743	73.00757	80.83480	-1050.18303	159.36419	-2509.06125	1
248	C	90.06208	71.23806	80.23751	-706.77696	-252.88343	-245.16230	1
249	H	90.80603	71.28862	81.06667	-1624.64039	-1665.49085	1417.86935	1
250	H	89.29490	70.48118	80.52272	2566.10521	598.51109	693.22305	1
251	H	90.59172	70.84634	79.33452	-1972.69758	107.10018	-1876.34312	1
252	C	90.60057	73.59902	79.61222	412.85148	672.58832	-27.69222	1
253	H	91.34114	73.64595	80.44493	1447.02277	1762.76533	-1490.78944	1
254	H	91.14854	73.27360	78.69690	1320.77379	-145.20455	2378.68491	1
255	H	90.23401	74.63993	79.43561	-1512.10848	1470.52031	1724.75147	1
256	C	88.22973	71.06713	78.17089	-607.11113	499.56689	73.73769	1
257	O	89.13681	70.49770	77.60634	357.97126	460.81534	356.68785	1
258	N	86.99425	70.56482	78.43338	536.55407	-368.62270	332.76306	1
259	H	86.41618	71.19193	78.99748	524.38866	2297.69985	1367.20941	1
260	C	87.03344	69.16656	78.80907	46.50277	-774.29190	-147.97904	1
261	H	88.07079	68.99788	79.17225	1676.51875	1883.29066	1032.55549	1
262	C	85.88926	68.91871	79.91377	-559.41456	-34.19198	-556.30433	1
263	H	84.93458	69.38119	79.56337	-64.66664	395.18769	2695.05373	1
264	H	85.68279	67.82588	80.01945	-2703.44278	-60.40056	333.79418	1
265	C	86.30903	69.50508	81.23886	-519.76435	377.31045	459.42366	1
266	H	86.69562	70.53518	81.06971	-1746.74323	1667.50644	-1261.73691	1
267	C	85.11050	69.58758	82.17566	570.95554	16.46261	-545.27700	1
268	H	85.39159	70.01444	83.17295	2391.58273	28.05277	-1305.07271	1
269	H	84.29898	70.23540	81.75298	175.75588	917.63458	2559.43867	1
270	H	84.66378	68.57660	82.36231	-1063.97851	-2155.34650	1283.00462	1
271	C	87.40461	68.66713	81.88323	193.76014	2.62946	-765.53141	1
272	H	87.72265	69.09135	82.87057	507.39394	-846.55087	2539.60089	1
273	H	87.06125	67.61654	82.06964	1337.57841	1818.19054	1526.01994	1
274	H	88.31838	68.60527	81.23833	1100.88635	-1172.91350	-2199.08909	1
275	C	86.68522	68.26905	77.54407	-549.21115	475.64486	-309.38218	1
276	O	85.90233	68.61523	76.66716	556.06106	-390.37755	-78.24250	1
277	O	87.14294	66.94816	77.59051	-572.27940	-310.19032	-209.75862	1
278	H	87.72036	67.01615	78.41275	-1380.08193	2212.14486	790.85944	1

Listing 113: C00113.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.3894	0.0000	300.0000
3	H	75.23134	71.44033	83.84587	-2043.14101	-1757.64893	399.89339		1
4	N	75.53238	71.95895	84.66977	426.75047	490.45733	-334.42467		1
5	H	75.60646	71.22542	85.38266	442.25559	-1110.30854	-2448.52907		1
6	C	76.75403	72.65265	84.50708	415.32972	-666.39213	83.73172		1
7	H	76.95180	72.71135	83.41366	879.32219	2491.00447	667.35213		1
8	C	76.61363	74.11166	85.18911	31.35357	477.41777	628.23362		1
9	H	76.30411	73.98799	86.25409	1168.38489	2240.25337	-1019.71136		1
10	H	77.60188	74.63013	85.21178	-360.43770	2534.90498	931.67112		1
11	C	75.60013	74.93058	84.43676	463.18208	512.70242	-382.34388		1

12	H	74.67084	74.32585	84.33300	1725.29117	1863.52247	-987.07854	1
13	C	75.27476	76.19504	85.22356	710.42801	-144.27427	-313.15367	1
14	H	74.50893	76.82608	84.70562	364.20195	-1033.13725	2494.72524	1
15	H	74.87302	75.95572	86.24191	2567.61904	335.80679	847.48802	1
16	H	76.18467	76.83243	85.36848	-2587.99029	680.92867	-512.16411	1
17	C	76.10575	75.30004	83.04912	268.17616	741.64379	-40.42634	1
18	H	75.35585	75.90912	82.47938	1283.54314	-1945.37420	-1411.27812	1
19	H	77.05114	75.90078	83.09849	-1258.57796	1317.15249	-2026.02085	1
20	H	76.32744	74.39418	82.42800	-2502.84526	909.80597	575.92391	1
21	C	77.83599	71.78037	85.33006	619.36578	-458.64843	-172.09273	1
22	O	77.50941	70.75699	85.94822	-81.40433	433.87611	522.34594	1
23	N	79.02537	72.30047	85.14981	175.23996	-622.20190	341.55523	1
24	H	79.03961	73.14807	84.58117	-876.57256	-303.22879	-2561.90213	1
25	C	80.11400	72.10159	86.06607	-571.88214	-534.10783	-106.15033	1
26	H	79.75056	72.49924	87.03951	-2713.20841	-16.25800	-248.80809	1
27	C	80.41637	70.53913	86.19620	166.60354	288.16399	-716.09568	1
28	H	80.11339	70.06084	85.22177	-2097.85574	1636.78449	-586.18044	1
29	O	79.62619	69.84686	87.17104	-317.80580	-363.38227	484.43082	1
30	H	78.68246	70.01778	86.78528	1863.74748	-1451.84923	1357.29467	1
31	C	81.97027	70.46363	86.39238	503.80731	517.99032	318.51606	1
32	H	82.32714	69.40777	86.42629	640.61020	-2157.10410	-1536.29104	1
33	H	82.52390	70.97741	85.57168	1687.88455	465.60692	2087.56452	1
34	H	82.27890	70.94963	87.34791	-1293.07895	-1899.88581	-1463.57452	1
35	C	81.34289	72.98299	85.47896	-153.07550	-733.68902	248.70981	1
36	O	82.05051	73.48843	86.31198	186.15459	-480.78787	-449.34387	1
37	N	81.51806	72.93972	84.14969	-487.53139	543.18517	42.03850	1
38	C	82.36497	73.89574	83.50257	-699.35871	69.34393	360.10701	1
39	H	83.13239	74.21442	84.24677	2.81126	-221.99807	-2715.58072	1
40	C	82.90019	73.05247	82.26088	-507.46439	-592.59194	122.07761	1
41	H	83.28194	73.69383	81.43575	-1975.08116	525.87560	-1801.71556	1
42	H	83.73526	72.37860	82.55481	1588.27743	-1913.22100	1113.83566	1
43	C	81.62752	72.24142	81.87179	-613.62442	-457.55993	-194.14490	1
44	H	80.89426	72.88330	81.33340	1707.54637	-721.27992	1996.92523	1
45	H	81.83535	71.36848	81.21254	758.23357	2100.81767	1560.55011	1
46	C	81.08995	71.82859	83.30940	-352.41524	704.96076	49.21465	1
47	H	79.98242	71.73425	83.38513	1714.76886	-2070.42778	443.35792	1
48	H	81.56115	70.91382	83.73810	1224.15040	1801.50881	1636.97633	1
49	C	81.47016	75.13419	82.92962	566.85117	537.05831	117.62814	1
50	O	80.25046	75.07230	82.79910	-550.26779	-406.08867	4.21666	1
51	N	82.29649	76.09575	82.59427	566.34832	-425.77725	180.18749	1
52	H	83.28524	75.93501	82.76818	644.44502	2646.80550	-52.73430	1
53	C	81.79937	77.35365	82.13433	612.34801	-281.48662	411.56221	1
54	H	80.92762	77.52374	82.80516	1667.23498	-1490.75142	1556.16753	1
55	C	82.96235	78.43340	82.25063	-714.45746	-175.43074	286.98927	1
56	H	83.78444	78.16030	81.53418	-787.09484	1763.03619	-1922.46060	1
57	O	83.57685	78.55137	83.54851	-429.46514	516.51932	-128.40526	1
58	H	84.50818	78.34052	83.34162	1981.82785	436.16847	-1818.18182	1
59	C	82.22465	79.72199	81.72788	630.79189	-468.94448	76.03230	1
60	H	82.91676	80.59418	81.67678	-1775.71861	2062.30353	131.89849	1
61	H	81.80252	79.57281	80.70468	-1855.14608	88.94118	1993.53760	1
62	H	81.38096	80.00855	82.39776	-1504.82350	-780.94249	-2132.90992	1
63	C	81.32134	77.15066	80.57818	288.57638	618.62814	-397.00270	1
64	O	81.94654	77.56022	79.63200	321.70495	-185.26452	574.37218	1
65	N	80.19254	76.45216	80.60472	-447.05792	-446.53431	367.76425	1
66	H	79.78023	76.12337	81.51484	350.31316	1975.63644	-1843.31522	1
67	C	79.38843	76.47352	79.43260	-511.23061	374.03917	-471.51480	1
68	H	80.07038	76.76200	78.59627	2234.79579	-898.70890	-1273.45190	1
69	C	78.80868	74.97509	79.35350	529.53781	-159.34528	563.72604	1
70	H	78.18436	74.88492	78.42554	654.59388	2347.94251	1217.51488	1
71	H	79.70164	74.31203	79.20051	-1526.55661	2103.42026	817.87394	1
72	O	78.03814	74.51565	80.49084	-554.84278	14.12789	399.58769	1
73	H	78.74278	74.54171	81.17457	1297.06236	2061.84854	1220.68812	1

74	C	78.20531	77.54748	79.69519	-662.15484	-412.13544	123.62687	1
75	O	77.98832	78.06276	80.78024	-540.01537	-317.05804	274.91456	1
76	N	77.45130	77.71125	78.56488	-202.76299	-690.00100	-131.49145	1
77	H	77.94918	77.08181	77.91763	-702.62132	-2617.37191	281.70413	1
78	C	77.13846	79.08742	78.08992	-491.73914	576.34187	222.73509	1
79	H	78.01997	79.68254	78.42346	1977.17978	-1823.58850	-434.68928	1
80	C	77.03472	78.99340	76.59157	-649.50797	-328.66843	306.11224	1
81	H	76.49238	78.05213	76.34521	2075.07803	1452.16490	-1004.45904	1
82	C	76.26296	80.14451	75.96471	-615.18735	-489.99689	-70.96352	1
83	H	76.41768	80.19483	74.85086	-1226.32661	-1724.38906	-1716.47170	1
84	H	75.15277	80.04503	76.13886	2381.64273	-969.84735	900.46860	1
85	H	76.57738	81.13570	76.39587	2122.74991	1702.23946	-141.36228	1
86	C	78.40795	78.91185	75.94353	-501.86074	-479.61276	-376.42482	1
87	H	78.33602	78.75053	74.83288	993.79261	-2246.95401	-1177.81305	1
88	H	78.99556	79.85743	76.10300	42.71279	-626.15391	-2651.37258	1
89	H	79.02092	78.06843	76.36403	-2026.39012	-1590.33709	-887.82922	1
90	C	75.76402	79.62644	78.80597	-672.89153	382.57394	-156.34072	1
91	O	75.16353	80.55010	78.31442	410.04627	221.86223	500.35950	1
92	N	75.57240	79.03799	79.97249	-378.11782	-443.79414	-441.10984	1
93	H	76.29607	78.36231	80.29298	2404.15973	-568.14894	1149.30085	1
94	C	74.29880	79.00674	80.62480	-544.54484	466.16019	331.29119	1
95	H	74.57606	78.85531	81.69043	-1409.80988	-170.17955	2325.32679	1
96	C	73.52525	80.35905	80.33601	-184.48284	116.78282	-758.89137	1
97	H	74.21439	81.23073	80.42143	1893.78641	1861.14652	611.04528	1
98	H	73.14426	80.37497	79.28612	-2170.79665	-974.19311	1327.50117	1
99	C	72.35094	80.43927	81.36056	389.51668	672.81878	-138.49152	1
100	H	71.69217	79.54850	81.25639	510.64577	1933.03327	1851.02484	1
101	H	72.74389	80.37031	82.39860	-2302.30869	-1105.72939	-948.89774	1
102	C	71.48693	81.74865	81.22103	-559.93427	-126.34590	542.30857	1
103	O	70.51791	81.89452	81.92309	-670.36003	-111.83166	76.36448	1
104	N	71.94804	82.62229	80.30014	-216.06729	-537.07037	446.51379	1
105	H	72.76270	82.55235	79.67922	-1251.96487	1074.12894	-2168.52500	1
106	H	71.51066	83.52843	80.10240	-2451.83023	-720.73851	944.84612	1
107	C	73.42076	77.78090	80.01979	546.24052	-563.88337	-85.11809	1
108	O	73.14102	77.73750	78.83037	71.70702	-307.40463	606.69673	1
109	N	73.02554	76.96231	80.99289	479.90863	-504.50129	222.86849	1
110	C	72.48765	75.66570	80.68435	75.51268	-600.91904	506.73700	1
111	H	73.13157	75.28958	79.85663	-2033.61562	1795.30103	254.89480	1
112	C	72.61732	74.89753	82.06351	523.79067	517.99274	284.45581	1
113	H	71.88933	74.06052	82.15913	1599.61665	-1127.00911	1895.98173	1
114	H	73.63072	74.45612	82.19398	-1881.83093	1275.82488	-1501.55016	1
115	C	72.36246	76.04880	83.08699	-600.05639	-404.05026	316.64485	1
116	H	71.27754	76.28922	83.15061	-2597.05260	496.36221	657.73249	1
117	H	72.69856	75.81029	84.12105	-1666.24518	1294.38985	-1723.90591	1
118	C	73.17843	77.23491	82.41653	493.57570	-129.95376	-602.56394	1
119	H	72.79001	78.25688	82.63057	-1469.08415	-637.84797	2204.22581	1
120	H	74.27617	77.20811	82.61870	-1038.97840	1068.88701	-2280.71789	1
121	C	70.92717	75.80343	80.21087	188.88100	241.05089	-727.87821	1
122	O	70.04504	75.35890	80.90214	531.88613	-49.19943	427.07960	1
123	N	70.84089	76.38822	79.02065	708.14833	26.93417	-179.73509	1
124	H	71.67634	76.81572	78.55149	-2232.69501	-1179.09831	1023.94816	1
125	C	69.54455	76.43684	78.43001	-738.32412	259.92548	104.42456	1
126	H	68.95559	75.62280	78.91400	2028.89123	1260.02983	1311.33324	1
127	C	68.95760	77.87495	78.80569	-258.65678	-345.52513	661.28459	1
128	H	69.78321	78.60848	78.92769	-1826.06090	-1801.46097	-918.64554	1
129	C	67.92253	78.36750	77.74079	-541.23400	531.92970	-218.41428	1
130	H	67.43312	79.32078	78.05112	1311.73218	-2219.18200	882.19023	1
131	H	68.41331	78.55075	76.75650	-1048.71298	1223.58118	-2196.97971	1
132	H	67.11427	77.61696	77.57401	419.06414	1903.92898	1903.44670	1
133	C	68.14900	77.70963	80.13612	-423.86431	152.66566	-648.55262	1
134	H	67.76407	78.68753	80.51119	105.68386	-2342.50080	1387.51238	1
135	H	67.26888	77.03742	79.99970	-1695.63603	-1484.73621	-1531.02793	1

136	H	68.78219	77.26364	80.94263	-1853.57121	-487.39031	1936.59343	1
137	C	69.70767	76.28936	76.81356	539.71428	-510.58232	267.58633	1
138	O	70.69037	76.69948	76.20451	-15.93758	-278.34085	-624.49402	1
139	N	68.60485	75.74077	76.35124	-676.81886	12.05292	276.17960	1
140	H	67.92285	75.48444	77.06360	-1694.44250	-373.84189	-2100.66098	1
141	C	68.25230	75.70057	74.97845	412.33078	-664.70360	108.35451	1
142	H	67.18897	75.37332	74.99050	1765.77476	1294.44366	1621.76594	1
143	C	68.46041	77.15308	74.37931	-179.66635	-721.95667	-264.73915	1
144	H	67.77014	77.88484	74.85504	-607.34922	2587.87032	-598.10018	1
145	H	69.48872	77.52729	74.60052	-359.69332	-1479.13954	-2259.74260	1
146	C	68.22310	77.07824	72.83617	-240.01076	616.02425	431.85322	1
147	H	68.86013	76.26883	72.37056	-1359.17131	782.54425	2227.99181	1
148	H	67.16626	76.81464	72.60533	-820.36667	85.81767	-2596.78715	1
149	C	68.61356	78.47877	72.21424	-513.07015	236.18570	-551.87280	1
150	H	67.92371	79.28400	72.55683	1816.11944	-1183.11722	-1650.94321	1
151	H	69.63362	78.79002	72.53838	-1800.04429	-1361.53473	1526.34643	1
152	C	68.56130	78.29576	70.67928	726.08972	-253.19732	-179.64713	1
153	H	69.31330	77.58575	70.27789	1224.27271	-456.51798	-2390.90304	1
154	H	67.55745	78.05007	70.27894	1206.40339	-1150.93514	-2154.90344	1
155	N	68.92392	79.66918	70.02390	329.70796	-633.68968	-155.67358	1
156	H	68.89916	79.69019	68.96373	1348.31305	1938.76845	1359.00643	1
157	H	68.31248	80.50308	70.26468	2096.92035	1446.54551	-966.48890	1
158	H	69.89809	80.04561	70.21335	-1197.07217	-2303.53719	827.28733	1
159	C	69.19747	74.64017	74.14449	-378.01186	-556.17301	-413.96481	1
160	O	68.67510	73.65432	73.68506	-409.44433	-307.55053	-453.30833	1
161	N	70.44943	75.05436	74.08250	-429.02477	524.70884	274.08502	1
162	H	70.74727	75.87866	74.65890	1706.34263	-1425.96036	1574.38926	1
163	C	71.38080	74.43459	73.20902	-45.25864	-626.22952	478.93267	1
164	H	72.37164	74.78300	73.57821	1988.63164	570.90773	1772.87287	1
165	C	71.15922	72.87122	73.34302	551.77128	-20.49526	-564.54996	1
166	H	71.01046	72.60748	74.41475	1434.61535	-1753.10253	1513.99471	1
167	H	70.21491	72.55897	72.82825	-714.67738	1819.09770	1898.36494	1
168	C	72.37746	72.09162	72.74505	446.99263	-555.77305	338.97221	1
169	H	72.39697	72.16278	71.63077	1953.68466	1892.25957	-161.67766	1
170	H	73.34732	72.50553	73.10121	-403.03785	2688.07032	-188.43591	1
171	C	72.18769	70.59760	73.22695	567.86262	335.74681	434.04421	1
172	H	72.29093	70.52439	74.33447	-1080.02275	1568.26081	-1948.78900	1
173	H	71.14709	70.24502	72.99899	-919.54108	2111.34692	1456.13463	1
174	C	73.23234	69.70499	72.51896	195.81897	173.33862	-745.11536	1
175	H	73.12183	69.64779	71.41741	1405.67949	-2301.21089	-390.08113	1
176	H	74.28628	69.92343	72.78359	-940.37328	-1118.32446	2299.72133	1
177	N	72.97800	68.24751	73.03198	319.26422	656.36007	-42.02424	1
178	H	73.61317	67.49729	72.63393	1961.03633	619.91968	1787.09422	1
179	H	73.08701	68.08129	74.07472	854.14343	-2156.80752	1429.08711	1
180	H	72.01798	67.83323	72.84874	1237.02905	-1378.50857	-1998.28500	1
181	C	71.11716	74.86843	71.64559	532.53319	-268.57236	517.55729	1
182	O	70.06371	75.25323	71.18191	266.16714	-290.73804	-558.88002	1
183	N	72.26980	74.68109	71.02422	-226.25352	640.49678	-270.32839	1
184	H	73.05597	74.32129	71.56162	2007.69063	-1035.27229	1523.50231	1
185	C	72.34431	74.84311	69.61995	-540.76542	-573.33303	49.50000	1
186	H	71.35040	75.22833	69.29236	-2374.20950	-1036.76023	843.75774	1
187	C	73.56028	75.86146	69.37045	-77.09082	666.87422	-415.84136	1
188	H	74.47527	75.44322	69.87263	-985.81834	617.19825	2463.91927	1
189	O	73.37486	77.17900	69.91927	293.29899	-391.65602	-477.80926	1
190	H	74.09962	77.21112	70.57528	2528.72714	-681.76262	-751.27122	1
191	C	73.76692	75.80650	67.81395	252.47363	-605.14473	440.05134	1
192	H	74.61445	76.45491	67.49178	-2052.65063	1456.49051	-1043.51830	1
193	H	73.99477	74.77256	67.46901	-2152.98800	-1661.97574	-161.70652	1
194	H	72.85969	76.15099	67.26558	-473.12726	-1584.27339	2165.61725	1
195	C	72.73692	73.37014	69.02031	360.36307	488.46713	505.10056	1
196	O	73.42812	72.59174	69.63592	-200.08817	-528.03552	-385.82850	1
197	N	72.28154	73.27017	67.77114	-597.54095	-226.44775	355.20479	1

198	H	71.70670	74.02823	67.40291	2179.23655	-1300.70981	-991.33835	1
199	C	72.31319	71.99837	67.15767	-687.68921	297.39807	-249.45179	1
200	H	73.03192	71.40306	67.76862	-349.16256	-2467.37713	-1101.72831	1
201	C	70.83135	71.38733	67.11144	672.47345	361.54328	-201.62880	1
202	H	70.13538	72.10002	66.61290	1541.41502	582.18425	2169.97026	1
203	H	70.83610	70.45439	66.49791	-2534.67717	60.25153	997.72295	1
204	C	70.37914	71.10478	68.55210	574.26774	-389.43119	-377.02542	1
205	C	70.78978	69.90098	69.19926	688.82679	-287.33580	-257.96133	1
206	H	71.43162	69.16987	68.67498	331.14182	1470.38163	2269.80013	1
207	C	69.58317	72.06102	69.25145	-383.52382	-675.04808	144.24917	1
208	H	69.28896	73.00916	68.76690	4.09847	1517.59662	2262.86397	1
209	C	70.36119	69.66574	70.50752	-134.76730	428.45285	-649.50303	1
210	H	70.67617	68.73073	71.00288	-903.23433	1600.49020	2011.53387	1
211	C	69.18312	71.78158	70.56218	-335.53281	-615.00040	-364.39058	1
212	H	68.56769	72.53105	71.09218	1596.45398	-1369.33862	1732.02659	1
213	C	69.53916	70.57639	71.23217	585.48547	-340.24194	-406.23938	1
214	O	69.12051	70.27740	72.56462	-419.15649	-173.04408	-511.94141	1
215	H	68.63695	71.11281	72.77199	-1071.84350	1559.71507	-1960.13012	1
216	C	72.64938	72.10156	65.55644	291.41878	-183.13091	710.72246	1
217	O	72.05820	71.36748	64.79487	379.87695	523.47396	-222.23622	1
218	N	73.62375	72.96372	65.29501	564.30591	373.09380	277.24371	1
219	H	73.97773	73.49958	66.08537	-120.59931	-2436.07824	-1214.35098	1
220	C	73.95692	73.27313	63.93997	404.07514	-299.37480	608.84009	1
221	H	73.83378	72.29756	63.41672	-1071.07882	-841.69025	2359.66467	1
222	C	72.90014	74.33524	63.41375	-683.12807	68.71770	-390.13096	1
223	H	71.86283	73.99509	63.63117	2068.88918	1596.58590	770.89603	1
224	H	73.01873	75.30524	63.94633	1379.86429	2342.49779	-179.85638	1
225	C	73.12379	74.50905	61.88020	-176.39967	537.49466	550.97268	1
226	H	74.17765	74.82724	61.67501	-396.28051	1942.22168	1869.33314	1
227	H	72.98997	73.54124	61.34679	-94.44700	586.00678	-2659.20016	1
228	C	72.08596	75.59982	61.34643	-291.69381	-718.18079	-150.72929	1
229	H	71.00201	75.33818	61.44680	-2303.38776	1089.76242	964.62032	1
230	H	72.23173	76.63280	61.75392	884.16729	2568.80533	-207.74283	1
231	N	72.39954	75.63295	59.97875	-594.49522	-252.81478	342.29276	1
232	H	73.22429	75.12990	59.68952	-1735.17426	2084.05705	-263.71605	1
233	C	71.73145	76.25560	59.09544	595.23177	-271.52487	442.22352	1
234	N	70.59603	76.95960	59.50990	585.53813	-424.79750	-105.81303	1
235	H	70.20769	77.06849	60.44614	959.88797	1327.56823	-2177.11905	1
236	H	69.98720	77.50131	58.89524	1578.48647	16.27378	-2220.76233	1
237	N	72.30380	76.09865	57.82549	-452.17763	-390.33541	-421.51853	1
238	H	73.13351	75.58920	57.52419	470.26107	1974.25629	-1817.92087	1
239	H	71.91738	76.52426	56.98179	1856.67307	-1573.97321	-1224.35416	1
240	C	75.45557	73.90340	63.90680	-531.47271	-581.45780	-55.06206	1
241	O	75.76832	74.69875	63.04899	-243.00837	192.73507	609.52485	1
242	N	76.20519	73.38763	64.86362	343.49288	-644.25607	38.09164	1
243	H	75.88513	72.62713	65.48680	-1691.16043	-1535.97525	-1484.73099	1
244	C	77.44986	73.99347	65.23223	542.66492	350.14337	454.42563	1
245	H	78.00689	74.13927	64.28011	1209.57979	-2396.95920	463.86744	1
246	C	77.18435	75.38481	65.95184	-737.14309	145.93010	242.71942	1
247	H	76.60922	75.22895	66.88986	-1050.18303	159.36419	-2509.06125	1
248	C	78.53602	76.11952	66.24856	-706.77696	-252.88343	-245.16230	1
249	H	78.36909	77.18547	66.53039	-1624.64039	-1665.49085	1417.86935	1
250	H	79.08596	75.64418	67.09703	2566.10521	598.51109	693.22305	1
251	H	79.21119	76.11484	65.36033	-1972.69758	107.10018	-1876.34312	1
252	C	76.40872	76.35381	64.99133	412.85148	672.58832	-27.69222	1
253	H	76.38760	77.39651	65.38769	1447.02277	1762.76533	-1490.78944	1
254	H	76.88254	76.39231	63.97886	1320.77379	-145.20455	2378.68491	1
255	H	75.34738	76.03491	64.85473	-1512.10848	1470.52031	1724.75147	1
256	C	78.01346	72.83238	66.21819	-607.11113	499.56689	73.73769	1
257	O	77.37580	71.79928	66.35323	357.97126	460.81534	356.68785	1
258	N	79.18411	73.16714	66.75102	536.55407	-368.62270	332.76306	1
259	H	79.54274	74.10137	66.55701	524.38866	2297.69985	1367.20941	1

260	C	79.63615	72.43703	67.89022	46.50277	-774.29190	-147.97904	1
261	H	79.62232	71.37947	67.54905	1676.51875	1883.29066	1032.55549	1
262	C	81.07028	72.99060	68.35513	-559.41456	-34.19198	-556.30433	1
263	H	80.90884	73.96673	68.87408	-64.66664	395.18769	2695.05373	1
264	H	81.50690	72.31236	69.12750	-2703.44278	-60.40056	333.79418	1
265	C	82.03296	73.18630	67.20725	-519.76435	377.31045	459.42366	1
266	H	81.50730	73.72233	66.38651	-1746.74323	1667.50644	-1261.73691	1
267	C	83.20706	74.04513	67.66088	570.95554	16.46261	-545.27700	1
268	H	83.92839	74.23757	66.82547	2391.58273	28.05277	-1305.07271	1
269	H	82.86668	75.04244	68.04271	175.75588	917.63458	2559.43867	1
270	H	83.78099	73.55353	68.48819	-1063.97851	-2155.34650	1283.00462	1
271	C	82.53651	71.85597	66.66711	193.76014	2.62946	-765.53141	1
272	H	83.25581	72.00130	65.81956	507.39394	-846.55087	2539.60089	1
273	H	83.06930	71.26493	67.45640	1337.57841	1818.19054	1526.01994	1
274	H	81.69476	71.22191	66.28528	1100.88635	-1172.91350	-2199.08909	1
275	C	78.61576	72.69822	69.11094	-549.21115	475.64486	-309.38218	1
276	O	78.05298	73.74483	69.30008	556.06106	-390.37755	-78.24250	1
277	O	78.57713	71.67357	70.08802	-572.27940	-310.19032	-209.75862	1
278	H	79.12653	70.98866	69.61755	-1380.08193	2212.14486	790.85944	1

Listing 114: C00114.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.9840	3936
		0.2500	300.00	0.00	0.00	0.00	-1293.3814	0.0000	300.0000
3	H	68.56733	81.73815	68.34202	-2043.14101	-1757.64893	399.89339		1
4	N	68.95824	82.58432	68.75224	426.75047	490.45733	-334.42467		1
5	H	69.22829	82.25454	69.67721	442.25559	-1110.30854	-2448.52907		1
6	C	69.99112	83.18254	67.99895	415.32972	-666.39213	83.73172		1
7	H	69.80747	82.87326	66.94876	879.32219	2491.00447	667.35213		1
8	C	69.91944	84.77595	68.21433	31.35357	477.41777	628.23362		1
9	H	70.08907	85.01590	69.29119	1168.38489	2240.25337	-1019.71136		1
10	H	70.74208	85.28449	67.65539	-360.43770	2534.90498	931.67112		1
11	C	68.56691	85.27924	67.77371	463.18208	512.70242	-382.34388		1
12	H	67.79312	84.57742	68.15966	1725.29117	1863.52247	-987.07854		1
13	C	68.29839	86.65906	68.35979	710.42801	-144.27427	-313.15367		1
14	H	67.29644	87.05362	68.04907	364.20195	-1033.13725	2494.72524		1
15	H	68.31625	86.64332	69.48049	2567.61904	335.80679	847.48802		1
16	H	69.06618	87.40438	68.02667	-2587.99029	680.92867	-512.16411		1
17	C	68.46819	85.33402	66.25587	268.17616	741.64379	-40.42634		1
18	H	67.46717	85.70959	65.91922	1283.54314	-1945.37420	-1411.27812		1
19	H	69.24222	86.01619	65.81781	-1258.57796	1317.15249	-2026.02085		1
20	H	68.61690	84.32422	65.79329	-2502.84526	909.80597	575.92391		1
21	C	71.41490	82.63782	68.59722	619.36578	-458.64843	-172.09273		1
22	O	72.23680	82.08496	67.90227	-81.40433	433.87611	522.34594		1
23	N	71.47766	82.92571	69.89403	175.23996	-622.20190	341.55523		1
24	H	70.68000	83.37407	70.34262	-876.57256	-303.22879	-2561.90213		1
25	C	72.62052	82.54588	70.63603	-571.88214	-534.10783	-106.15033		1
26	H	73.32827	82.08342	69.90945	-2713.20841	-16.25800	-248.80809		1
27	C	73.15273	83.88373	71.35362	166.60354	288.16399	-716.09568		1
28	H	72.33102	84.25904	72.02316	-2097.85574	1636.78449	-586.18044		1
29	O	73.47474	84.97420	70.47483	-317.80580	-363.38227	484.43082		1
30	H	72.79090	85.62708	70.72703	1863.74748	-1451.84923	1357.29467		1
31	C	74.34166	83.36180	72.23796	503.80731	517.99032	318.51606		1
32	H	74.73485	84.16681	72.90138	640.61020	-2157.10410	-1536.29104		1
33	H	74.04322	82.50106	72.90111	1687.88455	465.60692	2087.56452		1
34	H	75.19329	83.01698	71.60679	-1293.07895	-1899.88581	-1463.57452		1
35	C	72.05394	81.57062	71.82289	-153.07550	-733.68902	248.70981		1
36	O	71.06558	81.90500	72.42042	186.15459	-480.78787	-449.34387		1
37	N	72.86121	80.52648	72.03418	-487.53139	543.18517	42.03850		1
38	C	72.62496	79.63556	73.13808	-699.35871	69.34393	360.10701		1
39	H	71.53306	79.41185	73.15511	2.81126	-221.99807	-2715.58072		1

40	C	73.56436	78.40004	72.78793	-507.46439	-592.59194	122.07761	1
41	H	73.86946	77.82321	73.68986	-1975.08116	525.87560	-1801.71556	1
42	H	73.05467	77.67979	72.11004	1588.27743	-1913.22100	1113.83566	1
43	C	74.76013	79.09951	72.07358	-613.62442	-457.55993	-194.14490	1
44	H	75.43493	79.58694	72.81267	1707.54637	-721.27992	1996.92523	1
45	H	75.39018	78.40615	71.47223	758.23357	2100.81767	1560.55011	1
46	C	73.99412	80.17948	71.19133	-352.41524	704.96076	49.21465	1
47	H	74.58012	81.09875	70.96191	1714.76886	-2070.42778	443.35792	1
48	H	73.55343	79.77915	70.24712	1224.15040	1801.50881	1636.97633	1
49	C	73.12282	80.37399	74.49660	566.85117	537.05831	117.62814	1
50	O	73.98728	81.22954	74.50023	-550.26779	-406.08867	4.21666	1
51	N	72.54212	79.76021	75.52904	566.34832	-425.77725	180.18749	1
52	H	71.81179	79.08861	75.27813	644.44502	2646.80550	-52.73430	1
53	C	72.22440	80.59668	76.67014	612.34801	-281.48662	411.56221	1
54	H	71.63595	81.44590	76.25924	1667.23498	-1490.75142	1556.16753	1
55	C	71.39712	79.65385	77.63944	-714.45746	-175.43074	286.98927	1
56	H	72.09622	78.90329	78.10107	-787.09484	1763.03619	-1922.46060	1
57	O	70.34670	78.87248	77.02535	-429.46514	516.51932	-128.40526	1
58	H	70.62841	77.96512	77.25074	1981.82785	436.16847	-1818.18182	1
59	C	70.94408	80.70252	78.72273	630.79189	-468.94448	76.03230	1
60	H	70.49766	80.20417	79.61417	-1775.71861	2062.30353	131.89849	1
61	H	71.79468	81.32863	79.07856	-1855.14608	88.94118	1993.53760	1
62	H	70.17410	81.39686	78.31381	-1504.82350	-780.94249	-2132.90992	1
63	C	73.63207	81.03409	77.35327	288.57638	618.62814	-397.00270	1
64	O	74.50123	80.23547	77.62502	321.70495	-185.26452	574.37218	1
65	N	73.65809	82.39515	77.62820	-447.05792	-446.53431	367.76425	1
66	H	72.69671	82.63893	77.34112	350.31316	1975.63644	-1843.31522	1
67	C	74.67989	83.04126	76.80598	-511.23061	374.03917	-471.51480	1
68	H	74.60518	82.45908	75.83803	2234.79579	-898.70890	-1273.45190	1
69	C	74.19397	84.54027	76.68054	529.53781	-159.34528	563.72604	1
70	H	74.94016	85.13848	76.09657	654.59388	2347.94251	1217.51488	1
71	H	73.25945	84.53810	76.05647	-1526.55661	2103.42026	817.87394	1
72	O	73.86851	85.25065	77.92792	-554.84278	14.12789	399.58769	1
73	H	73.47558	84.51482	78.42290	1297.06236	2061.84854	1220.68812	1
74	C	76.12019	82.86218	77.51669	-662.15484	-412.13544	123.62687	1
75	O	76.51997	83.67516	78.35132	-540.01537	-317.05804	274.91456	1
76	N	76.71468	81.79258	77.03322	-202.76299	-690.00100	-131.49145	1
77	H	76.14994	81.22101	76.40208	-702.62132	-2617.37191	281.70413	1
78	C	78.04202	81.39404	77.31562	-491.73914	576.34187	222.73509	1
79	H	78.23757	80.60685	76.55565	1977.17978	-1823.58850	-434.68928	1
80	C	78.98458	82.66774	77.17345	-649.50797	-328.66843	306.11224	1
81	H	78.57847	83.51843	77.77052	2075.07803	1452.16490	-1004.45904	1
82	C	80.43324	82.30531	77.64634	-615.18735	-489.99689	-70.96352	1
83	H	81.14111	83.15286	77.48919	-1226.32661	-1724.38906	-1716.47170	1
84	H	80.45514	82.05168	78.73251	2381.64273	-969.84735	900.46860	1
85	H	80.83980	81.42586	77.09683	2122.74991	1702.23946	-141.36228	1
86	C	79.05003	83.05762	75.65716	-501.86074	-479.61276	-376.42482	1
87	H	79.69721	83.94982	75.48806	993.79261	-2246.95401	-1177.81305	1
88	H	79.46045	82.22814	75.03739	42.71279	-626.15391	-2651.37258	1
89	H	78.03668	83.30046	75.25932	-2026.39012	-1590.33709	-887.82922	1
90	C	78.19002	80.79660	78.84321	-672.89153	382.57394	-156.34072	1
91	O	78.70363	79.71654	79.02494	410.04627	221.86223	500.35950	1
92	N	77.70999	81.66027	79.70693	-378.11782	-443.79414	-441.10984	1
93	H	77.34379	82.58101	79.35206	2404.15973	-568.14894	1149.30085	1
94	C	77.87469	81.46460	81.11876	-544.54484	466.16019	331.29119	1
95	H	78.97629	81.40629	81.25782	-1409.80988	-170.17955	2325.32679	1
96	C	77.21872	82.78641	81.70311	-184.48284	116.78282	-758.89137	1
97	H	77.99479	83.55347	81.92373	1893.78641	1861.14652	611.04528	1
98	H	76.57456	83.24071	80.91623	-2170.79665	-974.19311	1327.50117	1
99	C	76.36880	82.49433	82.97693	389.51668	672.81878	-138.49152	1
100	H	76.03570	81.43219	82.98281	510.64577	1933.03327	1851.02484	1
101	H	76.99681	82.57775	83.89105	-2302.30869	-1105.72939	-948.89774	1

102	C	75.10267	83.42320	83.09965	-559.93427	-126.34590	542.30857	1
103	O	74.37998	83.29989	84.05458	-670.36003	-111.83166	76.36448	1
104	N	74.91719	84.28427	82.07459	-216.06729	-537.07037	446.51379	1
105	H	75.47515	84.48427	81.23461	-1251.96487	1074.12894	-2168.52500	1
106	H	74.13279	84.94618	82.04012	-2451.83023	-720.73851	944.84612	1
107	C	77.20254	80.08733	81.65525	546.24052	-563.88337	-85.11809	1
108	O	77.79507	79.55820	82.56223	71.70702	-307.40463	606.69673	1
109	N	75.99424	79.76548	81.16463	479.90863	-504.50129	222.86849	1
110	C	75.33197	78.60194	81.66930	75.51268	-600.91904	506.73700	1
111	H	75.83055	78.38845	82.64488	-2033.61562	1795.30103	254.89480	1
112	C	73.83266	79.12132	81.72571	523.79067	517.99274	284.45581	1
113	H	73.08886	78.29565	81.77204	1599.61665	-1127.00911	1895.98173	1
114	H	73.65484	79.76602	82.61496	-1881.83093	1275.82488	-1501.55016	1
115	C	73.75611	79.94601	80.40365	-600.05639	-404.05026	316.64485	1
116	H	73.65621	79.27268	79.51780	-2597.05260	496.36221	657.73249	1
117	H	72.89703	80.65084	80.37331	-1666.24518	1294.38985	-1723.90591	1
118	C	75.16390	80.67938	80.39244	493.57570	-129.95376	-602.56394	1
119	H	75.63455	80.78766	79.38071	-1469.08415	-637.84797	2204.22581	1
120	H	75.18525	81.66354	80.91541	-1038.97840	1068.88701	-2280.71789	1
121	C	75.42739	77.35656	80.60087	188.88100	241.05089	-727.87821	1
122	O	74.68931	77.29417	79.62323	531.88613	-49.19943	427.07960	1
123	N	76.31249	76.49453	81.03618	708.14833	26.93417	-179.73509	1
124	H	76.82202	76.77813	81.87263	-2232.69501	-1179.09831	1023.94816	1
125	C	76.68869	75.32037	80.33120	-738.32412	259.92548	104.42456	1
126	H	77.33859	74.77821	81.05341	2028.89123	1260.02983	1311.33324	1
127	C	75.39794	74.49859	79.88190	-258.65678	-345.52513	661.28459	1
128	H	74.70318	75.15572	79.30945	-1826.06090	-1801.46097	-918.64554	1
129	C	75.86100	73.28154	79.01115	-541.23400	531.92970	-218.41428	1
130	H	74.99437	72.70198	78.60613	1311.73218	-2219.18200	882.19023	1
131	H	76.47406	73.59993	78.13052	-1048.71298	1223.58118	-2196.97971	1
132	H	76.49062	72.57063	79.59639	419.06414	1903.92898	1903.44670	1
133	C	74.66541	73.92683	81.14184	-423.86431	152.66566	-648.55262	1
134	H	73.75610	73.34582	80.85797	105.68386	-2342.50080	1387.51238	1
135	H	75.32479	73.24590	81.72933	-1695.63603	-1484.73621	-1531.02793	1
136	H	74.33760	74.74507	81.82545	-1853.57121	-487.39031	1936.59343	1
137	C	77.50208	75.72742	78.97253	539.71428	-510.58232	267.58633	1
138	O	78.68567	75.42534	78.90417	-15.93758	-278.34085	-624.49402	1
139	N	76.71008	76.30809	78.10893	-676.81886	12.05292	276.17960	1
140	H	75.74025	76.56393	78.41021	-1694.44250	-373.84189	-2100.66098	1
141	C	77.11276	76.66136	76.79848	412.33078	-664.70360	108.35451	1
142	H	76.24622	77.25440	76.42815	1765.77476	1294.44366	1621.76594	1
143	C	78.45586	77.49229	76.91532	-179.66635	-721.95667	-264.73915	1
144	H	78.38148	78.28688	77.71426	-607.34922	2587.87032	-598.10018	1
145	H	79.30256	76.83753	77.23002	-359.69332	-1479.13954	-2259.74260	1
146	C	78.72029	78.12720	75.51153	-240.01076	616.02425	431.85322	1
147	H	78.79436	77.34339	74.72447	-1359.17131	782.54425	2227.99181	1
148	H	77.87181	78.78305	75.21217	-820.36667	85.81767	-2596.78715	1
149	C	80.06456	78.95427	75.61794	-513.07015	236.18570	-551.87280	1
150	H	80.04947	79.62711	76.50535	1816.11944	-1183.11722	-1650.94321	1
151	H	80.93958	78.28084	75.76798	-1800.04429	-1361.53473	1526.34643	1
152	C	80.18879	79.75917	74.30354	726.08972	-253.19732	-179.64713	1
153	H	80.37052	79.14098	73.40198	1224.27271	-456.51798	-2390.90304	1
154	H	79.34961	80.45694	74.11417	1206.40339	-1150.93514	-2154.90344	1
155	N	81.45255	80.67827	74.40971	329.70796	-633.68968	-155.67358	1
156	H	81.63741	81.29004	73.56300	1348.31305	1938.76845	1359.00643	1
157	H	81.48175	81.39602	75.19060	2096.92035	1446.54551	-966.48890	1
158	H	82.39030	80.19431	74.52359	-1197.07217	-2303.53719	827.28733	1
159	C	77.41690	75.34754	75.84419	-378.01186	-556.17301	-413.96481	1
160	O	76.84533	75.23826	74.79017	-409.44433	-307.55053	-453.30833	1
161	N	78.37849	74.60129	76.35889	-429.02477	524.70884	274.08502	1
162	H	78.78195	74.82176	77.30205	1706.34263	-1425.96036	1574.38926	1
163	C	78.72451	73.39079	75.69894	-45.25864	-626.22952	478.93267	1

164	H	78.50470	73.54929	74.61889	1988.63164	570.90773	1772.87287	1
165	C	80.23762	73.16249	76.09812	551.77128	-20.49526	-564.54996	1
166	H	80.86280	74.00991	75.73800	1434.61535	-1753.10253	1513.99471	1
167	H	80.32943	73.18102	77.20772	-714.67738	1819.09770	1898.36494	1
168	C	80.79078	71.80723	75.54758	446.99263	-555.77305	338.97221	1
169	H	80.13178	70.95868	75.84015	1953.68466	1892.25957	-161.67766	1
170	H	80.83059	71.80547	74.43719	-403.03785	2688.07032	-188.43591	1
171	C	82.24165	71.63149	76.15425	567.86262	335.74681	434.04421	1
172	H	82.87355	72.52178	75.93130	-1080.02275	1568.26081	-1948.78900	1
173	H	82.19948	71.56152	77.26556	-919.54108	2111.34692	1456.13463	1
174	C	82.86724	70.35535	75.54610	195.81897	173.33862	-745.11536	1
175	H	82.34208	69.41432	75.80487	1405.67949	-2301.21089	-390.08113	1
176	H	83.04272	70.40275	74.45281	-940.37328	-1118.32446	2299.72133	1
177	N	84.29575	70.19808	76.16996	319.26422	656.36007	-42.02424	1
178	H	84.85349	69.35965	75.83673	1961.03633	619.91968	1787.09422	1
179	H	84.98630	70.98671	76.00293	854.14343	-2156.80752	1429.08711	1
180	H	84.34979	70.07905	77.22327	1237.02905	-1378.50857	-1998.28500	1
181	C	77.83013	72.17806	76.36954	532.53319	-268.57236	517.55729	1
182	O	77.89609	71.90780	77.54519	266.16714	-290.73804	-558.88002	1
183	N	77.16940	71.56203	75.39753	-226.25352	640.49678	-270.32839	1
184	H	77.21124	71.95745	74.45946	2007.69063	-1035.27229	1523.50231	1
185	C	76.26848	70.52221	75.73970	-540.76542	-573.33303	49.50000	1
186	H	76.51737	70.27023	76.79629	-2374.20950	-1036.76023	843.75774	1
187	C	74.80146	71.13718	75.57166	-77.09082	666.87422	-415.84136	1
188	H	74.69660	71.53767	74.52612	-985.81834	617.19825	2463.91927	1
189	O	74.48248	72.25176	76.43108	293.29899	-391.65602	-477.80926	1
190	H	74.44664	72.98210	75.78262	2528.72714	-681.76262	-751.27122	1
191	C	73.89921	69.86163	75.73793	252.47363	-605.14473	440.05134	1
192	H	72.82371	70.09771	75.56512	-2052.65063	1456.49051	-1043.51830	1
193	H	74.18173	69.05839	75.01952	-2152.98800	-1661.97574	-161.70652	1
194	H	73.98544	69.43425	76.76368	-473.12726	-1584.27339	2165.61725	1
195	C	76.50479	69.28290	74.67885	360.36307	488.46713	505.10056	1
196	O	76.80864	68.19960	75.11610	-200.08817	-528.03552	-385.82850	1
197	N	76.22983	69.63060	73.42302	-597.54095	-226.44775	355.20479	1
198	H	76.00896	70.61754	73.29280	2179.23655	-1300.70981	-991.33835	1
199	C	76.73264	68.89011	72.32347	-687.68921	297.39807	-249.45179	1
200	H	76.52714	69.54914	71.45107	-349.16256	-2467.37713	-1101.72831	1
201	C	78.29958	68.62216	72.53199	672.47345	361.54328	-201.62880	1
202	H	78.51415	68.42057	73.60960	1541.41502	582.18425	2169.97026	1
203	H	78.61047	67.72361	71.94758	-2534.67717	60.25153	997.72295	1
204	C	79.01490	69.88207	72.02807	574.26774	-389.43119	-377.02542	1
205	C	79.43251	69.96146	70.66500	688.82679	-287.33580	-257.96133	1
206	H	79.28854	69.10671	69.97944	331.14182	1470.38163	2269.80013	1
207	C	79.18947	70.99628	72.90178	-383.52382	-675.04808	144.24917	1
208	H	78.85683	70.93413	73.95312	4.09847	1517.59662	2262.86397	1
209	C	80.01676	71.14445	70.21455	-134.76730	428.45285	-649.50303	1
210	H	80.33938	71.20586	69.16049	-903.23433	1600.49020	2011.53387	1
211	C	79.77266	72.16331	72.40145	-335.53281	-615.00040	-364.39058	1
212	H	79.89615	73.02432	73.08117	1596.45398	-1369.33862	1732.02659	1
213	C	80.21232	72.28194	71.05128	585.48547	-340.24194	-406.23938	1
214	O	80.81433	73.45976	70.53678	-419.15649	-173.04408	-511.94141	1
215	H	80.78630	74.02699	71.34305	-1071.84350	1559.71507	-1960.13012	1
216	C	76.09173	67.40548	72.15362	291.41878	-183.13091	710.72246	1
217	O	76.61652	66.60709	71.39611	379.87695	523.47396	-222.23622	1
218	N	74.86358	67.27253	72.73817	564.30591	373.09380	277.24371	1
219	H	74.83993	68.10385	73.34259	-120.59931	-2436.07824	-1214.35098	1
220	C	74.61376	65.96193	73.32069	404.07514	-299.37480	608.84009	1
221	H	75.57266	65.66601	73.80060	-1071.07882	-841.69025	2359.66467	1
222	C	73.44905	66.18463	74.35517	-683.12807	68.71770	-390.13096	1
223	H	73.75452	66.92168	75.13199	2068.88918	1596.58590	770.89603	1
224	H	72.56760	66.63592	73.84582	1379.86429	2342.49779	-179.85638	1
225	C	73.05297	64.82823	75.02183	-176.39967	537.49466	550.97268	1

226	H	72.74707	64.07704	74.25846	-396.28051	1942.22168	1869.33314	1
227	H	73.91644	64.37420	75.55617	-94.44700	586.00678	-2659.20016	1
228	C	71.85071	65.15212	76.02530	-291.69381	-718.18079	-150.72929	1
229	H	72.16914	65.72669	76.93291	-2303.38776	1089.76242	964.62032	1
230	H	70.95103	65.64562	75.57945	884.16729	2568.80533	-207.74283	1
231	N	71.50017	63.85742	76.43158	-594.49522	-252.81478	342.29276	1
232	H	72.23791	63.16917	76.41212	-1735.17426	2084.05705	-263.71605	1
233	C	70.35176	63.49982	76.84660	595.23177	-271.52487	442.22352	1
234	N	69.33134	64.45408	76.89628	585.53813	-424.79750	-105.81303	1
235	H	69.36229	65.45221	76.69290	959.88797	1327.56823	-2177.11905	1
236	H	68.38558	64.27410	77.23458	1578.48647	16.27378	-2220.76233	1
237	N	70.34652	62.13866	77.18058	-452.17763	-390.33541	-421.51853	1
238	H	71.09015	61.44223	77.16844	470.26107	1974.25629	-1817.92087	1
239	H	69.52504	61.66200	77.55403	1856.67307	-1573.97321	-1224.35416	1
240	C	74.14820	64.91323	72.18776	-531.47271	-581.45780	-55.06206	1
241	O	74.09948	63.71200	72.45444	-243.00837	192.73507	609.52485	1
242	N	73.75837	65.50891	71.07320	343.49288	-644.25607	38.09164	1
243	H	73.90645	66.51647	71.10911	-1691.16043	-1535.97525	-1484.73099	1
244	C	73.47033	64.81841	69.82976	542.66492	350.14337	454.42563	1
245	H	73.42606	65.63001	69.06488	1209.57979	-2396.95920	463.86744	1
246	C	74.57122	63.79723	69.57069	-737.14309	145.93010	242.71942	1
247	H	74.66799	63.15774	70.48273	-1050.18303	159.36419	-2509.06125	1
248	C	74.23837	62.90226	68.39437	-706.77696	-252.88343	-245.16230	1
249	H	75.03119	62.12218	68.22723	-1624.64039	-1665.49085	1417.86935	1
250	H	73.24788	62.35038	68.54557	2566.10521	598.51109	693.22305	1
251	H	74.14546	63.49080	67.44036	-1972.69758	107.10018	-1876.34312	1
252	C	75.91251	64.46674	69.35222	412.85148	672.58832	-27.69222	1
253	H	76.74679	63.71562	69.28316	1447.02277	1762.76533	-1490.78944	1
254	H	75.92505	65.06587	68.40060	1320.77379	-145.20455	2378.68491	1
255	H	76.16650	65.19122	70.21205	-1512.10848	1470.52031	1724.75147	1
256	C	71.98110	64.08903	70.03999	-607.11113	499.56689	73.73769	1
257	O	71.03025	64.56912	69.48579	357.97126	460.81534	356.68785	1
258	N	72.07126	63.05054	70.84967	536.55407	-368.62270	332.76306	1
259	H	72.95903	62.88461	71.37550	524.38866	2297.69985	1367.20941	1
260	C	71.00370	62.12006	70.94596	46.50277	-774.29190	-147.97904	1
261	H	71.40601	61.35660	71.64787	1676.51875	1883.29066	1032.55549	1
262	C	69.71240	62.88580	71.55277	-559.41456	-34.19198	-556.30433	1
263	H	69.51668	63.81685	70.96382	-64.66664	395.18769	2695.05373	1
264	H	68.79042	62.26266	71.46909	-2703.44278	-60.40056	333.79418	1
265	C	70.00929	63.20563	72.98963	-519.76435	377.31045	459.42366	1
266	H	70.99618	63.72006	73.03569	-1746.74323	1667.50644	-1261.73691	1
267	C	68.94821	64.13503	73.56785	570.95554	16.46261	-545.27700	1
268	H	69.15158	64.36633	74.64489	2391.58273	28.05277	-1305.07271	1
269	H	68.90454	65.11009	73.01780	175.75588	917.63458	2559.43867	1
270	H	67.92696	63.67675	73.51621	-1063.97851	-2155.34650	1283.00462	1
271	C	70.07186	61.94213	73.83923	193.76014	2.62946	-765.53141	1
272	H	70.24009	62.18443	74.91936	507.39394	-846.55087	2539.60089	1
273	H	69.11997	61.35429	73.77717	1337.57841	1818.19054	1526.01994	1
274	H	70.90369	61.26222	73.52415	1100.88635	-1172.91350	-2199.08909	1
275	C	70.69370	61.48667	69.50500	-549.21115	475.64486	-309.38218	1
276	O	71.52089	61.41618	68.62501	556.06106	-390.37755	-78.24250	1
277	O	69.44795	60.83909	69.35847	-572.27940	-310.19032	-209.75862	1
278	H	69.06423	61.04056	70.25654	-1380.08193	2212.14486	790.85944	1

Listing 115: C00115.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.3772	0.0000	300.0000
3	H	83.89417	78.01318	75.65562	-2043.14101	-1757.64893	399.89339		1
4	N	83.69350	78.76603	74.99664	426.75047	490.45733	-334.42467		1
5	H	83.03913	79.37508	75.51038	442.25559	-1110.30854	-2448.52907		1

6	C	84.87720	79.41395	74.55229	415.32972	-666.39213	83.73172	1
7	H	85.42737	78.55110	74.11399	879.32219	2491.00447	667.35213	1
8	C	84.50074	80.53956	73.44621	31.35357	477.41777	628.23362	1
9	H	83.77755	81.26673	73.88481	1168.38489	2240.25337	-1019.71136	1
10	H	85.40060	81.12996	73.15486	-360.43770	2534.90498	931.67112	1
11	C	83.91399	79.85761	72.24656	463.18208	512.70242	-382.34388	1
12	H	83.15532	79.12159	72.59784	1725.29117	1863.52247	-987.07854	1
13	C	83.22708	80.87280	71.33918	710.42801	-144.27427	-313.15367	1
14	H	82.77498	80.38349	70.43866	364.20195	-1033.13725	2494.72524	1
15	H	82.40422	81.41462	71.87214	2567.61904	335.80679	847.48802	1
16	H	83.94770	81.64619	70.96845	-2587.99029	680.92867	-512.16411	1
17	C	84.98521	79.12346	71.44838	268.17616	741.64379	-40.42634	1
18	H	84.55736	78.63049	70.53812	1283.54314	-1945.37420	-1411.27812	1
19	H	85.78843	79.82176	71.09896	-1258.57796	1317.15249	-2026.02085	1
20	H	85.48319	78.32394	72.05362	-2502.84526	909.80597	575.92391	1
21	C	85.62301	79.93238	75.85202	619.36578	-458.64843	-172.09273	1
22	O	85.69321	79.26301	76.94623	-81.40433	433.87611	522.34594	1
23	N	86.21532	81.08849	75.69752	175.23996	-622.20190	341.55523	1
24	H	86.19814	81.54208	74.78703	-876.57256	-303.22879	-2561.90213	1
25	C	87.32941	81.22440	76.59435	-571.88214	-534.10783	-106.15033	1
26	H	88.08462	80.58577	76.09184	-2713.20841	-16.25800	-248.80809	1
27	C	87.80576	82.71998	76.56558	166.60354	288.16399	-716.09568	1
28	H	86.95624	83.41019	76.83639	-2097.85574	1636.78449	-586.18044	1
29	O	88.23763	83.21568	75.26590	-317.80580	-363.38227	484.43082	1
30	H	87.63190	83.96453	75.13592	1863.74748	-1451.84923	1357.29467	1
31	C	88.89270	82.71110	77.70475	503.80731	517.99032	318.51606	1
32	H	89.27188	83.73764	77.91663	640.61020	-2157.10410	-1536.29104	1
33	H	88.49198	82.29635	78.65982	1687.88455	465.60692	2087.56452	1
34	H	89.77094	82.08631	77.42011	-1293.07895	-1899.88581	-1463.57452	1
35	C	86.86469	80.42163	78.02234	-153.07550	-733.68902	248.70981	1
36	O	87.76418	79.75905	78.56168	186.15459	-480.78787	-449.34387	1
37	N	85.95901	81.14678	78.77400	-487.53139	543.18517	42.03850	1
38	C	85.53156	80.63276	80.01550	-699.35871	69.34393	360.10701	1
39	H	86.37165	79.98215	80.36270	2.81126	-221.99807	-2715.58072	1
40	C	85.25356	81.97302	80.84119	-507.46439	-592.59194	122.07761	1
41	H	84.57413	81.81132	81.70792	-1975.08116	525.87560	-1801.71556	1
42	H	86.19432	82.40881	81.24448	1588.27743	-1913.22100	1113.83566	1
43	C	84.63494	82.87941	79.73806	-613.62442	-457.55993	-194.14490	1
44	H	83.57133	82.60955	79.55181	1707.54637	-721.27992	1996.92523	1
45	H	84.65062	83.96325	79.98883	758.23357	2100.81767	1560.55011	1
46	C	85.55964	82.50668	78.49008	-352.41524	704.96076	49.21465	1
47	H	85.05597	82.51821	77.49285	1714.76886	-2070.42778	443.35792	1
48	H	86.50364	83.09995	78.43574	1224.15040	1801.50881	1636.97633	1
49	C	84.08874	79.82065	79.95500	566.85117	537.05831	117.62814	1
50	O	83.83757	79.01720	80.82090	-550.26779	-406.08867	4.21666	1
51	N	83.31896	80.21332	78.94960	566.34832	-425.77725	180.18749	1
52	H	83.73695	80.87964	78.30298	644.44502	2646.80550	-52.73430	1
53	C	81.91300	80.00188	79.05662	612.34801	-281.48662	411.56221	1
54	H	81.80489	79.16292	79.78414	1667.23498	-1490.75142	1556.16753	1
55	C	81.23306	81.36096	79.57718	-714.45746	-175.43074	286.98927	1
56	H	81.33699	82.14812	78.78191	-787.09484	1763.03619	-1922.46060	1
57	O	81.77073	81.93019	80.78214	-429.46514	516.51932	-128.40526	1
58	H	81.90677	82.85991	80.50832	1981.82785	436.16847	-1818.18182	1
59	C	79.72760	80.91969	79.67149	630.79189	-468.94448	76.03230	1
60	H	79.07462	81.76627	79.98631	-1775.71861	2062.30353	131.89849	1
61	H	79.33937	80.54766	78.69519	-1855.14608	88.94118	1993.53760	1
62	H	79.58884	80.10391	80.41874	-1504.82350	-780.94249	-2132.90992	1
63	C	81.40104	79.70917	77.54330	288.57638	618.62814	-397.00270	1
64	O	81.83117	80.31808	76.57660	321.70495	-185.26452	574.37218	1
65	N	80.38366	78.84019	77.56845	-447.05792	-446.53431	367.76425	1
66	H	80.17718	78.43922	78.48627	350.31316	1975.63644	-1843.31522	1
67	C	80.36519	77.93057	76.45931	-511.23061	374.03917	-471.51480	1

68	H	80.77388	78.53338	75.61563	2234.79579	-898.70890	-1273.45190	1
69	C	81.34759	76.73671	76.87381	529.53781	-159.34528	563.72604	1
70	H	81.29971	75.99227	76.03388	654.59388	2347.94251	1217.51488	1
71	H	82.39086	77.15114	76.88475	-1526.55661	2103.42026	817.87394	1
72	O	81.06589	76.06267	78.12482	-554.84278	14.12789	399.58769	1
73	H	81.68260	76.53924	78.71261	1297.06236	2061.84854	1220.68812	1
74	C	78.85042	77.39895	76.19589	-662.15484	-412.13544	123.62687	1
75	O	78.68033	76.40744	75.51662	-540.01537	-317.05804	274.91456	1
76	N	77.94714	78.22178	76.71073	-202.76299	-690.00100	-131.49145	1
77	H	78.33200	79.01228	77.22531	-702.62132	-2617.37191	281.70413	1
78	C	76.56418	78.21513	76.35759	-491.73914	576.34187	222.73509	1
79	H	76.38757	79.30140	76.19969	1977.17978	-1823.58850	-434.68928	1
80	C	76.27197	77.35650	75.06059	-649.50797	-328.66843	306.11224	1
81	H	76.61269	76.30033	75.19821	2075.07803	1452.16490	-1004.45904	1
82	C	74.74795	77.42150	74.68780	-615.18735	-489.99689	-70.96352	1
83	H	74.52454	76.82052	73.77535	-1226.32661	-1724.38906	-1716.47170	1
84	H	74.09831	77.03205	75.50553	2381.64273	-969.84735	900.46860	1
85	H	74.42355	78.46830	74.48420	2122.74991	1702.23946	-141.36228	1
86	C	77.00610	78.02334	73.84343	-501.86074	-479.61276	-376.42482	1
87	H	76.78479	77.49484	72.88734	993.79261	-2246.95401	-1177.81305	1
88	H	76.70324	79.08844	73.71356	42.71279	-626.15391	-2651.37258	1
89	H	78.11360	78.00563	73.98381	-2026.39012	-1590.33709	-887.82922	1
90	C	75.75876	77.79237	77.71714	-672.89153	382.57394	-156.34072	1
91	O	75.76906	78.54137	78.66701	410.04627	221.86223	500.35950	1
92	N	75.07559	76.65757	77.57382	-378.11782	-443.79414	-441.10984	1
93	H	75.24879	76.07990	76.75295	2404.15973	-568.14894	1149.30085	1
94	C	74.42667	76.11356	78.71738	-544.54484	466.16019	331.29119	1
95	H	74.40621	76.92493	79.48139	-1409.80988	-170.17955	2325.32679	1
96	C	72.99455	75.64090	78.20872	-184.48284	116.78282	-758.89137	1
97	H	72.42486	76.49617	77.78162	1893.78641	1861.14652	611.04528	1
98	H	73.10111	74.91246	77.37592	-2170.79665	-974.19311	1327.50117	1
99	C	72.22684	74.99907	79.40400	389.51668	672.81878	-138.49152	1
100	H	72.90895	74.35495	79.99743	510.64577	1933.03327	1851.02484	1
101	H	71.89885	75.78924	80.11458	-2302.30869	-1105.72939	-948.89774	1
102	C	70.99368	74.12455	78.95430	-559.93427	-126.34590	542.30857	1
103	O	70.58243	73.26034	79.69002	-670.36003	-111.83166	76.36448	1
104	N	70.50527	74.45488	77.74396	-216.06729	-537.07037	446.51379	1
105	H	70.80270	75.21089	77.11560	-1251.96487	1074.12894	-2168.52500	1
106	H	69.68277	74.01890	77.31162	-2451.83023	-720.73851	944.84612	1
107	C	75.29834	74.79557	79.13818	546.24052	-563.88337	-85.11809	1
108	O	75.65297	74.02891	78.28076	71.70702	-307.40463	606.69673	1
109	N	75.40775	74.68305	80.46738	479.90863	-504.50129	222.86849	1
110	C	76.27298	73.70612	81.05944	75.51268	-600.91904	506.73700	1
111	H	77.15195	73.61315	80.38026	-2033.61562	1795.30103	254.89480	1
112	C	76.57325	74.33635	82.48530	523.79067	517.99274	284.45581	1
113	H	76.88567	73.57447	83.23471	1599.61665	-1127.00911	1895.98173	1
114	H	77.38790	75.09328	82.43768	-1881.83093	1275.82488	-1501.55016	1
115	C	75.20078	75.00135	82.81273	-600.05639	-404.05026	316.64485	1
116	H	74.44122	74.23854	83.09724	-2597.05260	496.36221	657.73249	1
117	H	75.24468	75.73897	83.64533	-1666.24518	1294.38985	-1723.90591	1
118	C	74.86886	75.66069	81.40509	493.57570	-129.95376	-602.56394	1
119	H	73.78505	75.81205	81.19541	-1469.08415	-637.84797	2204.22581	1
120	H	75.41903	76.61020	81.20152	-1038.97840	1068.88701	-2280.71789	1
121	C	75.55093	72.26524	81.31667	188.88100	241.05089	-727.87821	1
122	O	76.12024	71.39422	81.92963	531.88613	-49.19943	427.07960	1
123	N	74.23600	72.21357	80.90349	708.14833	26.93417	-179.73509	1
124	H	74.19546	73.05036	80.30861	-2232.69501	-1179.09831	1023.94816	1
125	C	73.78905	70.90404	80.37256	-738.32412	259.92548	104.42456	1
126	H	74.54769	70.19430	80.78178	2028.89123	1260.02983	1311.33324	1
127	C	72.38200	70.66974	80.87252	-258.65678	-345.52513	661.28459	1
128	H	71.78074	71.59285	80.69188	-1826.06090	-1801.46097	-918.64554	1
129	C	71.71285	69.52069	80.14038	-541.23400	531.92970	-218.41428	1

130	H	70.66273	69.35046	80.50610	1311.73218	-2219.18200	882.19023	1
131	H	71.65179	69.71670	79.03284	-1048.71298	1223.58118	-2196.97971	1
132	H	72.27662	68.55682	80.27704	419.06414	1903.92898	1903.44670	1
133	C	72.36671	70.41478	82.36976	-423.86431	152.66566	-648.55262	1
134	H	71.31871	70.31327	82.76624	105.68386	-2342.50080	1387.51238	1
135	H	72.91909	69.47110	82.63468	-1695.63603	-1484.73621	-1531.02793	1
136	H	72.86152	71.25608	82.93024	-1853.57121	-487.39031	1936.59343	1
137	C	73.84553	71.02543	78.72957	539.71428	-510.58232	267.58633	1
138	O	74.72313	70.44261	78.10975	-15.93758	-278.34085	-624.49402	1
139	N	72.88659	71.80046	78.28802	-676.81886	12.05292	276.17960	1
140	H	72.25411	72.19840	78.98469	-1694.44250	-373.84189	-2100.66098	1
141	C	72.61012	71.99688	76.90637	412.33078	-664.70360	108.35451	1
142	H	71.76366	72.72079	76.91376	1765.77476	1294.44366	1621.76594	1
143	C	73.92815	72.57225	76.23148	-179.66635	-721.95667	-264.73915	1
144	H	74.24632	73.51819	76.73032	-607.34922	2587.87032	-598.10018	1
145	H	74.79066	71.87936	76.36887	-359.69332	-1479.13954	-2259.74260	1
146	C	73.61532	72.80233	74.71797	-240.01076	616.02425	431.85322	1
147	H	73.42340	71.83127	74.20243	-1359.17131	782.54425	2227.99181	1
148	H	72.68570	73.40386	74.58584	-820.36667	85.81767	-2596.78715	1
149	C	74.86077	73.54507	74.08631	-513.07015	236.18570	-551.87280	1
150	H	75.07847	74.49271	74.63096	1816.11944	-1183.11722	-1650.94321	1
151	H	75.78250	72.92595	74.18140	-1800.04429	-1361.53473	1526.34643	1
152	C	74.53348	73.82659	72.60079	726.08972	-253.19732	-179.64713	1
153	H	74.34312	72.92302	71.98581	1224.27271	-456.51798	-2390.90304	1
154	H	73.72739	74.56983	72.43949	1206.40339	-1150.93514	-2154.90344	1
155	N	75.81243	74.47197	71.97378	329.70796	-633.68968	-155.67358	1
156	H	75.74178	74.75302	70.95375	1348.31305	1938.76845	1359.00643	1
157	H	76.18355	75.36084	72.42015	2096.92035	1446.54551	-966.48890	1
158	H	76.67849	73.86002	71.95755	-1197.07217	-2303.53719	827.28733	1
159	C	72.17323	70.56998	76.23811	-378.01186	-556.17301	-413.96481	1
160	O	70.98531	70.39816	75.99838	-409.44433	-307.55053	-453.30833	1
161	N	73.20180	69.77775	76.07296	-429.02477	524.70884	274.08502	1
162	H	74.12403	70.04410	76.48595	1706.34263	-1425.96036	1574.38926	1
163	C	73.10462	68.55311	75.36504	-45.25864	-626.22952	478.93267	1
164	H	74.08877	68.06992	75.55653	1988.63164	570.90773	1772.87287	1
165	C	71.88096	67.76713	75.99259	551.77128	-20.49526	-564.54996	1
166	H	71.92121	67.83325	77.10330	1434.61535	-1753.10253	1513.99471	1
167	H	70.91047	68.23750	75.70398	-714.67738	1819.09770	1898.36494	1
168	C	71.93376	66.27720	75.52144	446.99263	-555.77305	338.97221	1
169	H	71.72877	66.19432	74.42988	1953.68466	1892.25957	-161.67766	1
170	H	72.94615	65.84281	75.68048	-403.03785	2688.07032	-188.43591	1
171	C	70.85007	65.50251	76.37591	567.86262	335.74681	434.04421	1
172	H	71.04751	65.62658	77.46554	-1080.02275	1568.26081	-1948.78900	1
173	H	69.83440	65.92713	76.20366	-919.54108	2111.34692	1456.13463	1
174	C	70.89201	64.00714	75.98704	195.81897	173.33862	-745.11536	1
175	H	70.53892	63.78649	74.95999	1405.67949	-2301.21089	-390.08113	1
176	H	71.86557	63.50945	76.16813	-940.37328	-1118.32446	2299.72133	1
177	N	69.88892	63.25510	76.92707	319.26422	656.36007	-42.02424	1
178	H	69.80381	62.21027	76.76591	1961.03633	619.91968	1787.09422	1
179	H	70.08669	63.28793	77.96952	854.14343	-2156.80752	1429.08711	1
180	H	68.87167	63.55523	76.88773	1237.02905	-1378.50857	-1998.28500	1
181	C	72.87688	68.83263	73.75588	532.53319	-268.57236	517.55729	1
182	O	73.65811	68.37640	72.96003	266.16714	-290.73804	-558.88002	1
183	N	71.78621	69.55040	73.54831	-226.25352	640.49678	-270.32839	1
184	H	71.20367	69.87904	74.35238	2007.69063	-1035.27229	1523.50231	1
185	C	71.40837	69.85306	72.21785	-540.76542	-573.33303	49.50000	1
186	H	72.10341	69.28826	71.55315	-2374.20950	-1036.76023	843.75774	1
187	C	69.88429	69.35213	72.15836	-77.09082	666.87422	-415.84136	1
188	H	69.30894	69.86357	72.97839	-985.81834	617.19825	2463.91927	1
189	O	69.70761	67.93934	72.38865	293.29899	-391.65602	-477.80926	1
190	H	69.13026	67.94977	73.17649	2528.72714	-681.76262	-751.27122	1
191	C	69.34912	69.87018	70.77785	252.47363	-605.14473	440.05134	1

192	H	68.27311	69.59209	70.64586	-2052.65063	1456.49051	-1043.51830	1
193	H	69.40917	70.99686	70.69728	-2152.98800	-1661.97574	-161.70652	1
194	H	69.91869	69.43224	69.92431	-473.12726	-1584.27339	2165.61725	1
195	C	71.52337	71.47919	72.07020	360.36307	488.46713	505.10056	1
196	O	71.50458	72.22390	73.02460	-200.08817	-528.03552	-385.82850	1
197	N	71.61396	71.80556	70.78459	-597.54095	-226.44775	355.20479	1
198	H	71.57514	71.06994	70.08186	2179.23655	-1300.70981	-991.33835	1
199	C	71.45953	73.19866	70.46756	-687.68921	297.39807	-249.45179	1
200	H	72.21419	73.73281	71.08532	-349.16256	-2467.37713	-1101.72831	1
201	C	71.63757	73.38309	68.89070	672.47345	361.54328	-201.62880	1
202	H	70.92020	72.73356	68.34101	1541.41502	582.18425	2169.97026	1
203	H	71.39454	74.43580	68.61703	-2534.67717	60.25153	997.72295	1
204	C	73.08345	73.05196	68.49439	574.26774	-389.43119	-377.02542	1
205	C	74.12927	73.95695	68.84693	688.82679	-287.33580	-257.96133	1
206	H	73.91053	74.88003	69.41390	331.14182	1470.38163	2269.80013	1
207	C	73.36920	71.85538	67.77042	-383.52382	-675.04808	144.24917	1
208	H	72.56058	71.15095	67.50333	4.09847	1517.59662	2262.86397	1
209	C	75.43174	73.65214	68.45331	-134.76730	428.45285	-649.50303	1
210	H	76.24235	74.35376	68.71599	-903.23433	1600.49020	2011.53387	1
211	C	74.69103	71.59650	67.39925	-335.53281	-615.00040	-364.39058	1
212	H	74.90263	70.67225	66.83367	1596.45398	-1369.33862	1732.02659	1
213	C	75.76555	72.47640	67.72050	585.48547	-340.24194	-406.23938	1
214	O	77.11119	72.22374	67.34664	-419.15649	-173.04408	-511.94141	1
215	H	76.99214	71.37478	66.85922	-1071.84350	1559.71507	-1960.13012	1
216	C	69.94989	73.65458	70.82046	291.41878	-183.13091	710.72246	1
217	O	68.96774	72.91773	70.61088	379.87695	523.47396	-222.23622	1
218	N	69.97218	74.90838	71.19727	564.30591	373.09380	277.24371	1
219	H	70.90395	75.31980	71.22553	-120.59931	-2436.07824	-1214.35098	1
220	C	68.94018	75.44279	72.03704	404.07514	-299.37480	608.84009	1
221	H	68.63783	74.56355	72.64885	-1071.07882	-841.69025	2359.66467	1
222	C	69.58447	76.63299	72.84599	-683.12807	68.71770	-390.13096	1
223	H	70.49114	76.29509	73.39795	2068.88918	1596.58590	770.89603	1
224	H	69.93555	77.42382	72.14486	1379.86429	2342.49779	-179.85638	1
225	C	68.51715	77.21320	73.82848	-176.39967	537.49466	550.97268	1
226	H	67.58291	77.48029	73.28273	-396.28051	1942.22168	1869.33314	1
227	H	68.21888	76.46175	74.59308	-94.44700	586.00678	-2659.20016	1
228	C	69.16595	78.50873	74.50003	-291.69381	-718.18079	-150.72929	1
229	H	70.01421	78.30454	75.20242	-2303.38776	1089.76242	964.62032	1
230	H	69.48706	79.31667	73.79435	884.16729	2568.80533	-207.74283	1
231	N	68.08803	79.00461	75.24835	-594.49522	-252.81478	342.29276	1
232	H	67.28467	78.40249	75.34226	-1735.17426	2084.05705	-263.71605	1
233	C	68.05855	80.14422	75.81101	595.23177	-271.52487	442.22352	1
234	N	69.18267	80.96734	75.68444	585.53813	-424.79750	-105.81303	1
235	H	70.06014	80.79508	75.19557	959.88797	1327.56823	-2177.11905	1
236	H	69.27372	81.89852	76.09190	1578.48647	16.27378	-2220.76233	1
237	N	66.84213	80.34406	76.47931	-452.17763	-390.33541	-421.51853	1
238	H	66.01713	79.75122	76.55645	470.26107	1974.25629	-1817.92087	1
239	H	66.61533	81.20336	76.98116	1856.67307	-1573.97321	-1224.35416	1
240	C	67.70528	75.97991	71.10185	-531.47271	-581.45780	-55.06206	1
241	O	67.39275	77.14503	71.02979	-243.00837	192.73507	609.52485	1
242	N	67.13066	74.90347	70.58876	343.49288	-644.25607	38.09164	1
243	H	67.58944	73.99016	70.78279	-1691.16043	-1535.97525	-1484.73099	1
244	C	66.25116	75.02013	69.46545	542.66492	350.14337	454.42563	1
245	H	65.44632	75.70332	69.81480	1209.57979	-2396.95920	463.86744	1
246	C	67.03506	75.66750	68.23955	-737.14309	145.93010	242.71942	1
247	H	68.12727	75.48514	68.33444	-1050.18303	159.36419	-2509.06125	1
248	C	66.45559	75.06899	66.91101	-706.77696	-252.88343	-245.16230	1
249	H	66.94206	75.50805	66.00847	-1624.64039	-1665.49085	1417.86935	1
250	H	66.59340	73.96138	66.86566	2566.10521	598.51109	693.22305	1
251	H	65.35670	75.25672	66.82867	-1972.69758	107.10018	-1876.34312	1
252	C	66.71326	77.19885	68.17347	412.85148	672.58832	-27.69222	1
253	H	67.29881	77.71155	67.37404	1447.02277	1762.76533	-1490.78944	1

254	H	65.63298	77.38173	67.96166	1320.77379	-145.20455	2378.68491	1
255	H	66.95103	77.70735	69.15147	-1512.10848	1470.52031	1724.75147	1
256	C	65.72739	73.56567	68.97590	-607.11113	499.56689	73.73769	1
257	O	64.75886	73.56516	68.24561	357.97126	460.81534	356.68785	1
258	N	66.48968	72.52413	69.29855	536.55407	-368.62270	332.76306	1
259	H	67.35227	72.55135	69.87322	524.38866	2297.69985	1367.20941	1
260	C	66.04044	71.26416	68.83204	46.50277	-774.29190	-147.97904	1
261	H	65.22163	71.47773	68.10242	1676.51875	1883.29066	1032.55549	1
262	C	67.30718	70.45230	68.24042	-559.41456	-34.19198	-556.30433	1
263	H	67.97792	70.18027	69.08960	-64.66664	395.18769	2695.05373	1
264	H	66.97995	69.48438	67.79104	-2703.44278	-60.40056	333.79418	1
265	C	68.06545	71.29102	67.24557	-519.76435	377.31045	459.42366	1
266	H	68.08995	72.34084	67.61631	-1746.74323	1667.50644	-1261.73691	1
267	C	69.50235	70.79766	67.13024	570.95554	16.46261	-545.27700	1
268	H	70.09455	71.41018	66.40261	2391.58273	28.05277	-1305.07271	1
269	H	70.03396	70.84393	68.11543	175.75588	917.63458	2559.43867	1
270	H	69.54586	69.73378	66.78186	-1063.97851	-2155.34650	1283.00462	1
271	C	67.38524	71.26199	65.88410	193.76014	2.62946	-765.53141	1
272	H	67.92736	71.89577	65.13571	507.39394	-846.55087	2539.60089	1
273	H	67.34307	70.22190	65.46829	1337.57841	1818.19054	1526.01994	1
274	H	66.33130	71.63924	65.94103	1100.88635	-1172.91350	-2199.08909	1
275	C	65.57758	70.40141	70.12508	-549.21115	475.64486	-309.38218	1
276	O	66.09532	70.49582	71.20666	556.06106	-390.37755	-78.24250	1
277	O	64.64885	69.36960	69.86058	-572.27940	-310.19032	-209.75862	1
278	H	64.45622	69.57785	68.90346	-1380.08193	2212.14486	790.85944	1

Listing 116: C00116.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.3770	0.0000	300.0000
3	H	73.38581	70.28863	75.72308	-2043.14101	-1757.64893	399.89339		1
4	N	73.54253	70.28434	74.71356	426.75047	490.45733	-334.42467		1
5	H	72.59068	70.33455	74.26268	442.25559	-1110.30854	-2448.52907		1
6	C	74.54329	71.15160	74.25170	415.32972	-666.39213	83.73172		1
7	H	75.23381	71.29739	75.10909	879.32219	2491.00447	667.35213		1
8	C	75.22384	70.52134	72.93645	31.35357	477.41777	628.23362		1
9	H	74.46927	70.52461	72.11112	1168.38489	2240.25337	-1019.71136		1
10	H	76.06013	71.17548	72.58789	-360.43770	2534.90498	931.67112		1
11	C	75.70718	69.11731	73.20778	463.18208	512.70242	-382.34388		1
12	H	74.83324	68.50072	73.51735	1725.29117	1863.52247	-987.07854		1
13	C	76.31007	68.51539	71.94573	710.42801	-144.27427	-313.15367		1
14	H	76.65035	67.46036	72.11094	364.20195	-1033.13725	2494.72524		1
15	H	75.57200	68.49894	71.10206	2567.61904	335.80679	847.48802		1
16	H	77.20020	69.09992	71.59557	-2587.99029	680.92867	-512.16411		1
17	C	76.73338	69.09927	74.33162	268.17616	741.64379	-40.42634		1
18	H	77.18044	68.08095	74.47206	1283.54314	-1945.37420	-1411.27812		1
19	H	77.57364	69.80954	74.12493	-1258.57796	1317.15249	-2026.02085		1
20	H	76.27899	69.40015	75.31132	-2502.84526	909.80597	575.92391		1
21	C	73.80114	72.51553	73.71997	619.36578	-458.64843	-172.09273		1
22	O	73.25422	72.53714	72.63295	-81.40433	433.87611	522.34594		1
23	N	73.89066	73.44420	74.65389	175.23996	-622.20190	341.55523		1
24	H	74.39309	73.17446	75.49999	-876.57256	-303.22879	-2561.90213		1
25	C	73.74213	74.84153	74.36561	-571.88214	-534.10783	-106.15033		1
26	H	74.22568	75.31707	75.24589	-2713.20841	-16.25800	-248.80809		1
27	C	74.56601	75.14523	73.04198	166.60354	288.16399	-716.09568		1
28	H	74.09663	74.58063	72.18059	-2097.85574	1636.78449	-586.18044		1
29	O	75.91186	74.58223	72.95928	-317.80580	-363.38227	484.43082		1
30	H	76.46887	75.38262	72.98904	1863.74748	-1451.84923	1357.29467		1
31	C	74.42890	76.69117	72.85662	503.80731	517.99032	318.51606		1
32	H	74.68061	77.00320	71.81228	640.61020	-2157.10410	-1536.29104		1
33	H	73.39953	77.06545	73.08799	1687.88455	465.60692	2087.56452		1

34	H	75.12967	77.23915	73.53124	-1293.07895	-1899.88581	-1463.57452	1
35	C	72.15530	75.16245	74.54172	-153.07550	-733.68902	248.70981	1
36	O	71.87636	75.61847	75.64408	186.15459	-480.78787	-449.34387	1
37	N	71.32378	74.89922	73.53080	-487.53139	543.18517	42.03850	1
38	C	69.93237	74.65531	73.75291	-699.35871	69.34393	360.10701	1
39	H	69.67827	75.02661	74.77106	2.81126	-221.99807	-2715.58072	1
40	C	69.31648	75.46529	72.53413	-507.46439	-592.59194	122.07761	1
41	H	68.25784	75.19278	72.32494	-1975.08116	525.87560	-1801.71556	1
42	H	69.33306	76.56063	72.72895	1588.27743	-1913.22100	1113.83566	1
43	C	70.28917	75.08292	71.37390	-613.62442	-457.55993	-194.14490	1
44	H	69.99928	74.11041	70.90876	1707.54637	-721.27992	1996.92523	1
45	H	70.30049	75.83102	70.54926	758.23357	2100.81767	1560.55011	1
46	C	71.68393	74.95988	72.11777	-352.41524	704.96076	49.21465	1
47	H	72.22968	73.98027	71.93163	1714.76886	-2070.42778	443.35792	1
48	H	72.37307	75.82306	71.97748	1224.15040	1801.50881	1636.97633	1
49	C	69.59060	73.06923	73.50068	566.85117	537.05831	117.62814	1
50	O	69.83520	72.53150	72.43798	-550.26779	-406.08867	4.21666	1
51	N	69.00544	72.53849	74.55779	566.34832	-425.77725	180.18749	1
52	H	68.81388	73.14128	75.35413	644.44502	2646.80550	-52.73430	1
53	C	68.41320	71.22963	74.40459	612.34801	-281.48662	411.56221	1
54	H	68.14941	71.24203	73.32014	1667.23498	-1490.75142	1556.16753	1
55	C	69.48101	70.14057	74.69888	-714.45746	-175.43074	286.98927	1
56	H	69.95927	70.23532	75.70836	-787.09484	1763.03619	-1922.46060	1
57	O	70.92702	70.24381	73.96033	-429.46514	516.51932	-128.40526	1
58	H	70.70703	70.97186	73.37561	1981.82785	436.16847	-1818.18182	1
59	C	68.82174	68.76300	74.46456	630.79189	-468.94448	76.03230	1
60	H	69.51485	67.93002	74.73977	-1775.71861	2062.30353	131.89849	1
61	H	67.88580	68.63840	75.06517	-1855.14608	88.94118	1993.53760	1
62	H	68.54575	68.62655	73.38951	-1504.82350	-780.94249	-2132.90992	1
63	C	67.10178	71.17260	75.40943	288.57638	618.62814	-397.00270	1
64	O	66.09250	71.72742	75.04866	321.70495	-185.26452	574.37218	1
65	N	67.33367	70.50117	76.52438	-447.05792	-446.53431	367.76425	1
66	H	68.24435	70.08003	76.69437	350.31316	1975.63644	-1843.31522	1
67	C	66.28136	70.34526	77.47015	-511.23061	374.03917	-471.51480	1
68	H	65.39850	70.72910	76.90567	2234.79579	-898.70890	-1273.45190	1
69	C	66.21918	68.78291	77.79455	529.53781	-159.34528	563.72604	1
70	H	65.32534	68.62030	78.45219	654.59388	2347.94251	1217.51488	1
71	H	66.02013	68.23978	76.83540	-1526.55661	2103.42026	817.87394	1
72	O	67.39148	68.20444	78.47546	-554.84278	14.12789	399.58769	1
73	H	67.88305	67.90468	77.69319	1297.06236	2061.84854	1220.68812	1
74	C	66.60258	71.29035	78.76350	-662.15484	-412.13544	123.62687	1
75	O	66.56156	72.49001	78.64765	-540.01537	-317.05804	274.91456	1
76	N	66.83716	70.59057	79.87378	-202.76299	-690.00100	-131.49145	1
77	H	66.91587	69.56803	79.80426	-702.62132	-2617.37191	281.70413	1
78	C	67.06066	71.27949	81.13386	-491.73914	576.34187	222.73509	1
79	H	66.89545	72.36075	80.90627	1977.17978	-1823.58850	-434.68928	1
80	C	66.13239	70.69158	82.18513	-649.50797	-328.66843	306.11224	1
81	H	66.32532	69.59611	82.23110	2075.07803	1452.16490	-1004.45904	1
82	C	66.41378	71.27890	83.55560	-615.18735	-489.99689	-70.96352	1
83	H	65.75166	70.82963	84.34650	-1226.32661	-1724.38906	-1716.47170	1
84	H	67.47986	71.09839	83.86912	2381.64273	-969.84735	900.46860	1
85	H	66.24658	72.39140	83.57195	2122.74991	1702.23946	-141.36228	1
86	C	64.67183	70.88578	81.82346	-501.86074	-479.61276	-376.42482	1
87	H	63.98711	70.41205	82.58041	993.79261	-2246.95401	-1177.81305	1
88	H	64.40288	71.97684	81.76626	42.71279	-626.15391	-2651.37258	1
89	H	64.43300	70.43314	80.82135	-2026.39012	-1590.33709	-887.82922	1
90	C	68.62912	70.89551	81.59201	-672.89153	382.57394	-156.34072	1
91	O	68.92989	69.74855	81.82498	410.04627	221.86223	500.35950	1
92	N	69.34530	71.99521	81.68176	-378.11782	-443.79414	-441.10984	1
93	H	68.86481	72.86843	81.47436	2404.15973	-568.14894	1149.30085	1
94	C	70.77905	71.99689	81.78254	-544.54484	466.16019	331.29119	1
95	H	70.96388	72.36611	82.81529	-1409.80988	-170.17955	2325.32679	1

96	C	71.35291	70.54441	81.54572	-184.48284	116.78282	-758.89137	1
97	H	71.08912	69.86942	82.39527	1893.78641	1861.14652	611.04528	1
98	H	70.86485	70.08842	80.65306	-2170.79665	-974.19311	1327.50117	1
99	C	72.90198	70.62147	81.35601	389.51668	672.81878	-138.49152	1
100	H	73.16565	71.45154	80.66031	510.64577	1933.03327	1851.02484	1
101	H	73.39525	70.90989	82.31054	-2302.30869	-1105.72939	-948.89774	1
102	C	73.51279	69.27599	80.81039	-559.93427	-126.34590	542.30857	1
103	O	74.67772	69.22888	80.50925	-670.36003	-111.83166	76.36448	1
104	N	72.62438	68.26163	80.72538	-216.06729	-537.07037	446.51379	1
105	H	71.63477	68.22754	80.99799	-1251.96487	1074.12894	-2168.52500	1
106	H	72.86711	67.31303	80.42010	-2451.83023	-720.73851	944.84612	1
107	C	71.38862	73.05372	80.70385	546.24052	-563.88337	-85.11809	1
108	O	72.42248	73.57930	81.03098	71.70702	-307.40463	606.69673	1
109	N	70.78370	73.08171	79.51411	479.90863	-504.50129	222.86849	1
110	C	71.06788	74.11917	78.55817	75.51268	-600.91904	506.73700	1
111	H	72.15118	74.35513	78.68185	-2033.61562	1795.30103	254.89480	1
112	C	70.67454	73.40406	77.18865	523.79067	517.99274	284.45581	1
113	H	70.43731	74.12092	76.37277	1599.61665	-1127.00911	1895.98173	1
114	H	71.49633	72.75649	76.80874	-1881.83093	1275.82488	-1501.55016	1
115	C	69.44033	72.56353	77.62831	-600.05639	-404.05026	316.64485	1
116	H	68.53994	73.20393	77.78178	-2597.05260	496.36221	657.73249	1
117	H	69.15266	71.77826	76.89792	-1666.24518	1294.38985	-1723.90591	1
118	C	69.98215	71.97764	79.00321	493.57570	-129.95376	-602.56394	1
119	H	69.19054	71.72942	79.74870	-1469.08415	-637.84797	2204.22581	1
120	H	70.67483	71.10921	78.90029	-1038.97840	1068.88701	-2280.71789	1
121	C	70.12760	75.40947	78.83827	188.88100	241.05089	-727.87821	1
122	O	69.47540	75.49980	79.84144	531.88613	-49.19943	427.07960	1
123	N	70.24948	76.25515	77.81219	708.14833	26.93417	-179.73509	1
124	H	70.90255	76.02187	77.01935	-2232.69501	-1179.09831	1023.94816	1
125	C	69.51422	77.52543	77.70933	-738.32412	259.92548	104.42456	1
126	H	69.18052	77.47188	76.64703	2028.89123	1260.02983	1311.33324	1
127	C	68.37244	77.65067	78.68754	-258.65678	-345.52513	661.28459	1
128	H	68.77523	77.46396	79.71644	-1826.06090	-1801.46097	-918.64554	1
129	C	67.76107	79.04221	78.66902	-541.23400	531.92970	-218.41428	1
130	H	66.90691	79.12989	79.39426	1311.73218	-2219.18200	882.19023	1
131	H	68.51503	79.83064	78.95000	-1048.71298	1223.58118	-2196.97971	1
132	H	67.36362	79.30839	77.65205	419.06414	1903.92898	1903.44670	1
133	C	67.27303	76.63630	78.41835	-423.86431	152.66566	-648.55262	1
134	H	66.44952	76.70687	79.18014	105.68386	-2342.50080	1387.51238	1
135	H	66.80597	76.78779	77.40745	-1695.63603	-1484.73621	-1531.02793	1
136	H	67.66362	75.58100	78.44985	-1853.57121	-487.39031	1936.59343	1
137	C	70.65072	78.72032	77.89746	539.71428	-510.58232	267.58633	1
138	O	70.69341	79.38943	78.90609	-15.93758	-278.34085	-624.49402	1
139	N	71.46361	78.76368	76.84867	-676.81886	12.05292	276.17960	1
140	H	71.24215	78.05618	76.14710	-1694.44250	-373.84189	-2100.66098	1
141	C	71.95668	80.03303	76.35725	412.33078	-664.70360	108.35451	1
142	H	71.11336	80.37725	75.71909	1765.77476	1294.44366	1621.76594	1
143	C	72.22568	81.03201	77.54290	-179.66635	-721.95667	-264.73915	1
144	H	71.29132	81.22205	78.12985	-607.34922	2587.87032	-598.10018	1
145	H	72.94078	80.57753	78.26601	-359.69332	-1479.13954	-2259.74260	1
146	C	72.75554	82.40840	76.99998	-240.01076	616.02425	431.85322	1
147	H	73.64750	82.27717	76.34617	-1359.17131	782.54425	2227.99181	1
148	H	71.99308	82.91398	76.36699	-820.36667	85.81767	-2596.78715	1
149	C	73.11295	83.27921	78.26907	-513.07015	236.18570	-551.87280	1
150	H	72.18853	83.58865	78.80892	1816.11944	-1183.11722	-1650.94321	1
151	H	73.70226	82.68217	79.00231	-1800.04429	-1361.53473	1526.34643	1
152	C	73.92650	84.51260	77.81113	726.08972	-253.19732	-179.64713	1
153	H	74.92362	84.27515	77.38953	1224.27271	-456.51798	-2390.90304	1
154	H	73.38494	85.20379	77.13476	1206.40339	-1150.93514	-2154.90344	1
155	N	74.23247	85.36510	79.08927	329.70796	-633.68968	-155.67358	1
156	H	74.83044	86.22778	78.93600	1348.31305	1938.76845	1359.00643	1
157	H	73.40030	85.77834	79.60245	2096.92035	1446.54551	-966.48890	1

158	H	74.75740	84.88533	79.87738	-1197.07217	-2303.53719	827.28733	1
159	C	73.20156	79.57272	75.42821	-378.01186	-556.17301	-413.96481	1
160	O	72.96075	78.82477	74.47990	-409.44433	-307.55053	-453.30833	1
161	N	74.33929	80.12559	75.79390	-429.02477	524.70884	274.08502	1
162	H	74.27847	80.72621	76.61892	1706.34263	-1425.96036	1574.38926	1
163	C	75.62226	79.57392	75.50743	-45.25864	-626.22952	478.93267	1
164	H	76.28570	80.09857	76.23155	1988.63164	570.90773	1772.87287	1
165	C	75.51483	78.01789	75.79536	551.77128	-20.49526	-564.54996	1
166	H	75.17213	77.83423	76.83848	1434.61535	-1753.10253	1513.99471	1
167	H	74.73440	77.55164	75.14739	-714.67738	1819.09770	1898.36494	1
168	C	76.92657	77.39528	75.54507	446.99263	-555.77305	338.97221	1
169	H	77.23662	77.53600	74.48240	1953.68466	1892.25957	-161.67766	1
170	H	77.69563	77.92003	76.15495	-403.03785	2688.07032	-188.43591	1
171	C	76.88595	75.85743	75.91435	567.86262	335.74681	434.04421	1
172	H	76.56219	75.70474	76.96973	-1080.02275	1568.26081	-1948.78900	1
173	H	76.14902	75.31152	75.28189	-919.54108	2111.34692	1456.13463	1
174	C	78.30682	75.29590	75.67640	195.81897	173.33862	-745.11536	1
175	H	78.62813	75.32509	74.60456	1405.67949	-2301.21089	-390.08113	1
176	H	79.09369	75.73831	76.32008	-940.37328	-1118.32446	2299.72133	1
177	N	78.28164	73.78148	76.06990	319.26422	656.36007	-42.02424	1
178	H	79.19900	73.25587	75.97576	1961.03633	619.91968	1787.09422	1
179	H	78.01539	73.54552	77.07004	854.14343	-2156.80752	1429.08711	1
180	H	77.62785	73.15605	75.51504	1237.02905	-1378.50857	-1998.28500	1
181	C	76.12661	79.82479	73.97223	532.53319	-268.57236	517.55729	1
182	O	77.28469	80.18203	73.80905	266.16714	-290.73804	-558.88002	1
183	N	75.19950	79.52252	73.10724	-226.25352	640.49678	-270.32839	1
184	H	74.26650	79.19535	73.47414	2007.69063	-1035.27229	1523.50231	1
185	C	75.31127	79.74242	71.71210	-540.76542	-573.33303	49.50000	1
186	H	74.27044	79.57520	71.35564	-2374.20950	-1036.76023	843.75774	1
187	C	75.81800	81.23918	71.45683	-77.09082	666.87422	-415.84136	1
188	H	76.84294	81.35625	71.90724	-985.81834	617.19825	2463.91927	1
189	O	75.00414	82.28005	72.02604	293.29899	-391.65602	-477.80926	1
190	H	75.60955	82.63883	72.70577	2528.72714	-681.76262	-751.27122	1
191	C	75.92584	81.24185	69.88818	252.47363	-605.14473	440.05134	1
192	H	76.34996	82.20056	69.51042	-2052.65063	1456.49051	-1043.51830	1
193	H	76.58000	80.41908	69.51290	-2152.98800	-1661.97574	-161.70652	1
194	H	74.92691	81.11327	69.41049	-473.12726	-1584.27339	2165.61725	1
195	C	76.34849	78.65699	71.04238	360.36307	488.46713	505.10056	1
196	O	75.93271	77.95469	70.15288	-200.08817	-528.03552	-385.82850	1
197	N	77.56412	78.73736	71.55671	-597.54095	-226.44775	355.20479	1
198	H	77.77413	79.39039	72.35027	2179.23655	-1300.70981	-991.33835	1
199	C	78.57678	77.92480	70.98022	-687.68921	297.39807	-249.45179	1
200	H	78.02139	77.36843	70.18684	-349.16256	-2467.37713	-1101.72831	1
201	C	79.71046	78.90216	70.39568	672.47345	361.54328	-201.62880	1
202	H	80.08654	79.58489	71.19121	1541.41502	582.18425	2169.97026	1
203	H	80.57971	78.30620	70.03596	-2534.67717	60.25153	997.72295	1
204	C	79.14456	79.70067	69.21540	574.26774	-389.43119	-377.02542	1
205	C	78.84359	78.99783	68.00922	688.82679	-287.33580	-257.96133	1
206	H	78.99173	77.90485	67.94192	331.14182	1470.38163	2269.80013	1
207	C	78.94938	81.11302	69.29708	-383.52382	-675.04808	144.24917	1
208	H	79.17364	81.66005	70.23041	4.09847	1517.59662	2262.86397	1
209	C	78.36342	79.71810	66.91746	-134.76730	428.45285	-649.50303	1
210	H	78.13290	79.17323	65.98522	-903.23433	1600.49020	2011.53387	1
211	C	78.47183	81.79047	68.17238	-335.53281	-615.00040	-364.39058	1
212	H	78.32982	82.88299	68.24248	1596.45398	-1369.33862	1732.02659	1
213	C	78.16118	81.12854	66.94866	585.48547	-340.24194	-406.23938	1
214	O	77.67266	81.80651	65.80183	-419.15649	-173.04408	-511.94141	1
215	H	77.66675	82.73107	66.14473	-1071.84350	1559.71507	-1960.13012	1
216	C	79.13705	76.95852	72.15894	291.41878	-183.13091	710.72246	1
217	O	78.37399	76.36657	72.89548	379.87695	523.47396	-222.23622	1
218	N	80.44916	76.83496	72.08133	564.30591	373.09380	277.24371	1
219	H	81.08123	77.33762	71.42775	-120.59931	-2436.07824	-1214.35098	1

220	C	81.14469	76.15177	73.14074	404.07514	-299.37480	608.84009	1
221	H	80.75681	76.57135	74.09585	-1071.07882	-841.69025	2359.66467	1
222	C	80.79243	74.61453	73.00479	-683.12807	68.71770	-390.13096	1
223	H	79.68911	74.49641	72.88354	2068.88918	1596.58590	770.89603	1
224	H	81.24582	74.18196	72.08426	1379.86429	2342.49779	-179.85638	1
225	C	81.29465	73.86983	74.28019	-176.39967	537.49466	550.97268	1
226	H	82.40636	73.84100	74.31339	-396.28051	1942.22168	1869.33314	1
227	H	80.97344	74.40676	75.20038	-94.44700	586.00678	-2659.20016	1
228	C	80.70199	72.38678	74.24535	-291.69381	-718.18079	-150.72929	1
229	H	79.59523	72.29466	74.10044	-2303.38776	1089.76242	964.62032	1
230	H	81.21022	71.68862	73.53240	884.16729	2568.80533	-207.74283	1
231	N	81.01126	71.98952	75.55667	-594.49522	-252.81478	342.29276	1
232	H	81.64252	72.58202	76.07405	-1735.17426	2084.05705	-263.71605	1
233	C	80.56894	70.93952	76.12264	595.23177	-271.52487	442.22352	1
234	N	79.71030	70.11943	75.38226	585.53813	-424.79750	-105.81303	1
235	H	79.43651	70.20806	74.40514	959.88797	1327.56823	-2177.11905	1
236	H	79.31485	69.23670	75.70698	1578.48647	16.27378	-2220.76233	1
237	N	81.05876	70.82992	77.43093	-452.17763	-390.33541	-421.51853	1
238	H	81.69545	71.42496	77.95886	470.26107	1974.25629	-1817.92087	1
239	H	80.82790	70.05254	78.05086	1856.67307	-1573.97321	-1224.35416	1
240	C	82.66761	76.56974	72.76306	-531.47271	-581.45780	-55.06206	1
241	O	82.86203	77.28280	71.78570	-243.00837	192.73507	609.52485	1
242	N	83.53567	76.11539	73.65311	343.49288	-644.25607	38.09164	1
243	H	83.16720	75.51823	74.39219	-1691.16043	-1535.97525	-1484.73099	1
244	C	84.92044	76.05981	73.31176	542.66492	350.14337	454.42563	1
245	H	85.13764	77.01666	72.78585	1209.57979	-2396.95920	463.86744	1
246	C	85.70539	75.85749	74.67532	-737.14309	145.93010	242.71942	1
247	H	85.37381	74.92113	75.17404	-1050.18303	159.36419	-2509.06125	1
248	C	87.25301	75.83682	74.43511	-706.77696	-252.88343	-245.16230	1
249	H	87.81442	75.78738	75.39801	-1624.64039	-1665.49085	1417.86935	1
250	H	87.57112	74.94034	73.81927	2566.10521	598.51109	693.22305	1
251	H	87.59768	76.75246	73.89907	-1972.69758	107.10018	-1876.34312	1
252	C	85.42136	77.10010	75.58922	412.85148	672.58832	-27.69222	1
253	H	85.93137	77.01164	76.57688	1447.02277	1762.76533	-1490.78944	1
254	H	85.77625	78.04459	75.11455	1320.77379	-145.20455	2378.68491	1
255	H	84.33014	77.22016	75.78482	-1512.10848	1470.52031	1724.75147	1
256	C	85.13365	74.76881	72.32569	-607.11113	499.56689	73.73769	1
257	O	84.37509	73.83079	72.25661	357.97126	460.81534	356.68785	1
258	N	86.27609	74.96330	71.67063	536.55407	-368.62270	332.76306	1
259	H	86.83355	75.78716	71.89034	524.38866	2297.69985	1367.20941	1
260	C	86.77287	73.90380	70.86825	46.50277	-774.29190	-147.97904	1
261	H	85.85843	73.33107	70.58906	1676.51875	1883.29066	1032.55549	1
262	C	87.61699	74.51157	69.63264	-559.41456	-34.19198	-556.30433	1
263	H	88.58263	74.91621	70.01964	-64.66664	395.18769	2695.05373	1
264	H	87.89764	73.70178	68.91768	-2703.44278	-60.40056	333.79418	1
265	C	86.84629	75.60069	68.93581	-519.76435	377.31045	459.42366	1
266	H	86.51585	76.34144	69.69873	-1746.74323	1667.50644	-1261.73691	1
267	C	87.73742	76.31210	67.92495	570.95554	16.46261	-545.27700	1
268	H	87.19739	77.15058	67.41442	2391.58273	28.05277	-1305.07271	1
269	H	88.64752	76.74996	68.41045	175.75588	917.63458	2559.43867	1
270	H	88.09390	75.61249	67.12571	-1063.97851	-2155.34650	1283.00462	1
271	C	85.61047	75.04947	68.23802	193.76014	2.62946	-765.53141	1
272	H	85.04456	75.85610	67.70399	507.39394	-846.55087	2539.60089	1
273	H	85.87728	74.27076	67.47763	1337.57841	1818.19054	1526.01994	1
274	H	84.90368	74.57662	68.96833	1100.88635	-1172.91350	-2199.08909	1
275	C	87.80729	73.03364	71.74344	-549.21115	475.64486	-309.38218	1
276	O	88.21358	73.36186	72.83370	556.06106	-390.37755	-78.24250	1
277	O	88.30306	71.86962	71.11831	-572.27940	-310.19032	-209.75862	1
278	H	87.76088	71.90662	70.27876	-1380.08193	2212.14486	790.85944	1

Listing 117: C00117.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.3754	0.0000	300.0000
3	H	70.97346	64.98471	80.28844	-2043.14101	-1757.64893	399.89339		1
4	N	71.43028	64.84826	79.38579	426.75047	490.45733	-334.42467		1
5	H	70.66029	64.90472	78.69637	442.25559	-1110.30854	-2448.52907		1
6	C	72.44509	65.79200	79.11690	415.32972	-666.39213	83.73172		1
7	H	72.72764	66.28626	80.07178	879.32219	2491.00447	667.35213		1
8	C	73.68091	65.02983	78.41073	31.35357	477.41777	628.23362		1
9	H	73.31620	64.51232	77.49174	1168.38489	2240.25337	-1019.71136		1
10	H	74.45138	65.76408	78.07309	-360.43770	2534.90498	931.67112		1
11	C	74.27783	64.02006	79.35410	463.18208	512.70242	-382.34388		1
12	H	73.45282	63.38452	79.74876	1725.29117	1863.52247	-987.07854		1
13	C	75.26395	63.13066	78.60578	710.42801	-144.27427	-313.15367		1
14	H	75.70272	62.34513	79.27325	364.20195	-1033.13725	2494.72524		1
15	H	74.77591	62.60252	77.74641	2567.61904	335.80679	847.48802		1
16	H	76.11726	63.72430	78.18756	-2587.99029	680.92867	-512.16411		1
17	C	74.98260	64.69028	80.52532	268.17616	741.64379	-40.42634		1
18	H	75.45312	63.93696	81.20874	1283.54314	-1945.37420	-1411.27812		1
19	H	75.79707	65.37698	80.17777	-1258.57796	1317.15249	-2026.02085		1
20	H	74.27391	65.29988	81.14267	-2502.84526	909.80597	575.92391		1
21	C	71.69512	66.74884	78.04655	619.36578	-458.64843	-172.09273		1
22	O	70.62844	66.38575	77.56512	-81.40433	433.87611	522.34594		1
23	N	72.40580	67.83500	77.77211	175.23996	-622.20190	341.55523		1
24	H	73.29530	67.96824	78.25384	-876.57256	-303.22879	-2561.90213		1
25	C	72.03715	68.63191	76.65819	-571.88214	-534.10783	-106.15033		1
26	H	71.02983	68.25495	76.36164	-2713.20841	-16.25800	-248.80809		1
27	C	72.11438	70.17957	77.07710	166.60354	288.16399	-716.09568		1
28	H	73.19429	70.42725	77.27845	-2097.85574	1636.78449	-586.18044		1
29	O	71.37851	70.54332	78.25608	-317.80580	-363.38227	484.43082		1
30	H	72.09865	70.84297	78.84744	1863.74748	-1451.84923	1357.29467		1
31	C	71.66190	70.90448	75.75613	503.80731	517.99032	318.51606		1
32	H	71.74481	72.01227	75.85126	640.61020	-2157.10410	-1536.29104		1
33	H	72.28559	70.60328	74.87972	1687.88455	465.60692	2087.56452		1
34	H	70.60007	70.67346	75.50674	-1293.07895	-1899.88581	-1463.57452		1
35	C	73.20904	68.46288	75.52698	-153.07550	-733.68902	248.70981		1
36	O	74.06611	69.30718	75.49087	186.15459	-480.78787	-449.34387		1
37	N	73.09720	67.33526	74.80624	-487.53139	543.18517	42.03850		1
38	C	73.92254	67.15335	73.65366	-699.35871	69.34393	360.10701		1
39	H	74.73162	67.91877	73.72048	2.81126	-221.99807	-2715.58072		1
40	C	74.38290	65.64029	73.83379	-507.46439	-592.59194	122.07761		1
41	H	74.73642	65.18176	72.88345	-1975.08116	525.87560	-1801.71556		1
42	H	75.22051	65.55704	74.56139	1588.27743	-1913.22100	1113.83566		1
43	C	73.08703	64.97419	74.39055	-613.62442	-457.55993	-194.14490		1
44	H	72.36285	64.76617	73.56978	1707.54637	-721.27992	1996.92523		1
45	H	73.27144	64.00256	74.90147	758.23357	2100.81767	1560.55011		1
46	C	72.55842	66.10289	75.37432	-352.41524	704.96076	49.21465		1
47	H	71.44729	66.19390	75.43985	1714.76886	-2070.42778	443.35792		1
48	H	72.97856	66.06661	76.40380	1224.15040	1801.50881	1636.97633		1
49	C	73.04091	67.27346	72.27946	566.85117	537.05831	117.62814		1
50	O	73.62897	67.57202	71.24134	-550.26779	-406.08867	4.21666		1
51	N	71.77614	66.98574	72.46105	566.34832	-425.77725	180.18749		1
52	H	71.53984	66.80106	73.43281	644.44502	2646.80550	-52.73430		1
53	C	70.80877	66.92573	71.42194	612.34801	-281.48662	411.56221		1
54	H	69.87242	66.66777	71.96362	1667.23498	-1490.75142	1556.16753		1
55	C	70.75442	68.42246	70.87308	-714.45746	-175.43074	286.98927		1
56	H	71.77731	68.65999	70.47490	-787.09484	1763.03619	-1922.46060		1
57	O	70.52517	69.40982	71.91449	-429.46514	516.51932	-128.40526		1
58	H	71.44140	69.67662	72.10982	1981.82785	436.16847	-1818.18182		1
59	C	69.70248	68.50304	69.71079	630.79189	-468.94448	76.03230		1
60	H	69.37374	69.55575	69.55318	-1775.71861	2062.30353	131.89849		1

61	H	70.11278	68.15762	68.73081	-1855.14608	88.94118	1993.53760	1
62	H	68.78411	67.91170	69.93735	-1504.82350	-780.94249	-2132.90992	1
63	C	71.27032	65.70585	70.44525	288.57638	618.62814	-397.00270	1
64	O	71.99351	64.81383	70.83042	321.70495	-185.26452	574.37218	1
65	N	70.61694	65.76590	69.28715	-447.05792	-446.53431	367.76425	1
66	H	69.95750	66.51846	69.10130	350.31316	1975.63644	-1843.31522	1
67	C	71.04396	64.89537	68.24823	-511.23061	374.03917	-471.51480	1
68	H	71.46373	64.00777	68.77663	2234.79579	-898.70890	-1273.45190	1
69	C	69.74258	64.60215	67.35645	529.53781	-159.34528	563.72604	1
70	H	70.05547	63.86130	66.57049	654.59388	2347.94251	1217.51488	1
71	H	68.99818	64.08541	68.01739	-1526.55661	2103.42026	817.87394	1
72	O	69.15162	65.73916	66.67986	-554.84278	14.12789	399.58769	1
73	H	68.51179	66.01977	67.36044	1297.06236	2061.84854	1220.68812	1
74	C	72.15896	65.58903	67.28410	-662.15484	-412.13544	123.62687	1
75	O	72.75320	64.89754	66.48984	-540.01537	-317.05804	274.91456	1
76	N	72.20570	66.95459	67.35869	-202.76299	-690.00100	-131.49145	1
77	H	71.72835	67.14536	68.24153	-702.62132	-2617.37191	281.70413	1
78	C	73.51482	67.62016	67.01952	-491.73914	576.34187	222.73509	1
79	H	74.24329	66.85659	67.38412	1977.17978	-1823.58850	-434.68928	1
80	C	73.61106	67.90716	65.53486	-649.50797	-328.66843	306.11224	1
81	H	72.88846	68.72502	65.30969	2075.07803	1452.16490	-1004.45904	1
82	C	75.00063	68.40172	65.17164	-615.18735	-489.99689	-70.96352	1
83	H	75.08173	68.65490	64.07963	-1226.32661	-1724.38906	-1716.47170	1
84	H	75.26583	69.33100	65.75161	2381.64273	-969.84735	900.46860	1
85	H	75.78783	67.63085	65.39473	2122.74991	1702.23946	-141.36228	1
86	C	73.23712	66.72070	64.66263	-501.86074	-479.61276	-376.42482	1
87	H	73.32044	66.96232	63.56697	993.79261	-2246.95401	-1177.81305	1
88	H	73.90336	65.83265	64.86400	42.71279	-626.15391	-2651.37258	1
89	H	72.17694	66.38963	64.85578	-2026.39012	-1590.33709	-887.82922	1
90	C	73.57553	69.01223	67.80175	-672.89153	382.57394	-156.34072	1
91	O	73.67800	70.12609	67.18908	410.04627	221.86223	500.35950	1
92	N	73.50870	68.89203	69.08783	-378.11782	-443.79414	-441.10984	1
93	H	73.42423	67.97699	69.60650	2404.15973	-568.14894	1149.30085	1
94	C	73.83146	70.09288	69.78915	-544.54484	466.16019	331.29119	1
95	H	73.12777	70.14884	70.64645	-1409.80988	-170.17955	2325.32679	1
96	C	75.30708	69.89648	70.27206	-184.48284	116.78282	-758.89137	1
97	H	75.42013	68.91857	70.79951	1893.78641	1861.14652	611.04528	1
98	H	76.00466	69.86560	69.40331	-2170.79665	-974.19311	1327.50117	1
99	C	75.63589	71.09831	71.22230	389.51668	672.81878	-138.49152	1
100	H	75.49148	72.06127	70.67787	510.64577	1933.03327	1851.02484	1
101	H	74.90050	71.14848	72.05655	-2302.30869	-1105.72939	-948.89774	1
102	C	77.08780	71.03584	71.80744	-559.93427	-126.34590	542.30857	1
103	O	77.44719	71.89315	72.58422	-670.36003	-111.83166	76.36448	1
104	N	77.82165	69.99709	71.36653	-216.06729	-537.07037	446.51379	1
105	H	77.56980	69.25073	70.70742	-1251.96487	1074.12894	-2168.52500	1
106	H	78.79204	69.81605	71.64735	-2451.83023	-720.73851	944.84612	1
107	C	73.75409	71.39420	68.69594	546.24052	-563.88337	-85.11809	1
108	O	74.75506	72.10002	68.52584	71.70702	-307.40463	606.69673	1
109	N	72.47788	71.91531	68.82192	479.90863	-504.50129	222.86849	1
110	C	72.10699	73.08786	68.13016	75.51268	-600.91904	506.73700	1
111	H	72.75169	73.15891	67.22201	-2033.61562	1795.30103	254.89480	1
112	C	70.54275	72.87842	67.86903	523.79067	517.99274	284.45581	1
113	H	69.99737	73.83636	67.71787	1599.61665	-1127.00911	1895.98173	1
114	H	70.36049	72.26066	66.96178	-1881.83093	1275.82488	-1501.55016	1
115	C	70.12033	72.12198	69.15953	-600.05639	-404.05026	316.64485	1
116	H	70.02237	72.81490	70.02485	-2597.05260	496.36221	657.73249	1
117	H	69.14911	71.58801	69.06775	-1666.24518	1294.38985	-1723.90591	1
118	C	71.37248	71.14046	69.33739	493.57570	-129.95376	-602.56394	1
119	H	71.59529	70.84608	70.39340	-1469.08415	-637.84797	2204.22581	1
120	H	71.34592	70.22127	68.70182	-1038.97840	1068.88701	-2280.71789	1
121	C	72.30036	74.39651	69.11866	188.88100	241.05089	-727.87821	1
122	O	72.16930	75.50503	68.65636	531.88613	-49.19943	427.07960	1

123	N	72.51550	74.04784	70.37823	708.14833	26.93417	-179.73509	1
124	H	72.55499	73.05357	70.59708	-2232.69501	-1179.09831	1023.94816	1
125	C	72.53003	75.06926	71.36733	-738.32412	259.92548	104.42456	1
126	H	72.90542	75.98561	70.85759	2028.89123	1260.02983	1311.33324	1
127	C	71.03144	75.23314	71.88222	-258.65678	-345.52513	661.28459	1
128	H	70.62362	74.24846	72.19620	-1826.06090	-1801.46097	-918.64554	1
129	C	71.02850	76.25475	73.06951	-541.23400	531.92970	-218.41428	1
130	H	69.99803	76.42967	73.45869	1311.73218	-2219.18200	882.19023	1
131	H	71.65008	75.89161	73.92198	-1048.71298	1223.58118	-2196.97971	1
132	H	71.43986	77.24380	72.75908	419.06414	1903.92898	1903.44670	1
133	C	70.15881	75.85528	70.73994	-423.86431	152.66566	-648.55262	1
134	H	69.08554	75.93511	71.03335	105.68386	-2342.50080	1387.51238	1
135	H	70.51030	76.87888	70.47023	-1695.63603	-1484.73621	-1531.02793	1
136	H	70.21096	75.24103	69.80821	-1853.57121	-487.39031	1936.59343	1
137	C	73.40690	74.53027	72.64462	539.71428	-510.58232	267.58633	1
138	O	73.20282	73.45561	73.15694	-15.93758	-278.34085	-624.49402	1
139	N	74.22252	75.50158	73.03796	-676.81886	12.05292	276.17960	1
140	H	74.30827	76.35207	72.48355	-1694.44250	-373.84189	-2100.66098	1
141	C	74.99744	75.29239	74.22292	412.33078	-664.70360	108.35451	1
142	H	74.34972	74.67304	74.88655	1765.77476	1294.44366	1621.76594	1
143	C	76.31412	74.55079	73.78223	-179.66635	-721.95667	-264.73915	1
144	H	76.08451	73.59941	73.24767	-607.34922	2587.87032	-598.10018	1
145	H	76.87455	75.17350	73.05046	-359.69332	-1479.13954	-2259.74260	1
146	C	77.19264	74.27692	75.08136	-240.01076	616.02425	431.85322	1
147	H	77.29088	75.20817	75.69313	-1359.17131	782.54425	2227.99181	1
148	H	76.69474	73.52025	75.73735	-820.36667	85.81767	-2596.78715	1
149	C	78.54445	73.79492	74.60517	-513.07015	236.18570	-551.87280	1
150	H	78.39166	72.94470	73.86526	1816.11944	-1183.11722	-1650.94321	1
151	H	79.03474	74.60218	74.01310	-1800.04429	-1361.53473	1526.34643	1
152	C	79.43686	73.37372	75.68274	726.08972	-253.19732	-179.64713	1
153	H	79.73851	74.18419	76.37688	1224.27271	-456.51798	-2390.90304	1
154	H	79.08206	72.49553	76.25943	1206.40339	-1150.93514	-2154.90344	1
155	N	80.77419	72.89278	75.03007	329.70796	-633.68968	-155.67358	1
156	H	81.53110	72.55712	75.69605	1348.31305	1938.76845	1359.00643	1
157	H	80.70373	72.06838	74.36346	2096.92035	1446.54551	-966.48890	1
158	H	81.30906	73.59997	74.44415	-1197.07217	-2303.53719	827.28733	1
159	C	75.44314	76.76173	74.80025	-378.01186	-556.17301	-413.96481	1
160	O	76.38998	77.36591	74.30802	-409.44433	-307.55053	-453.30833	1
161	N	74.75084	77.06100	75.88142	-429.02477	524.70884	274.08502	1
162	H	74.00142	76.39737	76.07780	1706.34263	-1425.96036	1574.38926	1
163	C	74.57595	78.45709	76.22209	-45.25864	-626.22952	478.93267	1
164	H	74.12148	78.92666	75.32204	1988.63164	570.90773	1772.87287	1
165	C	73.62948	78.47488	77.46733	551.77128	-20.49526	-564.54996	1
166	H	72.66506	77.97134	77.23600	1434.61535	-1753.10253	1513.99471	1
167	H	74.07880	77.87629	78.29031	-714.67738	1819.09770	1898.36494	1
168	C	73.37513	79.97193	77.95169	446.99263	-555.77305	338.97221	1
169	H	74.34851	80.49926	78.11972	1953.68466	1892.25957	-161.67766	1
170	H	72.84151	80.55737	77.16327	-403.03785	2688.07032	-188.43591	1
171	C	72.57546	79.90892	79.23264	567.86262	335.74681	434.04421	1
172	H	71.59693	79.41358	79.03839	-1080.02275	1568.26081	-1948.78900	1
173	H	73.09361	79.24369	79.96098	-919.54108	2111.34692	1456.13463	1
174	C	72.35233	81.21842	79.84608	195.81897	173.33862	-745.11536	1
175	H	73.27924	81.73940	80.16596	1405.67949	-2301.21089	-390.08113	1
176	H	71.72172	81.90634	79.24707	-940.37328	-1118.32446	2299.72133	1
177	N	71.55209	81.01781	81.17425	319.26422	656.36007	-42.02424	1
178	H	71.34405	81.89794	81.73243	1961.03633	619.91968	1787.09422	1
179	H	70.58144	80.59351	81.08997	854.14343	-2156.80752	1429.08711	1
180	H	71.99549	80.40033	81.91706	1237.02905	-1378.50857	-1998.28500	1
181	C	76.00598	79.14861	76.60386	532.53319	-268.57236	517.55729	1
182	O	76.06520	80.35449	76.73175	266.16714	-290.73804	-558.88002	1
183	N	76.92762	78.23427	76.89782	-226.25352	640.49678	-270.32839	1
184	H	76.62870	77.27987	76.70408	2007.69063	-1035.27229	1523.50231	1

185	C	78.30332	78.53349	77.09739	-540.76542	-573.33303	49.50000	1
186	H	78.80002	77.54017	77.02997	-2374.20950	-1036.76023	843.75774	1
187	C	78.75961	79.48105	75.91015	-77.09082	666.87422	-415.84136	1
188	H	78.18794	80.45493	75.96896	-985.81834	617.19825	2463.91927	1
189	O	78.44386	79.06238	74.55604	293.29899	-391.65602	-477.80926	1
190	H	77.63420	78.48207	74.71002	2528.72714	-681.76262	-751.27122	1
191	C	80.28104	79.72966	76.17519	252.47363	-605.14473	440.05134	1
192	H	80.70221	80.46573	75.45025	-2052.65063	1456.49051	-1043.51830	1
193	H	80.47550	80.12509	77.20229	-2152.98800	-1661.97574	-161.70652	1
194	H	80.86862	78.78759	76.06855	-473.12726	-1584.27339	2165.61725	1
195	C	78.50871	79.18518	78.59042	360.36307	488.46713	505.10056	1
196	O	79.63825	79.30126	79.01186	-200.08817	-528.03552	-385.82850	1
197	N	77.36961	79.53579	79.16520	-597.54095	-226.44775	355.20479	1
198	H	76.52328	79.34978	78.62342	2179.23655	-1300.70981	-991.33835	1
199	C	77.26283	79.97651	80.50481	-687.68921	297.39807	-249.45179	1
200	H	76.16516	80.00914	80.68699	-349.16256	-2467.37713	-1101.72831	1
201	C	78.03803	78.97061	81.48646	672.47345	361.54328	-201.62880	1
202	H	79.05350	78.73225	81.08786	1541.41502	582.18425	2169.97026	1
203	H	78.17896	79.46344	82.47735	-2534.67717	60.25153	997.72295	1
204	C	77.17739	77.70771	81.61935	574.26774	-389.43119	-377.02542	1
205	C	75.94525	77.78537	82.33625	688.82679	-287.33580	-257.96133	1
206	H	75.61990	78.73528	82.79789	331.14182	1470.38163	2269.80013	1
207	C	77.58983	76.48093	81.01741	-383.52382	-675.04808	144.24917	1
208	H	78.53905	76.42188	80.45465	4.09847	1517.59662	2262.86397	1
209	C	75.16113	76.63761	82.44046	-134.76730	428.45285	-649.50303	1
210	H	74.20910	76.69643	82.99628	-903.23433	1600.49020	2011.53387	1
211	C	76.77261	75.35638	81.15696	-335.53281	-615.00040	-364.39058	1
212	H	77.10451	74.40896	80.69759	1596.45398	-1369.33862	1732.02659	1
213	C	75.53663	75.38821	81.86642	585.48547	-340.24194	-406.23938	1
214	O	74.69521	74.25353	82.00465	-419.15649	-173.04408	-511.94141	1
215	H	75.25982	73.57357	81.56707	-1071.84350	1559.71507	-1960.13012	1
216	C	77.97778	81.42178	80.70936	291.41878	-183.13091	710.72246	1
217	O	78.36473	81.76058	81.80471	379.87695	523.47396	-222.23622	1
218	N	77.89458	82.18012	79.59584	564.30591	373.09380	277.24371	1
219	H	77.56274	81.65002	78.78663	-120.59931	-2436.07824	-1214.35098	1
220	C	78.97704	83.11735	79.43278	404.07514	-299.37480	608.84009	1
221	H	79.29020	83.33213	80.48141	-1071.07882	-841.69025	2359.66467	1
222	C	80.09759	82.39691	78.58445	-683.12807	68.71770	-390.13096	1
223	H	80.33440	81.39440	79.01724	2068.88918	1596.58590	770.89603	1
224	H	79.74261	82.20509	77.54622	1379.86429	2342.49779	-179.85638	1
225	C	81.35000	83.32891	78.58458	-176.39967	537.49466	550.97268	1
226	H	81.08598	84.33399	78.17636	-396.28051	1942.22168	1869.33314	1
227	H	81.71126	83.50941	79.62193	-94.44700	586.00678	-2659.20016	1
228	C	82.47983	82.63524	77.69543	-291.69381	-718.18079	-150.72929	1
229	H	82.91808	81.69159	78.11002	-2303.38776	1089.76242	964.62032	1
230	H	82.21863	82.45713	76.62098	884.16729	2568.80533	-207.74283	1
231	N	83.45734	83.64299	77.74755	-594.49522	-252.81478	342.29276	1
232	H	83.24079	84.45776	78.30158	-1735.17426	2084.05705	-263.71605	1
233	C	84.58020	83.60138	77.15038	595.23177	-271.52487	442.22352	1
234	N	84.86940	82.46605	76.38652	585.53813	-424.79750	-105.81303	1
235	H	84.30283	81.63398	76.22816	959.88797	1327.56823	-2177.11905	1
236	H	85.73326	82.31595	75.86482	1578.48647	16.27378	-2220.76233	1
237	N	85.31957	84.76547	77.40433	-452.17763	-390.33541	-421.51853	1
238	H	85.09055	85.59273	77.95294	470.26107	1974.25629	-1817.92087	1
239	H	86.24512	84.93903	77.01162	1856.67307	-1573.97321	-1224.35416	1
240	C	78.39538	84.41197	78.63850	-531.47271	-581.45780	-55.06206	1
241	O	79.02091	85.00932	77.79562	-243.00837	192.73507	609.52485	1
242	N	77.18448	84.79715	79.17389	343.49288	-644.25607	38.09164	1
243	H	76.98002	83.99564	79.78359	-1691.16043	-1535.97525	-1484.73099	1
244	C	76.15766	85.26741	78.20992	542.66492	350.14337	454.42563	1
245	H	76.40275	84.76669	77.24487	1209.57979	-2396.95920	463.86744	1
246	C	74.80886	84.88821	78.77336	-737.14309	145.93010	242.71942	1

247	H	74.79331	85.19290	79.84455	-1050.18303	159.36419	-2509.06125	1
248	C	73.68406	85.61767	78.06006	-706.77696	-252.88343	-245.16230	1
249	H	72.68968	85.44178	78.55581	-1624.64039	-1665.49085	1417.86935	1
250	H	73.86603	86.73021	78.03957	2566.10521	598.51109	693.22305	1
251	H	73.58953	85.28495	76.99018	-1972.69758	107.10018	-1876.34312	1
252	C	74.57161	83.38926	78.71436	412.85148	672.58832	-27.69222	1
253	H	73.59863	83.10652	79.20348	1447.02277	1762.76533	-1490.78944	1
254	H	74.53267	83.01781	77.65327	1320.77379	-145.20455	2378.68491	1
255	H	75.38749	82.81382	79.23248	-1512.10848	1470.52031	1724.75147	1
256	C	76.29041	86.90227	78.11790	-607.11113	499.56689	73.73769	1
257	O	75.85924	87.47866	77.14118	357.97126	460.81534	356.68785	1
258	N	76.74691	87.43226	79.24423	536.55407	-368.62270	332.76306	1
259	H	77.08214	86.79001	79.96251	524.38866	2297.69985	1367.20941	1
260	C	77.10960	88.80573	79.22455	46.50277	-774.29190	-147.97904	1
261	H	77.17466	89.05893	78.14128	1676.51875	1883.29066	1032.55549	1
262	C	75.99003	89.68280	79.99268	-559.41456	-34.19198	-556.30433	1
263	H	75.93738	89.35187	81.05698	-64.66664	395.18769	2695.05373	1
264	H	76.30020	90.75447	80.02295	-2703.44278	-60.40056	333.79418	1
265	C	74.64255	89.54151	79.33970	-519.76435	377.31045	459.42366	1
266	H	74.38035	88.45952	79.31534	-1746.74323	1667.50644	-1261.73691	1
267	C	73.57987	90.28054	80.14509	570.95554	16.46261	-545.27700	1
268	H	72.56155	90.15996	79.69358	2391.58273	28.05277	-1305.07271	1
269	H	73.52249	89.90592	81.19921	175.75588	917.63458	2559.43867	1
270	H	73.79110	91.37956	80.19454	-1063.97851	-2155.34650	1283.00462	1
271	C	74.64622	90.06798	77.91210	193.76014	2.62946	-765.53141	1
272	H	73.60838	90.13960	77.49541	507.39394	-846.55087	2539.60089	1
273	H	75.10296	91.08889	77.84339	1337.57841	1818.19054	1526.01994	1
274	H	75.23012	89.37929	77.22667	1100.88635	-1172.91350	-2199.08909	1
275	C	78.47414	88.94471	80.06842	-549.21115	475.64486	-309.38218	1
276	O	78.84045	88.12399	80.86877	556.06106	-390.37755	-78.24250	1
277	O	79.16826	90.17003	79.92275	-572.27940	-310.19032	-209.75862	1
278	H	78.60249	90.58530	79.21538	-1380.08193	2212.14486	790.85944	1

Listing 118: C00118.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.3750	0.0000	300.0000
3	H	68.44644	68.55395	83.54742	-2043.14101	-1757.64893	399.89339		1
4	N	69.33845	68.21722	83.90263	426.75047	490.45733	-334.42467		1
5	H	69.06137	67.77533	84.77655	442.25559	-1110.30854	-2448.52907		1
6	C	70.34468	69.20053	84.01987	415.32972	-666.39213	83.73172		1
7	H	70.28054	69.76083	83.06274	879.32219	2491.00447	667.35213		1
8	C	70.04505	70.14590	85.29302	31.35357	477.41777	628.23362		1
9	H	69.85734	69.51706	86.19624	1168.38489	2240.25337	-1019.71136		1
10	H	70.96251	70.74009	85.53058	-360.43770	2534.90498	931.67112		1
11	C	68.87906	71.06283	85.04086	463.18208	512.70242	-382.34388		1
12	H	67.95259	70.44804	84.98733	1725.29117	1863.52247	-987.07854		1
13	C	68.74897	72.04975	86.19632	710.42801	-144.27427	-313.15367		1
14	H	67.87318	72.73510	86.06031	364.20195	-1033.13725	2494.72524		1
15	H	68.61309	71.52491	87.17679	2567.61904	335.80679	847.48802		1
16	H	69.66172	72.69322	86.29082	-2587.99029	680.92867	-512.16411		1
17	C	69.00480	71.84200	83.73870	268.17616	741.64379	-40.42634		1
18	H	68.16422	72.57260	83.61614	1283.54314	-1945.37420	-1411.27812		1
19	H	69.95755	72.42836	83.69154	-1258.57796	1317.15249	-2026.02085		1
20	H	68.98344	71.16867	82.84391	-2502.84526	909.80597	575.92391		1
21	C	71.79122	68.52555	84.24168	619.36578	-458.64843	-172.09273		1
22	O	72.70227	69.19841	84.73537	-81.40433	433.87611	522.34594		1
23	N	71.83804	67.28157	83.81193	175.23996	-622.20190	341.55523		1
24	H	70.96070	66.89053	83.47426	-876.57256	-303.22879	-2561.90213		1
25	C	73.07349	66.57144	83.87037	-571.88214	-534.10783	-106.15033		1
26	H	73.54708	66.99117	84.78815	-2713.20841	-16.25800	-248.80809		1

27	C	72.72537	65.01125	83.96282	166.60354	288.16399	-716.09568	1
28	H	72.13634	64.70910	83.05176	-2097.85574	1636.78449	-586.18044	1
29	O	71.92086	64.62188	85.08989	-317.80580	-363.38227	484.43082	1
30	H	71.13415	64.25178	84.64217	1863.74748	-1451.84923	1357.29467	1
31	C	74.15938	64.37237	83.88244	503.80731	517.99032	318.51606	1
32	H	74.10940	63.26175	83.79985	640.61020	-2157.10410	-1536.29104	1
33	H	74.73366	64.75139	83.00162	1687.88455	465.60692	2087.56452	1
34	H	74.75870	64.61036	84.79185	-1293.07895	-1899.88581	-1463.57452	1
35	C	73.99862	66.92580	82.56868	-153.07550	-733.68902	248.70981	1
36	O	75.17984	66.98394	82.79810	186.15459	-480.78787	-449.34387	1
37	N	73.38243	66.99247	81.38027	-487.53139	543.18517	42.03850	1
38	C	74.08703	67.45326	80.22139	-699.35871	69.34393	360.10701	1
39	H	75.17250	67.32963	80.45115	2.81126	-221.99807	-2715.58072	1
40	C	73.48784	66.51535	79.08253	-507.46439	-592.59194	122.07761	1
41	H	73.64808	66.92739	78.06083	-1975.08116	525.87560	-1801.71556	1
42	H	73.94291	65.50011	79.10055	1588.27743	-1913.22100	1113.83566	1
43	C	71.98672	66.48009	79.50346	-613.62442	-457.55993	-194.14490	1
44	H	71.47110	67.41872	79.19916	1707.54637	-721.27992	1996.92523	1
45	H	71.41452	65.64198	79.04531	758.23357	2100.81767	1560.55011	1
46	C	72.09760	66.37087	81.08482	-352.41524	704.96076	49.21465	1
47	H	71.31440	66.93424	81.64181	1714.76886	-2070.42778	443.35792	1
48	H	72.15931	65.32877	81.47768	1224.15040	1801.50881	1636.97633	1
49	C	73.66005	68.98726	79.86994	566.85117	537.05831	117.62814	1
50	O	73.44108	69.31911	78.70468	-550.26779	-406.08867	4.21666	1
51	N	73.60321	69.74551	80.95364	566.34832	-425.77725	180.18749	1
52	H	73.84582	69.23669	81.80496	644.44502	2646.80550	-52.73430	1
53	C	73.98708	71.12232	80.75892	612.34801	-281.48662	411.56221	1
54	H	74.66538	71.10168	79.87668	1667.23498	-1490.75142	1556.16753	1
55	C	72.65813	71.92113	80.43365	-714.45746	-175.43074	286.98927	1
56	H	71.93193	71.85234	81.29330	-787.09484	1763.03619	-1922.46060	1
57	O	71.86045	71.41499	79.33390	-429.46514	516.51932	-128.40526	1
58	H	72.44039	70.63226	79.04922	1981.82785	436.16847	-1818.18182	1
59	C	73.14290	73.40468	80.29981	630.79189	-468.94448	76.03230	1
60	H	72.28158	74.10837	80.22803	-1775.71861	2062.30353	131.89849	1
61	H	73.76218	73.72648	81.17022	-1855.14608	88.94118	1993.53760	1
62	H	73.75859	73.54625	79.38144	-1504.82350	-780.94249	-2132.90992	1
63	C	74.72706	71.60937	82.12733	288.57638	618.62814	-397.00270	1
64	O	75.87864	71.98600	82.08677	321.70495	-185.26452	574.37218	1
65	N	73.92482	71.52677	83.23949	-447.05792	-446.53431	367.76425	1
66	H	73.13272	70.98807	82.85539	350.31316	1975.63644	-1843.31522	1
67	C	73.52819	72.81505	83.80437	-511.23061	374.03917	-471.51480	1
68	H	72.99574	73.33049	82.97673	2234.79579	-898.70890	-1273.45190	1
69	C	72.55835	72.38139	84.97041	529.53781	-159.34528	563.72604	1
70	H	72.18301	73.31630	85.46275	654.59388	2347.94251	1217.51488	1
71	H	71.67142	71.88502	84.49579	-1526.55661	2103.42026	817.87394	1
72	O	73.09794	71.50914	86.01071	-554.84278	14.12789	399.58769	1
73	H	73.02789	70.61399	85.51843	1297.06236	2061.84854	1220.68812	1
74	C	74.81266	73.65708	84.29281	-662.15484	-412.13544	123.62687	1
75	O	75.14846	74.60845	83.64108	-540.01537	-317.05804	274.91456	1
76	N	75.31973	73.21084	85.47006	-202.76299	-690.00100	-131.49145	1
77	H	74.76122	72.44060	85.88316	-702.62132	-2617.37191	281.70413	1
78	C	76.79387	73.05510	85.61290	-491.73914	576.34187	222.73509	1
79	H	76.84541	72.79187	86.69397	1977.17978	-1823.58850	-434.68928	1
80	C	77.23738	71.91270	84.73786	-649.50797	-328.66843	306.11224	1
81	H	77.02915	72.18008	83.66040	2075.07803	1452.16490	-1004.45904	1
82	C	78.72111	71.62964	84.90430	-615.18735	-489.99689	-70.96352	1
83	H	79.07476	70.83644	84.19085	-1226.32661	-1724.38906	-1716.47170	1
84	H	79.34886	72.54462	84.72366	2381.64273	-969.84735	900.46860	1
85	H	78.95717	71.27145	85.94322	2122.74991	1702.23946	-141.36228	1
86	C	76.45708	70.63645	85.00902	-501.86074	-479.61276	-376.42482	1
87	H	76.82828	69.78187	84.37965	993.79261	-2246.95401	-1177.81305	1
88	H	76.53392	70.31956	86.08463	42.71279	-626.15391	-2651.37258	1

89	H	75.36379	70.76317	84.77342	-2026.39012	-1590.33709	-887.82922	1
90	C	77.49785	74.51386	85.33825	-672.89153	382.57394	-156.34072	1
91	O	77.39123	75.37111	86.18321	410.04627	221.86223	500.35950	1
92	N	78.23443	74.55716	84.22159	-378.11782	-443.79414	-441.10984	1
93	H	78.14979	73.72717	83.63768	2404.15973	-568.14894	1149.30085	1
94	C	78.26765	75.85172	83.56118	-544.54484	466.16019	331.29119	1
95	H	77.20026	76.16300	83.52566	-1409.80988	-170.17955	2325.32679	1
96	C	79.15568	76.77513	84.47690	-184.48284	116.78282	-758.89137	1
97	H	78.65816	76.93785	85.46696	1893.78641	1861.14652	611.04528	1
98	H	80.12308	76.26869	84.69992	-2170.79665	-974.19311	1327.50117	1
99	C	79.40461	78.13068	83.74034	389.51668	672.81878	-138.49152	1
100	H	79.90446	77.93630	82.76114	510.64577	1933.03327	1851.02484	1
101	H	78.43908	78.60937	83.46401	-2302.30869	-1105.72939	-948.89774	1
102	C	80.26851	79.13248	84.59562	-559.93427	-126.34590	542.30857	1
103	O	80.51646	80.22748	84.15981	-670.36003	-111.83166	76.36448	1
104	N	80.66397	78.64303	85.79122	-216.06729	-537.07037	446.51379	1
105	H	80.48788	77.72835	86.22268	-1251.96487	1074.12894	-2168.52500	1
106	H	81.23276	79.16857	86.46404	-2451.83023	-720.73851	944.84612	1
107	C	78.94295	75.63464	82.10197	546.24052	-563.88337	-85.11809	1
108	O	80.13128	75.79663	81.98920	71.70702	-307.40463	606.69673	1
109	N	78.05563	75.24482	81.17150	479.90863	-504.50129	222.86849	1
110	C	78.43912	75.07295	79.80605	75.51268	-600.91904	506.73700	1
111	H	79.54859	74.95507	79.80670	-2033.61562	1795.30103	254.89480	1
112	C	77.58491	73.77563	79.43838	523.79067	517.99274	284.45581	1
113	H	77.50640	73.57985	78.34700	1599.61665	-1127.00911	1895.98173	1
114	H	78.01234	72.85820	79.90072	-1881.83093	1275.82488	-1501.55016	1
115	C	76.22606	74.15528	80.09556	-600.05639	-404.05026	316.64485	1
116	H	75.67077	74.89806	79.47815	-2597.05260	496.36221	657.73249	1
117	H	75.55413	73.27895	80.23020	-1666.24518	1294.38985	-1723.90591	1
118	C	76.71026	74.77817	81.47791	493.57570	-129.95376	-602.56394	1
119	H	76.10681	75.64446	81.84257	-1469.08415	-637.84797	2204.22581	1
120	H	76.83485	74.03597	82.30309	-1038.97840	1068.88701	-2280.71789	1
121	C	77.91810	76.36052	78.94602	188.88100	241.05089	-727.87821	1
122	O	77.67390	77.42293	79.46062	531.88613	-49.19943	427.07960	1
123	N	77.94801	76.07731	77.62786	708.14833	26.93417	-179.73509	1
124	H	78.17680	75.09818	77.46069	-2232.69501	-1179.09831	1023.94816	1
125	C	77.05737	76.81755	76.72409	-738.32412	259.92548	104.42456	1
126	H	77.10439	77.85923	77.12072	2028.89123	1260.02983	1311.33324	1
127	C	77.60401	76.64829	75.32253	-258.65678	-345.52513	661.28459	1
128	H	77.67816	75.55914	75.10356	-1826.06090	-1801.46097	-918.64554	1
129	C	76.69053	77.26293	74.27826	-541.23400	531.92970	-218.41428	1
130	H	77.13342	77.19352	73.24656	1311.73218	-2219.18200	882.19023	1
131	H	75.69117	76.73860	74.24236	-1048.71298	1223.58118	-2196.97971	1
132	H	76.49209	78.35036	74.48684	419.06414	1903.92898	1903.44670	1
133	C	79.00340	77.22809	75.20770	-423.86431	152.66566	-648.55262	1
134	H	79.45129	77.04633	74.19266	105.68386	-2342.50080	1387.51238	1
135	H	79.00564	78.33888	75.38212	-1695.63603	-1484.73621	-1531.02793	1
136	H	79.69641	76.77456	75.96897	-1853.57121	-487.39031	1936.59343	1
137	C	75.51778	76.20315	76.84917	539.71428	-510.58232	267.58633	1
138	O	74.61353	76.95518	77.13165	-15.93758	-278.34085	-624.49402	1
139	N	75.46244	74.89262	76.63385	-676.81886	12.05292	276.17960	1
140	H	76.36312	74.48157	76.39584	-1694.44250	-373.84189	-2100.66098	1
141	C	74.25063	74.33215	76.10866	412.33078	-664.70360	108.35451	1
142	H	74.44003	73.24607	76.25565	1765.77476	1294.44366	1621.76594	1
143	C	73.06897	74.89897	76.98688	-179.66635	-721.95667	-264.73915	1
144	H	73.45115	75.18578	77.99447	-607.34922	2587.87032	-598.10018	1
145	H	72.69298	75.85708	76.55697	-359.69332	-1479.13954	-2259.74260	1
146	C	71.92824	73.83104	77.09942	-240.01076	616.02425	431.85322	1
147	H	71.63018	73.44604	76.09852	-1359.17131	782.54425	2227.99181	1
148	H	72.26651	72.94168	77.68391	-820.36667	85.81767	-2596.78715	1
149	C	70.71149	74.53704	77.82034	-513.07015	236.18570	-551.87280	1
150	H	71.04714	75.06168	78.74383	1816.11944	-1183.11722	-1650.94321	1

151	H	70.26355	75.32518	77.17224	-1800.04429	-1361.53473	1526.34643	1
152	C	69.67878	73.43793	78.16439	726.08972	-253.19732	-179.64713	1
153	H	69.19872	72.96330	77.28535	1224.27271	-456.51798	-2390.90304	1
154	H	70.05301	72.65648	78.85885	1206.40339	-1150.93514	-2154.90344	1
155	N	68.50648	74.12061	78.94392	329.70796	-633.68968	-155.67358	1
156	H	67.71151	73.47824	79.22806	1348.31305	1938.76845	1359.00643	1
157	H	68.74464	74.57930	79.87120	2096.92035	1446.54551	-966.48890	1
158	H	67.97976	74.89557	78.44516	-1197.07217	-2303.53719	827.28733	1
159	C	74.19721	74.70137	74.51715	-378.01186	-556.17301	-413.96481	1
160	O	75.19005	74.54351	73.84558	-409.44433	-307.55053	-453.30833	1
161	N	73.00241	75.14461	74.12570	-429.02477	524.70884	274.08502	1
162	H	72.26904	75.16861	74.83176	1706.34263	-1425.96036	1574.38926	1
163	C	72.64433	74.99526	72.73735	-45.25864	-626.22952	478.93267	1
164	H	72.95929	73.96709	72.45410	1988.63164	570.90773	1772.87287	1
165	C	71.09492	75.25213	72.67282	551.77128	-20.49526	-564.54996	1
166	H	70.54540	74.53262	73.32121	1434.61535	-1753.10253	1513.99471	1
167	H	70.86586	76.25974	73.08794	-714.67738	1819.09770	1898.36494	1
168	C	70.59264	75.15255	71.19032	446.99263	-555.77305	338.97221	1
169	H	71.21284	75.78338	70.50948	1953.68466	1892.25957	-161.67766	1
170	H	70.67307	74.11357	70.79986	-403.03785	2688.07032	-188.43591	1
171	C	69.09325	75.65114	71.20480	567.86262	335.74681	434.04421	1
172	H	68.46280	74.99399	71.84754	-1080.02275	1568.26081	-1948.78900	1
173	H	69.02861	76.67565	71.65725	-919.54108	2111.34692	1456.13463	1
174	C	68.54898	75.68882	69.75789	195.81897	173.33862	-745.11536	1
175	H	69.09318	76.37805	69.08104	1405.67949	-2301.21089	-390.08113	1
176	H	68.42557	74.69940	69.27369	-940.37328	-1118.32446	2299.72133	1
177	N	67.10382	76.28458	69.85691	319.26422	656.36007	-42.02424	1
178	H	66.61422	76.51508	68.94362	1961.03633	619.91968	1787.09422	1
179	H	66.36993	75.69584	70.34769	854.14343	-2156.80752	1429.08711	1
180	H	67.02203	77.20332	70.38054	1237.02905	-1378.50857	-1998.28500	1
181	C	73.37295	76.14174	71.82253	532.53319	-268.57236	517.55729	1
182	O	73.37656	77.31851	72.09221	266.16714	-290.73804	-558.88002	1
183	N	73.79030	75.53554	70.71693	-226.25352	640.49678	-270.32839	1
184	H	73.72918	74.52210	70.62274	2007.69063	-1035.27229	1523.50231	1
185	C	74.26007	76.28094	69.61283	-540.76542	-573.33303	49.50000	1
186	H	74.54497	77.28315	70.00766	-2374.20950	-1036.76023	843.75774	1
187	C	75.42537	75.42766	68.90011	-77.09082	666.87422	-415.84136	1
188	H	75.14438	75.27176	67.82098	-985.81834	617.19825	2463.91927	1
189	O	75.67191	74.11780	69.43072	293.29899	-391.65602	-477.80926	1
190	H	75.49207	73.55613	68.64806	2528.72714	-681.76262	-751.27122	1
191	C	76.61199	76.45765	68.92475	252.47363	-605.14473	440.05134	1
192	H	77.52514	76.03165	68.44808	-2052.65063	1456.49051	-1043.51830	1
193	H	76.36575	77.39677	68.37024	-2152.98800	-1661.97574	-161.70652	1
194	H	76.88511	76.73956	69.96853	-473.12726	-1584.27339	2165.61725	1
195	C	73.06777	76.32755	68.48590	360.36307	488.46713	505.10056	1
196	O	72.14032	75.55436	68.43232	-200.08817	-528.03552	-385.82850	1
197	N	73.42104	77.27297	67.61322	-597.54095	-226.44775	355.20479	1
198	H	74.23241	77.83975	67.85450	2179.23655	-1300.70981	-991.33835	1
199	C	72.50312	77.62652	66.59659	-687.68921	297.39807	-249.45179	1
200	H	71.70899	76.84346	66.61644	-349.16256	-2467.37713	-1101.72831	1
201	C	71.96122	79.10499	66.91810	672.47345	361.54328	-201.62880	1
202	H	72.81936	79.81207	66.98120	1541.41502	582.18425	2169.97026	1
203	H	71.30154	79.46118	66.09423	-2534.67717	60.25153	997.72295	1
204	C	71.20051	79.05634	68.24852	574.26774	-389.43119	-377.02542	1
205	C	69.77636	78.96386	68.25158	688.82679	-287.33580	-257.96133	1
206	H	69.20825	78.95764	67.30382	331.14182	1470.38163	2269.80013	1
207	C	71.92355	79.05261	69.47988	-383.52382	-675.04808	144.24917	1
208	H	73.02660	79.11019	69.48186	4.09847	1517.59662	2262.86397	1
209	C	69.11809	78.87891	69.47961	-134.76730	428.45285	-649.50303	1
210	H	68.01638	78.81917	69.47792	-903.23433	1600.49020	2011.53387	1
211	C	71.21960	78.94102	70.68167	-335.53281	-615.00040	-364.39058	1
212	H	71.80068	78.90640	71.62321	1596.45398	-1369.33862	1732.02659	1

213	C	69.79843	78.85756	70.73080	585.48547	-340.24194	-406.23938	1
214	O	69.07178	78.74660	71.95483	-419.15649	-173.04408	-511.94141	1
215	H	69.82007	78.83114	72.59122	-1071.84350	1559.71507	-1960.13012	1
216	C	73.27733	77.78779	65.16974	291.41878	-183.13091	710.72246	1
217	O	72.65149	77.77242	64.13960	379.87695	523.47396	-222.23622	1
218	N	74.56248	78.06140	65.35240	564.30591	373.09380	277.24371	1
219	H	75.03801	78.09174	66.27593	-120.59931	-2436.07824	-1214.35098	1
220	C	75.46474	77.98394	64.23229	404.07514	-299.37480	608.84009	1
221	H	75.19355	77.08020	63.64141	-1071.07882	-841.69025	2359.66467	1
222	C	75.27200	79.31855	63.39980	-683.12807	68.71770	-390.13096	1
223	H	74.18641	79.47983	63.20707	2068.88918	1596.58590	770.89603	1
224	H	75.60311	80.19734	63.99731	1379.86429	2342.49779	-179.85638	1
225	C	76.05531	79.23873	62.05329	-176.39967	537.49466	550.97268	1
226	H	77.14559	79.05512	62.21836	-396.28051	1942.22168	1869.33314	1
227	H	75.69449	78.38507	61.43684	-94.44700	586.00678	-2659.20016	1
228	C	75.83803	80.62792	61.29441	-291.69381	-718.18079	-150.72929	1
229	H	74.77465	80.92245	61.10483	-2303.38776	1089.76242	964.62032	1
230	H	76.36527	81.50761	61.74473	884.16729	2568.80533	-207.74283	1
231	N	76.43107	80.35493	60.05247	-594.49522	-252.81478	342.29276	1
232	H	76.91560	79.47477	59.96622	-1735.17426	2084.05705	-263.71605	1
233	C	76.40085	81.13412	59.04815	595.23177	-271.52487	442.22352	1
234	N	75.74486	82.36108	59.19333	585.53813	-424.79750	-105.81303	1
235	H	75.26464	82.74501	60.00610	959.88797	1327.56823	-2177.11905	1
236	H	75.65968	83.06874	58.46308	1578.48647	16.27378	-2220.76233	1
237	N	77.08524	80.57512	57.95949	-452.17763	-390.33541	-421.51853	1
238	H	77.54990	79.67449	57.85510	470.26107	1974.25629	-1817.92087	1
239	H	77.16283	81.03573	57.05208	1856.67307	-1573.97321	-1224.35416	1
240	C	76.86127	77.91708	65.04470	-531.47271	-581.45780	-55.06206	1
241	O	76.86531	78.10522	66.25519	-243.00837	192.73507	609.52485	1
242	N	77.87681	77.60844	64.24323	343.49288	-644.25607	38.09164	1
243	H	77.67988	77.44966	63.25000	-1691.16043	-1535.97525	-1484.73099	1
244	C	79.14003	78.22174	64.52191	542.66492	350.14337	454.42563	1
245	H	78.99958	78.89174	65.40004	1209.57979	-2396.95920	463.86744	1
246	C	80.14278	77.01934	64.81562	-737.14309	145.93010	242.71942	1
247	H	79.92726	76.16352	64.14069	-1050.18303	159.36419	-2509.06125	1
248	C	81.62817	77.48979	64.66453	-706.77696	-252.88343	-245.16230	1
249	H	82.34717	76.68714	64.95323	-1624.64039	-1665.49085	1417.86935	1
250	H	81.86008	77.77991	63.61191	2566.10521	598.51109	693.22305	1
251	H	81.85093	78.38221	65.29983	-1972.69758	107.10018	-1876.34312	1
252	C	79.91898	76.62023	66.31395	412.85148	672.58832	-27.69222	1
253	H	80.51931	75.72503	66.60018	1447.02277	1762.76533	-1490.78944	1
254	H	80.20417	77.44804	67.00500	1320.77379	-145.20455	2378.68491	1
255	H	78.84569	76.38418	66.50869	-1512.10848	1470.52031	1724.75147	1
256	C	79.54695	78.97316	63.13198	-607.11113	499.56689	73.73769	1
257	O	79.21647	78.54778	62.04667	357.97126	460.81534	356.68785	1
258	N	80.25202	80.06699	63.42532	536.55407	-368.62270	332.76306	1
259	H	80.47338	80.24817	64.40586	524.38866	2297.69985	1367.20941	1
260	C	81.14413	80.55588	62.43256	46.50277	-774.29190	-147.97904	1
261	H	80.96123	79.92210	61.53494	1676.51875	1883.29066	1032.55549	1
262	C	80.83868	82.12427	62.18406	-559.41456	-34.19198	-556.30433	1
263	H	80.94274	82.68286	63.14460	-64.66664	395.18769	2695.05373	1
264	H	81.58926	82.56781	61.48739	-2703.44278	-60.40056	333.79418	1
265	C	79.44574	82.26714	61.63552	-519.76435	377.31045	459.42366	1
266	H	78.74785	81.70714	62.29891	-1746.74323	1667.50644	-1261.73691	1
267	C	79.02426	83.73126	61.61097	570.95554	16.46261	-545.27700	1
268	H	77.98017	83.85387	61.22242	2391.58273	28.05277	-1305.07271	1
269	H	79.05631	84.18973	62.63287	175.75588	917.63458	2559.43867	1
270	H	79.69577	84.34122	60.95331	-1063.97851	-2155.34650	1283.00462	1
271	C	79.34588	81.68977	60.22946	193.76014	2.62946	-765.53141	1
272	H	78.36087	81.93459	59.75633	507.39394	-846.55087	2539.60089	1
273	H	80.14510	82.09312	59.55564	1337.57841	1818.19054	1526.01994	1
274	H	79.43874	80.57256	60.23287	1100.88635	-1172.91350	-2199.08909	1

275	C	82.62635	80.43810	63.05139	-549.21115	475.64486	-309.38218	1
276	O	82.84057	80.12128	64.19347	556.06106	-390.37755	-78.24250	1
277	O	83.69335	80.77283	62.18448	-572.27940	-310.19032	-209.75862	1
278	H	83.16593	80.97247	61.36202	-1380.08193	2212.14486	790.85944	1

Listing 119: C00119.xmolout

1		276						
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750 11100
		0.2500	300.00	0.00	0.00	0.00	-1293.3688	0.0000 300.0000
3	H	66.57129	70.67049	68.15094	-2043.14101	-1757.64893	399.89339	1
4	N	67.08590	71.28089	68.78324	426.75047	490.45733	-334.42467	1
5	H	67.37864	70.63666	69.51673	442.25559	-1110.30854	-2448.52907	1
6	C	68.17676	71.95771	68.19783	415.32972	-666.39213	83.73172	1
7	H	67.90104	72.18254	67.14488	879.32219	2491.00447	667.35213	1
8	C	68.47323	73.26700	69.09020	31.35357	477.41777	628.23362	1
9	H	68.79932	72.93765	70.10612	1168.38489	2240.25337	-1019.71136	1
10	H	69.32777	73.84617	68.66439	-360.43770	2534.90498	931.67112	1
11	C	67.23433	74.12043	69.19419	463.18208	512.70242	-382.34388	1
12	H	66.37378	73.45292	69.42714	1725.29117	1863.52247	-987.07854	1
13	C	67.38181	75.12882	70.32651	710.42801	-144.27427	-313.15367	1
14	H	66.46472	75.76294	70.43904	364.20195	-1033.13725	2494.72524	1
15	H	67.55855	74.62256	71.31075	2567.61904	335.80679	847.48802	1
16	H	68.24465	75.82196	70.15102	-2587.99029	680.92867	-512.16411	1
17	C	66.94560	74.85112	67.89072	268.17616	741.64379	-40.42634	1
18	H	66.03070	75.49380	67.97190	1283.54314	-1945.37420	-1411.27812	1
19	H	67.79493	75.52039	67.59605	-1258.57796	1317.15249	-2026.02085	1
20	H	66.77555	74.13694	67.04419	-2502.84526	909.80597	575.92391	1
21	C	69.45807	70.96347	68.37050	619.36578	-458.64843	-172.09273	1
22	O	69.74004	70.44804	69.43972	-81.40433	433.87611	522.34594	1
23	N	70.12046	70.90806	67.22667	175.23996	-622.20190	341.55523	1
24	H	69.78273	71.44324	66.42822	-876.57256	-303.22879	-2561.90213	1
25	C	71.19722	69.98728	67.11041	-571.88214	-534.10783	-106.15033	1
26	H	71.10373	69.31712	67.99470	-2713.20841	-16.25800	-248.80809	1
27	C	71.05143	69.25706	65.69141	166.60354	288.16399	-716.09568	1
28	H	71.11596	70.03343	64.88070	-2097.85574	1636.78449	-586.18044	1
29	O	69.81977	68.54996	65.47464	-317.80580	-363.38227	484.43082	1
30	H	69.46646	69.01664	64.69001	1863.74748	-1451.84923	1357.29467	1
31	C	72.35995	68.38500	65.67951	503.80731	517.99032	318.51606	1
32	H	72.47895	67.83873	64.71522	640.61020	-2157.10410	-1536.29104	1
33	H	73.27003	69.01353	65.82157	1687.88455	465.60692	2087.56452	1
34	H	72.35094	67.62164	66.49242	-1293.07895	-1899.88581	-1463.57452	1
35	C	72.56517	70.89264	67.08375	-153.07550	-733.68902	248.70981	1
36	O	72.79755	71.55163	66.10538	186.15459	-480.78787	-449.34387	1
37	N	73.27848	70.77094	68.21851	-487.53139	543.18517	42.03850	1
38	C	74.46921	71.53747	68.39241	-699.35871	69.34393	360.10701	1
39	H	74.34105	72.39270	67.68991	2.81126	-221.99807	-2715.58072	1
40	C	74.38490	71.89890	69.93272	-507.46439	-592.59194	122.07761	1
41	H	75.38715	72.08422	70.38158	-1975.08116	525.87560	-1801.71556	1
42	H	73.80713	72.83786	70.07401	1588.27743	-1913.22100	1113.83566	1
43	C	73.62555	70.70543	70.59909	-613.62442	-457.55993	-194.14490	1
44	H	74.32367	69.94953	71.02272	1707.54637	-721.27992	1996.92523	1
45	H	72.99082	71.02895	71.45451	758.23357	2100.81767	1560.55011	1
46	C	72.76834	70.10442	69.40848	-352.41524	704.96076	49.21465	1
47	H	72.91380	69.00975	69.24394	1714.76886	-2070.42778	443.35792	1
48	H	71.65525	70.33011	69.45579	1224.15040	1801.50881	1636.97633	1
49	C	75.80954	70.66841	67.99900	566.85117	537.05831	117.62814	1
50	O	76.45745	71.02338	67.01728	-550.26779	-406.08867	4.21666	1
51	N	76.04402	69.68814	68.83817	566.34832	-425.77725	180.18749	1
52	H	75.32833	69.61474	69.55688	644.44502	2646.80550	-52.73430	1
53	C	76.98551	68.64941	68.63215	612.34801	-281.48662	411.56221	1
54	H	76.78025	67.94239	69.46567	1667.23498	-1490.75142	1556.16753	1

55	C	76.67824	68.01983	67.19399	-714.45746	-175.43074	286.98927	1
56	H	76.71937	68.83833	66.42060	-787.09484	1763.03619	-1922.46060	1
57	O	75.37684	67.41942	67.04710	-429.46514	516.51932	-128.40526	1
58	H	74.99165	67.98379	66.34795	1981.82785	436.16847	-1818.18182	1
59	C	77.90850	67.05924	67.00471	630.79189	-468.94448	76.03230	1
60	H	77.89812	66.57721	65.99978	-1775.71861	2062.30353	131.89849	1
61	H	78.87719	67.60371	67.09946	-1855.14608	88.94118	1993.53760	1
62	H	77.91061	66.24400	67.76501	-1504.82350	-780.94249	-2132.90992	1
63	C	78.52191	69.22385	68.68741	288.57638	618.62814	-397.00270	1
64	O	79.25318	68.82062	69.55720	321.70495	-185.26452	574.37218	1
65	N	78.79208	70.03631	67.67447	-447.05792	-446.53431	367.76425	1
66	H	78.04788	70.34673	67.00038	350.31316	1975.63644	-1843.31522	1
67	C	80.10185	70.55974	67.58139	-511.23061	374.03917	-471.51480	1
68	H	80.59904	70.26235	68.53502	2234.79579	-898.70890	-1273.45190	1
69	C	80.77981	69.88615	66.28803	529.53781	-159.34528	563.72604	1
70	H	81.86414	70.17243	66.31694	654.59388	2347.94251	1217.51488	1
71	H	80.73044	68.77232	66.42769	-1526.55661	2103.42026	817.87394	1
72	O	80.18297	70.19665	65.00557	-554.84278	14.12789	399.58769	1
73	H	80.58066	71.07916	64.85710	1297.06236	2061.84854	1220.68812	1
74	C	80.05581	72.17101	67.29861	-662.15484	-412.13544	123.62687	1
75	O	81.01236	72.74547	66.83591	-540.01537	-317.05804	274.91456	1
76	N	78.89707	72.68808	67.68899	-202.76299	-690.00100	-131.49145	1
77	H	78.22702	72.01668	68.07031	-702.62132	-2617.37191	281.70413	1
78	C	78.54709	74.08939	67.60656	-491.73914	576.34187	222.73509	1
79	H	79.43216	74.63938	67.20254	1977.17978	-1823.58850	-434.68928	1
80	C	77.29397	74.14556	66.73865	-649.50797	-328.66843	306.11224	1
81	H	76.52603	73.49951	67.22317	2075.07803	1452.16490	-1004.45904	1
82	C	76.74189	75.55353	66.63758	-615.18735	-489.99689	-70.96352	1
83	H	75.78316	75.58206	66.04876	-1226.32661	-1724.38906	-1716.47170	1
84	H	76.52475	75.98587	67.65432	2381.64273	-969.84735	900.46860	1
85	H	77.46650	76.24745	66.12824	2122.74991	1702.23946	-141.36228	1
86	C	77.54332	73.56342	65.35988	-501.86074	-479.61276	-376.42482	1
87	H	76.61023	73.56064	64.73121	993.79261	-2246.95401	-1177.81305	1
88	H	78.32758	74.14222	64.79810	42.71279	-626.15391	-2651.37258	1
89	H	77.90118	72.49740	65.43047	-2026.39012	-1590.33709	-887.82922	1
90	C	78.13430	74.44207	69.18468	-672.89153	382.57394	-156.34072	1
91	O	77.53540	73.61086	69.84355	410.04627	221.86223	500.35950	1
92	N	78.46850	75.66883	69.51193	-378.11782	-443.79414	-441.10984	1
93	H	78.92342	76.21951	68.78772	2404.15973	-568.14894	1149.30085	1
94	C	78.45232	76.04094	70.89360	-544.54484	466.16019	331.29119	1
95	H	78.45391	75.05698	71.41453	-1409.80988	-170.17955	2325.32679	1
96	C	79.71511	76.96144	71.16410	-184.48284	116.78282	-758.89137	1
97	H	80.66295	76.42178	70.93982	1893.78641	1861.14652	611.04528	1
98	H	79.70239	77.85276	70.49637	-2170.79665	-974.19311	1327.50117	1
99	C	79.63738	77.39134	72.66208	389.51668	672.81878	-138.49152	1
100	H	78.65877	77.89149	72.85060	510.64577	1933.03327	1851.02484	1
101	H	79.61895	76.49232	73.31665	-2302.30869	-1105.72939	-948.89774	1
102	C	80.80297	78.34811	73.11887	-559.93427	-126.34590	542.30857	1
103	O	80.79731	78.79543	74.23689	-670.36003	-111.83166	76.36448	1
104	N	81.74106	78.56923	72.17346	-216.06729	-537.07037	446.51379	1
105	H	81.79524	78.21888	71.20988	-1251.96487	1074.12894	-2168.52500	1
106	H	82.56491	79.16452	72.31150	-2451.83023	-720.73851	944.84612	1
107	C	77.12683	76.93378	71.21384	546.24052	-563.88337	-85.11809	1
108	O	77.15831	78.14753	71.08850	71.70702	-307.40463	606.69673	1
109	N	76.12909	76.17345	71.66064	479.90863	-504.50129	222.86849	1
110	C	74.75809	76.59068	71.54370	75.51268	-600.91904	506.73700	1
111	H	74.67964	77.12106	70.56597	-2033.61562	1795.30103	254.89480	1
112	C	73.96631	75.21945	71.67866	523.79067	517.99274	284.45581	1
113	H	72.91432	75.36810	72.01292	1599.61665	-1127.00911	1895.98173	1
114	H	73.92835	74.67565	70.70971	-1881.83093	1275.82488	-1501.55016	1
115	C	74.84189	74.46701	72.72997	-600.05639	-404.05026	316.64485	1
116	H	74.65091	74.85374	73.75685	-2597.05260	496.36221	657.73249	1

117	H	74.66262	73.36850	72.76054	-1666.24518	1294.38985	-1723.90591	1
118	C	76.30245	74.84886	72.24141	493.57570	-129.95376	-602.56394	1
119	H	77.07462	74.90765	73.04252	-1469.08415	-637.84797	2204.22581	1
120	H	76.69443	74.20723	71.38566	-1038.97840	1068.88701	-2280.71789	1
121	C	74.33262	77.52162	72.81232	188.88100	241.05089	-727.87821	1
122	O	73.37383	77.18541	73.45707	531.88613	-49.19943	427.07960	1
123	N	75.07985	78.61931	72.88056	708.14833	26.93417	-179.73509	1
124	H	75.87502	78.71010	72.20327	-2232.69501	-1179.09831	1023.94816	1
125	C	74.83220	79.67653	73.86908	-738.32412	259.92548	104.42456	1
126	H	75.21430	80.59643	73.36619	2028.89123	1260.02983	1311.33324	1
127	C	73.34534	79.74949	74.15704	-258.65678	-345.52513	661.28459	1
128	H	73.03806	78.79122	74.65689	-1826.06090	-1801.46097	-918.64554	1
129	C	72.96849	80.88546	75.08713	-541.23400	531.92970	-218.41428	1
130	H	71.86212	81.08683	75.06005	1311.73218	-2219.18200	882.19023	1
131	H	73.22328	80.63819	76.17447	-1048.71298	1223.58118	-2196.97971	1
132	H	73.48766	81.84496	74.81507	419.06414	1903.92898	1903.44670	1
133	C	72.53170	79.87146	72.87898	-423.86431	152.66566	-648.55262	1
134	H	71.42962	79.93333	73.09059	105.68386	-2342.50080	1387.51238	1
135	H	72.81357	80.78614	72.29021	-1695.63603	-1484.73621	-1531.02793	1
136	H	72.69192	78.97781	72.21317	-1853.57121	-487.39031	1936.59343	1
137	C	75.74068	79.31751	75.19837	539.71428	-510.58232	267.58633	1
138	O	76.10962	78.17345	75.44640	-15.93758	-278.34085	-624.49402	1
139	N	75.95276	80.40220	75.91241	-676.81886	12.05292	276.17960	1
140	H	75.54945	81.25257	75.52855	-1694.44250	-373.84189	-2100.66098	1
141	C	76.99249	80.38865	76.89022	412.33078	-664.70360	108.35451	1
142	H	77.36462	79.33524	76.89682	1765.77476	1294.44366	1621.76594	1
143	C	78.09057	81.43703	76.41910	-179.66635	-721.95667	-264.73915	1
144	H	78.32352	81.31601	75.33761	-607.34922	2587.87032	-598.10018	1
145	H	77.70411	82.47463	76.52967	-359.69332	-1479.13954	-2259.74260	1
146	C	79.36739	81.22357	77.29374	-240.01076	616.02425	431.85322	1
147	H	79.07907	81.11016	78.37228	-1359.17131	782.54425	2227.99181	1
148	H	79.89095	80.28188	77.01022	-820.36667	85.81767	-2596.78715	1
149	C	80.31864	82.47560	77.11727	-513.07015	236.18570	-551.87280	1
150	H	80.68880	82.55228	76.06907	1816.11944	-1183.11722	-1650.94321	1
151	H	79.76817	83.42356	77.31749	-1800.04429	-1361.53473	1526.34643	1
152	C	81.48952	82.30690	78.11300	726.08972	-253.19732	-179.64713	1
153	H	81.18654	82.27817	79.17897	1224.27271	-456.51798	-2390.90304	1
154	H	82.16711	81.45890	77.88919	1206.40339	-1150.93514	-2154.90344	1
155	N	82.39407	83.58043	78.00337	329.70796	-633.68968	-155.67358	1
156	H	83.24061	83.59751	78.64239	1348.31305	1938.76845	1359.00643	1
157	H	82.84028	83.77611	77.06051	2096.92035	1446.54551	-966.48890	1
158	H	81.94279	84.51360	78.23217	-1197.07217	-2303.53719	827.28733	1
159	C	76.45509	80.89247	78.34014	-378.01186	-556.17301	-413.96481	1
160	O	77.22555	81.03465	79.26234	-409.44433	-307.55053	-453.30833	1
161	N	75.15245	81.16321	78.32552	-429.02477	524.70884	274.08502	1
162	H	74.55726	80.90171	77.51798	1706.34263	-1425.96036	1574.38926	1
163	C	74.49251	81.17854	79.59990	-45.25864	-626.22952	478.93267	1
164	H	75.19941	80.74662	80.34539	1988.63164	570.90773	1772.87287	1
165	C	74.12219	82.69343	79.88048	551.77128	-20.49526	-564.54996	1
166	H	74.98967	83.35078	79.64772	1434.61535	-1753.10253	1513.99471	1
167	H	73.30720	83.02412	79.19845	-714.67738	1819.09770	1898.36494	1
168	C	73.69582	82.85674	81.37555	446.99263	-555.77305	338.97221	1
169	H	72.85933	82.16743	81.62623	1953.68466	1892.25957	-161.67766	1
170	H	74.53437	82.58998	82.05726	-403.03785	2688.07032	-188.43591	1
171	C	73.25208	84.36089	81.58841	567.86262	335.74681	434.04421	1
172	H	74.08296	85.06134	81.34197	-1080.02275	1568.26081	-1948.78900	1
173	H	72.41696	84.62733	80.90058	-919.54108	2111.34692	1456.13463	1
174	C	72.81681	84.51883	83.06344	195.81897	173.33862	-745.11536	1
175	H	71.97306	83.86732	83.36641	1405.67949	-2301.21089	-390.08113	1
176	H	73.64099	84.43808	83.79999	-940.37328	-1118.32446	2299.72133	1
177	N	72.26352	85.97357	83.24164	319.26422	656.36007	-42.02424	1
178	H	71.91135	86.21288	84.21317	1961.03633	619.91968	1787.09422	1

179	H	72.93526	86.77498	83.05995	854.14343	-2156.80752	1429.08711	1
180	H	71.42838	86.24637	82.64598	1237.02905	-1378.50857	-1998.28500	1
181	C	73.16768	80.29732	79.22304	532.53319	-268.57236	517.55729	1
182	O	72.88973	80.20487	78.02725	266.16714	-290.73804	-558.88002	1
183	N	72.53423	79.88634	80.29350	-226.25352	640.49678	-270.32839	1
184	H	72.97629	80.14821	81.17493	2007.69063	-1035.27229	1523.50231	1
185	C	71.42191	79.00523	80.31751	-540.76542	-573.33303	49.50000	1
186	H	70.90408	79.24942	81.27147	-2374.20950	-1036.76023	843.75774	1
187	C	70.51904	79.26112	79.02719	-77.09082	666.87422	-415.84136	1
188	H	71.14060	79.01515	78.11654	-985.81834	617.19825	2463.91927	1
189	O	70.07154	80.62725	78.86634	293.29899	-391.65602	-477.80926	1
190	H	70.74589	80.94742	78.22860	2528.72714	-681.76262	-751.27122	1
191	C	69.37351	78.19222	79.15455	252.47363	-605.14473	440.05134	1
192	H	68.69181	78.22343	78.27334	-2052.65063	1456.49051	-1043.51830	1
193	H	69.77764	77.15471	79.22086	-2152.98800	-1661.97574	-161.70652	1
194	H	68.74791	78.36846	80.06033	-473.12726	-1584.27339	2165.61725	1
195	C	71.99635	77.47265	80.32802	360.36307	488.46713	505.10056	1
196	O	72.96952	77.11736	79.70583	-200.08817	-528.03552	-385.82850	1
197	N	71.11219	76.65391	80.99657	-597.54095	-226.44775	355.20479	1
198	H	70.37840	77.33897	81.23547	2179.23655	-1300.70981	-991.33835	1
199	C	71.63946	75.99741	82.18077	-687.68921	297.39807	-249.45179	1
200	H	71.76880	76.82079	82.91400	-349.16256	-2467.37713	-1101.72831	1
201	C	70.48614	74.98679	82.58980	672.47345	361.54328	-201.62880	1
202	H	70.07266	74.49432	81.67955	1541.41502	582.18425	2169.97026	1
203	H	70.89714	74.18517	83.24616	-2534.67717	60.25153	997.72295	1
204	C	69.37006	75.75171	83.32313	574.26774	-389.43119	-377.02542	1
205	C	69.39446	75.80655	84.74793	688.82679	-287.33580	-257.96133	1
206	H	70.20355	75.31443	85.31768	331.14182	1470.38163	2269.80013	1
207	C	68.32345	76.38923	82.59210	-383.52382	-675.04808	144.24917	1
208	H	68.30305	76.34842	81.48781	4.09847	1517.59662	2262.86397	1
209	C	68.36982	76.48624	85.40731	-134.76730	428.45285	-649.50303	1
210	H	68.38367	76.52153	86.51054	-903.23433	1600.49020	2011.53387	1
211	C	67.32137	77.06145	83.29795	-335.53281	-615.00040	-364.39058	1
212	H	66.51483	77.54976	82.72355	1596.45398	-1369.33862	1732.02659	1
213	C	67.30270	77.13466	84.72134	585.48547	-340.24194	-406.23938	1
214	O	66.28994	77.81290	85.44968	-419.15649	-173.04408	-511.94141	1
215	H	65.72326	78.11781	84.70300	-1071.84350	1559.71507	-1960.13012	1
216	C	73.03169	75.22379	81.90111	291.41878	-183.13091	710.72246	1
217	O	74.07178	75.67970	82.37647	379.87695	523.47396	-222.23622	1
218	N	72.83718	74.09803	81.24005	564.30591	373.09380	277.24371	1
219	H	71.86621	73.95686	80.96097	-120.59931	-2436.07824	-1214.35098	1
220	C	73.85695	73.44410	80.48281	404.07514	-299.37480	608.84009	1
221	H	73.27258	72.71486	79.87682	-1071.07882	-841.69025	2359.66467	1
222	C	74.54837	74.56625	79.59112	-683.12807	68.71770	-390.13096	1
223	H	73.77429	75.22977	79.12950	2068.88918	1596.58590	770.89603	1
224	H	75.17801	75.24520	80.21084	1379.86429	2342.49779	-179.85638	1
225	C	75.39353	73.82438	78.51304	-176.39967	537.49466	550.97268	1
226	H	76.26771	73.31776	78.98128	-396.28051	1942.22168	1869.33314	1
227	H	74.80010	73.01025	78.04035	-94.44700	586.00678	-2659.20016	1
228	C	75.85745	74.88505	77.41127	-291.69381	-718.18079	-150.72929	1
229	H	75.04044	75.33188	76.78828	-2303.38776	1089.76242	964.62032	1
230	H	76.50683	75.72117	77.77638	884.16729	2568.80533	-207.74283	1
231	N	76.63462	74.05297	76.58955	-594.49522	-252.81478	342.29276	1
232	H	76.68839	73.08003	76.85011	-1735.17426	2084.05705	-263.71605	1
233	C	77.27800	74.43542	75.55950	595.23177	-271.52487	442.22352	1
234	N	77.19693	75.77974	75.20522	585.53813	-424.79750	-105.81303	1
235	H	76.62453	76.53624	75.65211	959.88797	1327.56823	-2177.11905	1
236	H	77.67391	76.19092	74.39522	1578.48647	16.27378	-2220.76233	1
237	N	77.97035	73.36891	74.96073	-452.17763	-390.33541	-421.51853	1
238	H	78.04840	72.39429	75.24561	470.26107	1974.25629	-1817.92087	1
239	H	78.57377	73.46705	74.14442	1856.67307	-1573.97321	-1224.35416	1
240	C	74.95101	72.69682	81.42116	-531.47271	-581.45780	-55.06206	1

241	O	75.08644	71.49869	81.27473	-243.00837	192.73507	609.52485	1
242	N	75.62284	73.52792	82.19728	343.49288	-644.25607	38.09164	1
243	H	75.31967	74.54281	82.21345	-1691.16043	-1535.97525	-1484.73099	1
244	C	76.35580	73.05152	83.37700	542.66492	350.14337	454.42563	1
245	H	76.55189	74.00056	83.92848	1209.57979	-2396.95920	463.86744	1
246	C	75.46031	72.10113	84.15088	-737.14309	145.93010	242.71942	1
247	H	75.16995	71.26551	83.47150	-1050.18303	159.36419	-2509.06125	1
248	C	76.17483	71.50341	85.34855	-706.77696	-252.88343	-245.16230	1
249	H	75.49760	70.83217	85.94544	-1624.64039	-1665.49085	1417.86935	1
250	H	77.06107	70.88715	85.03461	2566.10521	598.51109	693.22305	1
251	H	76.55419	72.30086	86.04565	-1972.69758	107.10018	-1876.34312	1
252	C	74.18235	72.79015	84.59504	412.85148	672.58832	-27.69222	1
253	H	73.47560	72.07701	85.10155	1447.02277	1762.76533	-1490.78944	1
254	H	74.39341	73.62382	85.31993	1320.77379	-145.20455	2378.68491	1
255	H	73.63702	73.24341	83.72052	-1512.10848	1470.52031	1724.75147	1
256	C	77.78141	72.35378	82.89351	-607.11113	499.56689	73.73769	1
257	O	78.80629	72.83129	83.31005	357.97126	460.81534	356.68785	1
258	N	77.61590	71.29131	82.12650	536.55407	-368.62270	332.76306	1
259	H	76.66732	70.97772	81.81294	524.38866	2297.69985	1367.20941	1
260	C	78.80249	70.68736	81.63126	46.50277	-774.29190	-147.97904	1
261	H	79.57888	71.48509	81.65884	1676.51875	1883.29066	1032.55549	1
262	C	79.18653	69.43154	82.57207	-559.41456	-34.19198	-556.30433	1
263	H	78.29120	68.77535	82.68818	-64.66664	395.18769	2695.05373	1
264	H	79.96348	68.80628	82.07050	-2703.44278	-60.40056	333.79418	1
265	C	79.67990	69.89794	83.91486	-519.76435	377.31045	459.42366	1
266	H	78.90195	70.55220	84.36773	-1746.74323	1667.50644	-1261.73691	1
267	C	79.91780	68.70481	84.83280	570.95554	16.46261	-545.27700	1
268	H	80.25460	69.02708	85.85172	2391.58273	28.05277	-1305.07271	1
269	H	78.98932	68.09241	84.96719	175.75588	917.63458	2559.43867	1
270	H	80.70779	68.02330	84.42413	-1063.97851	-2155.34650	1283.00462	1
271	C	80.96241	70.71058	83.79914	193.76014	2.62946	-765.53141	1
272	H	81.39952	70.93654	84.80605	507.39394	-846.55087	2539.60089	1
273	H	81.74675	70.17010	83.20885	1337.57841	1818.19054	1526.01994	1
274	H	80.77690	71.69697	83.29532	1100.88635	-1172.91350	-2199.08909	1
275	C	78.46151	70.09602	80.16553	-549.21115	475.64486	-309.38218	1
276	O	77.67606	69.20150	79.99453	556.06106	-390.37755	-78.24250	1
277	O	79.17660	70.65416	79.08148	-572.27940	-310.19032	-209.75862	1
278	H	79.72887	71.32061	79.57514	-1380.08193	2212.14486	790.85944	1

Listing 120: C00120.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.2750	1100
		0.2500	300.00	0.00	0.00	0.00	-1293.3685	0.0000	300.0000
3	H	78.67782	65.63576	71.09836	-2043.14101	-1757.64893	399.89339		1
4	N	78.85828	65.67139	70.09413	426.75047	490.45733	-334.42467		1
5	H	77.93537	65.86848	69.67036	442.25559	-1110.30854	-2448.52907		1
6	C	79.83755	66.61871	69.72496	415.32972	-666.39213	83.73172		1
7	H	80.32269	66.97757	70.65886	879.32219	2491.00447	667.35213		1
8	C	80.88171	65.94854	68.69491	31.35357	477.41777	628.23362		1
9	H	80.36575	65.73874	67.72793	1168.38489	2240.25337	-1019.71136		1
10	H	81.70826	66.65807	68.45238	-360.43770	2534.90498	931.67112		1
11	C	81.41579	64.67302	69.29437	463.18208	512.70242	-382.34388		1
12	H	80.54823	64.03850	69.58612	1725.29117	1863.52247	-987.07854		1
13	C	82.24846	63.91624	68.26760	710.42801	-144.27427	-313.15367		1
14	H	82.63863	62.95136	68.68245	364.20195	-1033.13725	2494.72524		1
15	H	81.65076	63.66804	67.35261	2567.61904	335.80679	847.48802		1
16	H	83.13365	64.51580	67.93216	-2587.99029	680.92867	-512.16411		1
17	C	82.25134	64.95466	70.53554	268.17616	741.64379	-40.42634		1
18	H	82.69255	64.01545	70.95801	1283.54314	-1945.37420	-1411.27812		1
19	H	83.10047	65.65079	70.31231	-1258.57796	1317.15249	-2026.02085		1
20	H	81.63856	65.42640	71.34640	-2502.84526	909.80597	575.92391		1

21	C	78.92843	67.72038	68.95719	619.36578	-458.64843	-172.09273	1
22	O	77.72778	67.48986	68.82787	-81.40433	433.87611	522.34594	1
23	N	79.66412	68.73650	68.55954	175.23996	-622.20190	341.55523	1
24	H	80.65991	68.67088	68.77504	-876.57256	-303.22879	-2561.90213	1
25	C	79.20717	69.81664	67.76408	-571.88214	-534.10783	-106.15033	1
26	H	80.14698	70.25510	67.36500	-2713.20841	-16.25800	-248.80809	1
27	C	78.24517	69.24431	66.61520	166.60354	288.16399	-716.09568	1
28	H	77.42495	68.65124	67.11427	-2097.85574	1636.78449	-586.18044	1
29	O	78.88611	68.36379	65.67638	-317.80580	-363.38227	484.43082	1
30	H	78.44545	67.51519	65.89159	1863.74748	-1451.84923	1357.29467	1
31	C	77.61497	70.55849	66.02718	503.80731	517.99032	318.51606	1
32	H	76.89955	70.33408	65.20190	640.61020	-2157.10410	-1536.29104	1
33	H	77.05192	71.12178	66.80888	1687.88455	465.60692	2087.56452	1
34	H	78.39436	71.23929	65.61249	-1293.07895	-1899.88581	-1463.57452	1
35	C	78.39650	70.84109	68.74656	-153.07550	-733.68902	248.70981	1
36	O	77.31113	70.52686	69.17398	186.15459	-480.78787	-449.34387	1
37	N	79.05797	71.99416	68.87888	-487.53139	543.18517	42.03850	1
38	C	78.70278	72.93591	69.90522	-699.35871	69.34393	360.10701	1
39	H	78.57454	72.34992	70.84301	2.81126	-221.99807	-2715.58072	1
40	C	79.94234	73.92866	69.90859	-507.46439	-592.59194	122.07761	1
41	H	79.67914	74.94350	70.28189	-1975.08116	525.87560	-1801.71556	1
42	H	80.76139	73.55399	70.56203	1588.27743	-1913.22100	1113.83566	1
43	C	80.37197	73.91694	68.40874	-613.62442	-457.55993	-194.14490	1
44	H	79.68873	74.54393	67.79237	1707.54637	-721.27992	1996.92523	1
45	H	81.40327	74.29899	68.23388	758.23357	2100.81767	1560.55011	1
46	C	80.20932	72.37201	68.07091	-352.41524	704.96076	49.21465	1
47	H	79.99476	72.14019	67.00140	1714.76886	-2070.42778	443.35792	1
48	H	81.05527	71.73628	68.42650	1224.15040	1801.50881	1636.97633	1
49	C	77.32500	73.71062	69.51622	566.85117	537.05831	117.62814	1
50	O	76.74971	74.37882	70.37272	-550.26779	-406.08867	4.21666	1
51	N	77.00118	73.53283	68.25535	566.34832	-425.77725	180.18749	1
52	H	77.61631	72.93010	67.71434	644.44502	2646.80550	-52.73430	1
53	C	75.78974	74.09339	67.75447	612.34801	-281.48662	411.56221	1
54	H	75.65362	74.96183	68.44168	1667.23498	-1490.75142	1556.16753	1
55	C	76.09476	74.47567	66.23249	-714.45746	-175.43074	286.98927	1
56	H	76.31645	73.53918	65.64869	-787.09484	1763.03619	-1922.46060	1
57	O	77.24793	75.31578	66.02111	-429.46514	516.51932	-128.40526	1
58	H	77.81596	74.72495	65.48988	1981.82785	436.16847	-1818.18182	1
59	C	74.71661	75.07587	65.77444	630.79189	-468.94448	76.03230	1
60	H	74.72165	75.32012	64.68670	-1775.71861	2062.30353	131.89849	1
61	H	73.87281	74.36880	65.95124	-1855.14608	88.94118	1993.53760	1
62	H	74.48434	76.01719	66.32468	-1504.82350	-780.94249	-2132.90992	1
63	C	74.60958	72.98797	67.98651	288.57638	618.62814	-397.00270	1
64	O	74.11146	72.88673	69.10168	321.70495	-185.26452	574.37218	1
65	N	74.34218	72.29406	66.90433	-447.05792	-446.53431	367.76425	1
66	H	74.88302	72.44102	66.05420	350.31316	1975.63644	-1843.31522	1
67	C	73.06291	71.67289	66.76614	-511.23061	374.03917	-471.51480	1
68	H	72.41574	72.28943	67.42962	2234.79579	-898.70890	-1273.45190	1
69	C	72.68890	71.73936	65.21780	529.53781	-159.34528	563.72604	1
70	H	71.85690	71.01133	65.04035	654.59388	2347.94251	1217.51488	1
71	H	72.25293	72.75955	65.03134	-1526.55661	2103.42026	817.87394	1
72	O	73.78004	71.58708	64.26055	-554.84278	14.12789	399.58769	1
73	H	73.54276	70.72827	63.87271	1297.06236	2061.84854	1220.68812	1
74	C	73.15942	70.14803	67.34652	-662.15484	-412.13544	123.62687	1
75	O	72.85444	69.17372	66.70221	-540.01537	-317.05804	274.91456	1
76	N	73.52870	70.23631	68.62017	-202.76299	-690.00100	-131.49145	1
77	H	73.71196	71.18618	69.01479	-702.62132	-2617.37191	281.70413	1
78	C	73.73220	69.02897	69.35207	-491.73914	576.34187	222.73509	1
79	H	72.88114	68.38415	69.03919	1977.17978	-1823.58850	-434.68928	1
80	C	75.10968	68.37297	68.90313	-649.50797	-328.66843	306.11224	1
81	H	75.97578	69.08364	69.06513	2075.07803	1452.16490	-1004.45904	1
82	C	75.23864	67.07550	69.77358	-615.18735	-489.99689	-70.96352	1

83	H	76.04674	66.39362	69.40585	-1226.32661	-1724.38906	-1716.47170	1
84	H	75.46835	67.32346	70.83950	2381.64273	-969.84735	900.46860	1
85	H	74.28889	66.49077	69.77083	2122.74991	1702.23946	-141.36228	1
86	C	75.06315	67.92278	67.40453	-501.86074	-479.61276	-376.42482	1
87	H	75.92511	67.25812	67.15357	993.79261	-2246.95401	-1177.81305	1
88	H	74.12762	67.35772	67.16983	42.71279	-626.15391	-2651.37258	1
89	H	75.10851	68.79830	66.71078	-2026.39012	-1590.33709	-887.82922	1
90	C	73.84228	69.29422	70.96052	-672.89153	382.57394	-156.34072	1
91	O	73.62901	68.36772	71.70888	410.04627	221.86223	500.35950	1
92	N	74.28353	70.50277	71.27709	-378.11782	-443.79414	-441.10984	1
93	H	74.44925	71.21857	70.57078	2404.15973	-568.14894	1149.30085	1
94	C	74.53291	70.77997	72.66147	-544.54484	466.16019	331.29119	1
95	H	75.02755	69.85906	73.03844	-1409.80988	-170.17955	2325.32679	1
96	C	75.44844	72.06914	72.62494	-184.48284	116.78282	-758.89137	1
97	H	76.37398	71.86934	72.03654	1893.78641	1861.14652	611.04528	1
98	H	74.93279	72.90212	72.09273	-2170.79665	-974.19311	1327.50117	1
99	C	75.79398	72.46238	74.09421	389.51668	672.81878	-138.49152	1
100	H	74.86090	72.73074	74.63966	510.64577	1933.03327	1851.02484	1
101	H	76.18652	71.57877	74.64250	-2302.30869	-1105.72939	-948.89774	1
102	C	76.83579	73.64170	74.21964	-559.93427	-126.34590	542.30857	1
103	O	77.32337	73.87334	75.29845	-670.36003	-111.83166	76.36448	1
104	N	77.09116	74.31221	73.07998	-216.06729	-537.07037	446.51379	1
105	H	76.71188	74.23350	72.09765	-1251.96487	1074.12894	-2168.52500	1
106	H	77.72185	75.12692	73.09875	-2451.83023	-720.73851	944.84612	1
107	C	73.09569	71.04933	73.39545	546.24052	-563.88337	-85.11809	1
108	O	72.40475	71.95405	73.00784	71.70702	-307.40463	606.69673	1
109	N	72.90357	70.22846	74.44035	479.90863	-504.50129	222.86849	1
110	C	71.59734	70.01586	74.98367	75.51268	-600.91904	506.73700	1
111	H	70.88250	70.07537	74.13169	-2033.61562	1795.30103	254.89480	1
112	C	71.73628	68.59474	75.67758	523.79067	517.99274	284.45581	1
113	H	70.99204	68.43959	76.49110	1599.61665	-1127.00911	1895.98173	1
114	H	71.59127	67.76548	74.94962	-1881.83093	1275.82488	-1501.55016	1
115	C	73.20845	68.64211	76.18996	-600.05639	-404.05026	316.64485	1
116	H	73.30452	69.29295	77.08825	-2597.05260	496.36221	657.73249	1
117	H	73.62205	67.64755	76.47039	-1666.24518	1294.38985	-1723.90591	1
118	C	73.90723	69.28380	74.91280	493.57570	-129.95376	-602.56394	1
119	H	74.85728	69.83332	75.11204	-1469.08415	-637.84797	2204.22581	1
120	H	74.05401	68.56869	74.06593	-1038.97840	1068.88701	-2280.71789	1
121	C	71.21325	71.07622	76.17504	188.88100	241.05089	-727.87821	1
122	O	70.05362	71.23054	76.48061	531.88613	-49.19943	427.07960	1
123	N	72.29689	71.53313	76.80247	708.14833	26.93417	-179.73509	1
124	H	73.18958	71.32249	76.35798	-2232.69501	-1179.09831	1023.94816	1
125	C	72.11366	72.60381	77.71870	-738.32412	259.92548	104.42456	1
126	H	71.03098	72.60254	77.98337	2028.89123	1260.02983	1311.33324	1
127	C	73.10324	72.35707	78.93367	-258.65678	-345.52513	661.28459	1
128	H	74.11901	72.11421	78.54963	-1826.06090	-1801.46097	-918.64554	1
129	C	73.13831	73.63345	79.84513	-541.23400	531.92970	-218.41428	1
130	H	73.80150	73.48302	80.72959	1311.73218	-2219.18200	882.19023	1
131	H	73.53876	74.51817	79.29301	-1048.71298	1223.58118	-2196.97971	1
132	H	72.12538	73.90535	80.22246	419.06414	1903.92898	1903.44670	1
133	C	72.57378	71.17398	79.81509	-423.86431	152.66566	-648.55262	1
134	H	73.26429	70.95803	80.66433	105.68386	-2342.50080	1387.51238	1
135	H	71.57196	71.39845	80.25017	-1695.63603	-1484.73621	-1531.02793	1
136	H	72.47395	70.23621	79.21930	-1853.57121	-487.39031	1936.59343	1
137	C	72.60296	73.95319	76.90206	539.71428	-510.58232	267.58633	1
138	O	73.75384	74.12905	76.57755	-15.93758	-278.34085	-624.49402	1
139	N	71.54975	74.74332	76.76733	-676.81886	12.05292	276.17960	1
140	H	70.64944	74.41805	77.11728	-1694.44250	-373.84189	-2100.66098	1
141	C	71.68032	75.97108	76.05321	412.33078	-664.70360	108.35451	1
142	H	72.43822	75.75178	75.26732	1765.77476	1294.44366	1621.76594	1
143	C	70.24053	76.32300	75.50358	-179.66635	-721.95667	-264.73915	1
144	H	69.83332	75.46333	74.92547	-607.34922	2587.87032	-598.10018	1

145	H	69.52769	76.47735	76.34439	-359.69332	-1479.13954	-2259.74260	1
146	C	70.31402	77.60501	74.60922	-240.01076	616.02425	431.85322	1
147	H	70.59590	78.49593	75.22108	-1359.17131	782.54425	2227.99181	1
148	H	71.10375	77.50478	73.83169	-820.36667	85.81767	-2596.78715	1
149	C	68.89112	77.78616	73.94099	-513.07015	236.18570	-551.87280	1
150	H	68.64278	76.90919	73.29986	1816.11944	-1183.11722	-1650.94321	1
151	H	68.09273	77.82747	74.71664	-1800.04429	-1361.53473	1526.34643	1
152	C	68.89686	79.08668	73.10522	726.08972	-253.19732	-179.64713	1
153	H	68.98473	80.01720	73.70153	1224.27271	-456.51798	-2390.90304	1
154	H	69.62783	79.09936	72.27229	1206.40339	-1150.93514	-2154.90344	1
155	N	67.50033	79.19479	72.40229	329.70796	-633.68968	-155.67358	1
156	H	67.35612	80.05481	71.79822	1348.31305	1938.76845	1359.00643	1
157	H	67.23410	78.41943	71.72759	2096.92035	1446.54551	-966.48890	1
158	H	66.64721	79.24025	73.03203	-1197.07217	-2303.53719	827.28733	1
159	C	72.21477	77.15745	77.05038	-378.01186	-556.17301	-413.96481	1
160	O	72.40581	78.26326	76.59699	-409.44433	-307.55053	-453.30833	1
161	N	72.40225	76.73348	78.29520	-429.02477	524.70884	274.08502	1
162	H	72.18058	75.75487	78.46842	1706.34263	-1425.96036	1574.38926	1
163	C	72.66466	77.65793	79.34102	-45.25864	-626.22952	478.93267	1
164	H	72.78753	78.63626	78.81965	1988.63164	570.90773	1772.87287	1
165	C	71.41004	77.60783	80.31338	551.77128	-20.49526	-564.54996	1
166	H	70.50967	77.99887	79.79010	1434.61535	-1753.10253	1513.99471	1
167	H	71.15841	76.56268	80.59754	-714.67738	1819.09770	1898.36494	1
168	C	71.74231	78.46809	81.57595	446.99263	-555.77305	338.97221	1
169	H	72.34233	77.88590	82.31952	1953.68466	1892.25957	-161.67766	1
170	H	72.37954	79.33207	81.28243	-403.03785	2688.07032	-188.43591	1
171	C	70.39543	78.97599	82.23416	567.86262	335.74681	434.04421	1
172	H	69.69456	79.36538	81.46381	-1080.02275	1568.26081	-1948.78900	1
173	H	69.85491	78.14775	82.74747	-919.54108	2111.34692	1456.13463	1
174	C	70.79419	80.09630	83.22168	195.81897	173.33862	-745.11536	1
175	H	71.49169	79.77879	84.02216	1405.67949	-2301.21089	-390.08113	1
176	H	71.17029	81.01597	82.73346	-940.37328	-1118.32446	2299.72133	1
177	N	69.51285	80.57566	83.98369	319.26422	656.36007	-42.02424	1
178	H	69.66219	81.36560	84.67584	1961.03633	619.91968	1787.09422	1
179	H	68.71848	80.96335	83.39823	854.14343	-2156.80752	1429.08711	1
180	H	69.01314	79.85998	84.58768	1237.02905	-1378.50857	-1998.28500	1
181	C	73.99567	77.16584	80.15411	532.53319	-268.57236	517.55729	1
182	O	74.16086	77.46910	81.31756	266.16714	-290.73804	-558.88002	1
183	N	74.81272	76.47114	79.37127	-226.25352	640.49678	-270.32839	1
184	H	74.56101	76.35719	78.39024	2007.69063	-1035.27229	1523.50231	1
185	C	76.05500	76.06227	79.93647	-540.76542	-573.33303	49.50000	1
186	H	75.84179	75.91460	81.01977	-2374.20950	-1036.76023	843.75774	1
187	C	76.56471	74.78163	79.13633	-77.09082	666.87422	-415.84136	1
188	H	76.77087	75.08492	78.07183	-985.81834	617.19825	2463.91927	1
189	O	75.63917	73.67839	79.03172	293.29899	-391.65602	-477.80926	1
190	H	75.33036	73.78330	78.10286	2528.72714	-681.76262	-751.27122	1
191	C	77.90735	74.47000	79.88974	252.47363	-605.14473	440.05134	1
192	H	78.46657	73.63983	79.40030	-2052.65063	1456.49051	-1043.51830	1
193	H	78.58640	75.35675	79.91850	-2152.98800	-1661.97574	-161.70652	1
194	H	77.72218	74.16577	80.94529	-473.12726	-1584.27339	2165.61725	1
195	C	77.14895	77.26355	79.64989	360.36307	488.46713	505.10056	1
196	O	77.29827	77.74754	78.55427	-200.08817	-528.03552	-385.82850	1
197	N	77.82151	77.47096	80.77444	-597.54095	-226.44775	355.20479	1
198	H	77.54051	76.92890	81.59151	2179.23655	-1300.70981	-991.33835	1
199	C	78.97313	78.28371	80.82599	-687.68921	297.39807	-249.45179	1
200	H	79.37212	78.14109	81.85521	-349.16256	-2467.37713	-1101.72831	1
201	C	80.02067	77.88833	79.67468	672.47345	361.54328	-201.62880	1
202	H	79.50410	77.80575	78.68789	1541.41502	582.18425	2169.97026	1
203	H	80.76872	78.71164	79.58046	-2534.67717	60.25153	997.72295	1
204	C	80.71416	76.56887	80.03836	574.26774	-389.43119	-377.02542	1
205	C	81.50262	76.49214	81.22638	688.82679	-287.33580	-257.96133	1
206	H	81.63476	77.37902	81.87184	331.14182	1470.38163	2269.80013	1

207	C	80.57542	75.42191	79.19797	-383.52382	-675.04808	144.24917	1
208	H	79.98515	75.47634	78.26336	4.09847	1517.59662	2262.86397	1
209	C	82.10085	75.27720	81.55973	-134.76730	428.45285	-649.50303	1
210	H	82.70489	75.22144	82.48237	-903.23433	1600.49020	2011.53387	1
211	C	81.19199	74.22534	79.57536	-335.53281	-615.00040	-364.39058	1
212	H	81.06797	73.34552	78.92086	1596.45398	-1369.33862	1732.02659	1
213	C	81.96853	74.10213	80.76430	585.48547	-340.24194	-406.23938	1
214	O	82.59489	72.89137	81.16075	-419.15649	-173.04408	-511.94141	1
215	H	82.31993	72.30863	80.41451	-1071.84350	1559.71507	-1960.13012	1
216	C	78.60617	79.83622	80.48458	291.41878	-183.13091	710.72246	1
217	O	79.49357	80.57249	80.11245	379.87695	523.47396	-222.23622	1
218	N	77.34053	80.14606	80.77427	564.30591	373.09380	277.24371	1
219	H	76.72416	79.37350	81.02690	-120.59931	-2436.07824	-1214.35098	1
220	C	76.86546	81.41133	80.31466	404.07514	-299.37480	608.84009	1
221	H	77.78534	82.04004	80.32523	-1071.07882	-841.69025	2359.66467	1
222	C	76.32184	81.19209	78.84652	-683.12807	68.71770	-390.13096	1
223	H	77.11860	80.76658	78.19449	2068.88918	1596.58590	770.89603	1
224	H	75.49537	80.44748	78.81739	1379.86429	2342.49779	-179.85638	1
225	C	75.85168	82.59165	78.33805	-176.39967	537.49466	550.97268	1
226	H	75.05770	83.00697	78.99905	-396.28051	1942.22168	1869.33314	1
227	H	76.68730	83.32583	78.37396	-94.44700	586.00678	-2659.20016	1
228	C	75.30740	82.40940	76.84868	-291.69381	-718.18079	-150.72929	1
229	H	76.02051	81.95201	76.11616	-2303.38776	1089.76242	964.62032	1
230	H	74.32193	81.87987	76.76327	884.16729	2568.80533	-207.74283	1
231	N	75.10034	83.74635	76.47549	-594.49522	-252.81478	342.29276	1
232	H	75.15742	84.43849	77.20624	-1735.17426	2084.05705	-263.71605	1
233	C	74.82280	84.13248	75.29596	595.23177	-271.52487	442.22352	1
234	N	74.73495	83.15545	74.29690	585.53813	-424.79750	-105.81303	1
235	H	74.79048	82.14197	74.38697	959.88797	1327.56823	-2177.11905	1
236	H	74.46797	83.33131	73.32846	1578.48647	16.27378	-2220.76233	1
237	N	74.66503	85.52446	75.24748	-452.17763	-390.33541	-421.51853	1
238	H	74.70675	86.22504	75.98613	470.26107	1974.25629	-1817.92087	1
239	H	74.41059	86.02900	74.39767	1856.67307	-1573.97321	-1224.35416	1
240	C	75.69608	81.94805	81.34764	-531.47271	-581.45780	-55.06206	1
241	O	76.04324	82.75189	82.18631	-243.00837	192.73507	609.52485	1
242	N	74.51083	81.42471	81.11484	343.49288	-644.25607	38.09164	1
243	H	74.48468	80.72685	80.37499	-1691.16043	-1535.97525	-1484.73099	1
244	C	73.34140	81.65557	81.90374	542.66492	350.14337	454.42563	1
245	H	73.06657	80.60167	82.13184	1209.57979	-2396.95920	463.86744	1
246	C	73.63244	82.51098	83.20179	-737.14309	145.93010	242.71942	1
247	H	74.24392	83.41384	82.94540	-1050.18303	159.36419	-2509.06125	1
248	C	72.33103	82.94902	83.96038	-706.77696	-252.88343	-245.16230	1
249	H	72.56878	83.61347	84.82427	-1624.64039	-1665.49085	1417.86935	1
250	H	71.63657	83.51769	83.28893	2566.10521	598.51109	693.22305	1
251	H	71.77004	82.07469	84.36424	-1972.69758	107.10018	-1876.34312	1
252	C	74.39740	81.56291	84.19144	412.85148	672.58832	-27.69222	1
253	H	74.63533	82.07461	85.15293	1447.02277	1762.76533	-1490.78944	1
254	H	73.79935	80.65311	84.43631	1320.77379	-145.20455	2378.68491	1
255	H	75.36377	81.22365	83.74495	-1512.10848	1470.52031	1724.75147	1
256	C	72.19776	82.30913	80.93177	-607.11113	499.56689	73.73769	1
257	O	71.71910	83.39772	81.16889	357.97126	460.81534	356.68785	1
258	N	71.93190	81.48710	79.92032	536.55407	-368.62270	332.76306	1
259	H	72.48467	80.63130	79.92938	524.38866	2297.69985	1367.20941	1
260	C	70.63942	81.40891	79.30762	46.50277	-774.29190	-147.97904	1
261	H	70.23705	80.44035	79.67158	1676.51875	1883.29066	1032.55549	1
262	C	69.67151	82.65000	79.62603	-559.41456	-34.19198	-556.30433	1
263	H	70.26944	83.59781	79.58612	-64.66664	395.18769	2695.05373	1
264	H	68.89408	82.74018	78.82781	-2703.44278	-60.40056	333.79418	1
265	C	68.99861	82.49675	80.96831	-519.76435	377.31045	459.42366	1
266	H	69.77258	82.19884	81.71171	-1746.74323	1667.50644	-1261.73691	1
267	C	68.39936	83.82723	81.40734	570.95554	16.46261	-545.27700	1
268	H	67.92748	83.75550	82.42128	2391.58273	28.05277	-1305.07271	1

269	H	69.17878	84.63120	81.45748	175.75588	917.63458	2559.43867	1
270	H	67.60570	84.17601	80.69637	-1063.97851	-2155.34650	1283.00462	1
271	C	67.89651	81.44792	80.92790	193.76014	2.62946	-765.53141	1
272	H	67.37219	81.35929	81.91421	507.39394	-846.55087	2539.60089	1
273	H	67.11479	81.70205	80.16609	1337.57841	1818.19054	1526.01994	1
274	H	68.28928	80.43294	80.66774	1100.88635	-1172.91350	-2199.08909	1
275	C	70.88638	81.35659	77.72620	-549.21115	475.64486	-309.38218	1
276	O	71.89889	81.71844	77.18455	556.06106	-390.37755	-78.24250	1
277	O	69.76577	80.94689	76.95415	-572.27940	-310.19032	-209.75862	1
278	H	69.13500	80.74561	77.69669	-1380.08193	2212.14486	790.85944	1

Listing 121: C00121.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.3649	0.0000	300.0000
3	H	56.46556	75.37115	71.76407	-2043.14101	-1757.64893	399.89339		1
4	N	57.28378	75.20829	72.35232	426.75047	490.45733	-334.42467		1
5	H	57.51930	74.21291	72.19371	442.25559	-1110.30854	-2448.52907		1
6	C	58.37126	76.05840	72.05387	415.32972	-666.39213	83.73172		1
7	H	57.99882	76.86376	71.38380	879.32219	2491.00447	667.35213		1
8	C	58.99808	76.62929	73.42709	31.35357	477.41777	628.23362		1
9	H	59.34904	75.77774	74.05691	1168.38489	2240.25337	-1019.71136		1
10	H	59.90170	77.24876	73.21247	-360.43770	2534.90498	931.67112		1
11	C	57.96612	77.42505	74.18002	463.18208	512.70242	-382.34388		1
12	H	57.07372	76.77669	74.33391	1725.29117	1863.52247	-987.07854		1
13	C	58.51791	77.83176	75.54152	710.42801	-144.27427	-313.15367		1
14	H	57.75795	78.38893	76.14739	364.20195	-1033.13725	2494.72524		1
15	H	58.83543	76.94120	76.14286	2567.61904	335.80679	847.48802		1
16	H	59.41290	78.49814	75.43946	-2587.99029	680.92867	-512.16411		1
17	C	57.53612	78.66799	73.41324	268.17616	741.64379	-40.42634		1
18	H	56.80523	79.28198	74.00038	1283.54314	-1945.37420	-1411.27812		1
19	H	58.40924	79.32877	73.17544	-1258.57796	1317.15249	-2026.02085		1
20	H	57.04205	78.40602	72.44250	-2502.84526	909.80597	575.92391		1
21	C	59.40007	75.01699	71.36064	619.36578	-458.64843	-172.09273		1
22	O	59.12738	73.82173	71.33198	-81.40433	433.87611	522.34594		1
23	N	60.50831	75.62513	70.95287	175.23996	-622.20190	341.55523		1
24	H	60.59199	76.63359	71.08097	-876.57256	-303.22879	-2561.90213		1
25	C	61.59746	74.83885	70.50008	-571.88214	-534.10783	-106.15033		1
26	H	61.16955	73.81739	70.36533	-2713.20841	-16.25800	-248.80809		1
27	C	62.20162	75.53783	69.18737	166.60354	288.16399	-716.09568		1
28	H	62.66528	76.51565	69.49993	-2097.85574	1636.78449	-586.18044		1
29	O	61.25549	75.84511	68.15053	-317.80580	-363.38227	484.43082		1
30	H	61.31440	76.82198	68.12098	1863.74748	-1451.84923	1357.29467		1
31	C	63.34473	74.53575	68.78407	503.80731	517.99032	318.51606		1
32	H	63.93599	74.92058	67.92071	640.61020	-2157.10410	-1536.29104		1
33	H	64.05923	74.36422	69.62621	1687.88455	465.60692	2087.56452		1
34	H	62.93154	73.54426	68.48532	-1293.07895	-1899.88581	-1463.57452		1
35	C	62.79685	74.94535	71.61194	-153.07550	-733.68902	248.70981		1
36	O	63.66763	75.74943	71.40194	186.15459	-480.78787	-449.34387		1
37	N	62.60893	74.15453	72.68125	-487.53139	543.18517	42.03850		1
38	C	63.64723	73.98395	73.64644	-699.35871	69.34393	360.10701		1
39	H	64.42905	74.72312	73.34943	2.81126	-221.99807	-2715.58072		1
40	C	62.83942	74.31628	74.97665	-507.46439	-592.59194	122.07761		1
41	H	63.36907	74.01947	75.90977	-1975.08116	525.87560	-1801.71556		1
42	H	62.63240	75.40608	75.06139	1588.27743	-1913.22100	1113.83566		1
43	C	61.52990	73.50979	74.71955	-613.62442	-457.55993	-194.14490		1
44	H	61.68774	72.41963	74.88542	1707.54637	-721.27992	1996.92523		1
45	H	60.68505	73.81257	75.37812	758.23357	2100.81767	1560.55011		1
46	C	61.27509	73.84154	73.18748	-352.41524	704.96076	49.21465		1
47	H	60.85543	73.00186	72.58158	1714.76886	-2070.42778	443.35792		1
48	H	60.67323	74.76126	73.00283	1224.15040	1801.50881	1636.97633		1

49	C	64.17254	72.42585	73.59041	566.85117	537.05831	117.62814	1
50	O	64.33068	71.88075	72.52281	-550.26779	-406.08867	4.21666	1
51	N	64.50789	72.00960	74.80273	566.34832	-425.77725	180.18749	1
52	H	64.32145	72.65176	75.57139	644.44502	2646.80550	-52.73430	1
53	C	64.88947	70.67730	75.11627	612.34801	-281.48662	411.56221	1
54	H	64.76705	70.62645	76.22097	1667.23498	-1490.75142	1556.16753	1
55	C	63.89368	69.66584	74.37778	-714.45746	-175.43074	286.98927	1
56	H	64.00831	69.79587	73.26515	-787.09484	1763.03619	-1922.46060	1
57	O	62.49761	69.87313	74.67082	-429.46514	516.51932	-128.40526	1
58	H	62.16184	70.12551	73.78777	1981.82785	436.16847	-1818.18182	1
59	C	64.45284	68.25621	74.79101	630.79189	-468.94448	76.03230	1
60	H	63.84724	67.43229	74.34665	-1775.71861	2062.30353	131.89849	1
61	H	65.50751	68.10648	74.45600	-1855.14608	88.94118	1993.53760	1
62	H	64.43376	68.11845	75.89740	-1504.82350	-780.94249	-2132.90992	1
63	C	66.45684	70.47248	74.71472	288.57638	618.62814	-397.00270	1
64	O	67.07002	69.54215	75.18568	321.70495	-185.26452	574.37218	1
65	N	66.89335	71.37206	73.83057	-447.05792	-446.53431	367.76425	1
66	H	66.24318	72.09514	73.50955	350.31316	1975.63644	-1843.31522	1
67	C	68.28899	71.66750	73.86443	-511.23061	374.03917	-471.51480	1
68	H	68.72735	71.02845	74.66557	2234.79579	-898.70890	-1273.45190	1
69	C	68.76643	71.21405	72.40237	529.53781	-159.34528	563.72604	1
70	H	69.87912	71.33619	72.32588	654.59388	2347.94251	1217.51488	1
71	H	68.56648	70.10855	72.35932	-1526.55661	2103.42026	817.87394	1
72	O	68.13113	71.85884	71.26822	-554.84278	14.12789	399.58769	1
73	H	67.19846	71.64476	71.47025	1297.06236	2061.84854	1220.68812	1
74	C	68.39616	73.26335	74.15707	-662.15484	-412.13544	123.62687	1
75	O	67.66041	74.08537	73.67386	-540.01537	-317.05804	274.91456	1
76	N	69.36112	73.45452	75.08389	-202.76299	-690.00100	-131.49145	1
77	H	69.90918	72.61337	75.27331	-702.62132	-2617.37191	281.70413	1
78	C	70.02269	74.77369	75.17930	-491.73914	576.34187	222.73509	1
79	H	69.77912	75.20263	74.17888	1977.17978	-1823.58850	-434.68928	1
80	C	69.42235	75.56996	76.31653	-649.50797	-328.66843	306.11224	1
81	H	69.76917	75.11411	77.27136	2075.07803	1452.16490	-1004.45904	1
82	C	69.86461	77.02314	76.28766	-615.18735	-489.99689	-70.96352	1
83	H	69.50909	77.58222	77.19567	-1226.32661	-1724.38906	-1716.47170	1
84	H	70.98526	77.12440	76.25067	2381.64273	-969.84735	900.46860	1
85	H	69.45646	77.55953	75.38848	2122.74991	1702.23946	-141.36228	1
86	C	67.90361	75.51307	76.31451	-501.86074	-479.61276	-376.42482	1
87	H	67.45976	76.07086	77.18359	993.79261	-2246.95401	-1177.81305	1
88	H	67.47975	75.95886	75.37306	42.71279	-626.15391	-2651.37258	1
89	H	67.53393	74.45270	76.36523	-2026.39012	-1590.33709	-887.82922	1
90	C	71.60733	74.36446	75.36152	-672.89153	382.57394	-156.34072	1
91	O	72.09678	73.54206	74.62178	410.04627	221.86223	500.35950	1
92	N	72.21413	75.02478	76.33629	-378.11782	-443.79414	-441.10984	1
93	H	71.72533	75.73586	76.87647	2404.15973	-568.14894	1149.30085	1
94	C	73.63155	74.80287	76.45565	-544.54484	466.16019	331.29119	1
95	H	73.69167	73.69179	76.46403	-1409.80988	-170.17955	2325.32679	1
96	C	74.31679	75.40434	75.13660	-184.48284	116.78282	-758.89137	1
97	H	73.88103	74.91656	74.22941	1893.78641	1861.14652	611.04528	1
98	H	74.10621	76.49584	75.03793	-2170.79665	-974.19311	1327.50117	1
99	C	75.78919	75.13564	75.27687	389.51668	672.81878	-138.49152	1
100	H	76.17439	75.62723	76.19966	510.64577	1933.03327	1851.02484	1
101	H	75.95446	74.05290	75.47393	-2302.30869	-1105.72939	-948.89774	1
102	C	76.65396	75.55754	74.10712	-559.93427	-126.34590	542.30857	1
103	O	77.84615	75.45724	74.31656	-670.36003	-111.83166	76.36448	1
104	N	76.06634	75.97937	72.92416	-216.06729	-537.07037	446.51379	1
105	H	75.07696	75.83597	72.69937	-1251.96487	1074.12894	-2168.52500	1
106	H	76.54943	75.89020	72.02391	-2451.83023	-720.73851	944.84612	1
107	C	74.17012	75.52022	77.79190	546.24052	-563.88337	-85.11809	1
108	O	74.74793	76.59306	77.69872	71.70702	-307.40463	606.69673	1
109	N	73.92506	74.80603	78.88956	479.90863	-504.50129	222.86849	1
110	C	74.14610	75.36722	80.18917	75.51268	-600.91904	506.73700	1

111	H	74.12174	76.47202	80.04612	-2033.61562	1795.30103	254.89480	1
112	C	72.93128	74.75535	81.00551	523.79067	517.99274	284.45581	1
113	H	73.10167	74.77313	82.10561	1599.61665	-1127.00911	1895.98173	1
114	H	71.98928	75.31711	80.81581	-1881.83093	1275.82488	-1501.55016	1
115	C	72.85422	73.31129	80.41585	-600.05639	-404.05026	316.64485	1
116	H	73.64132	72.65863	80.85464	-2597.05260	496.36221	657.73249	1
117	H	71.88140	72.80419	80.60734	-1666.24518	1294.38985	-1723.90591	1
118	C	73.11616	73.58840	78.87659	493.57570	-129.95376	-602.56394	1
119	H	73.68880	72.79332	78.34530	-1469.08415	-637.84797	2204.22581	1
120	H	72.20427	73.83819	78.28506	-1038.97840	1068.88701	-2280.71789	1
121	C	75.53906	74.86611	80.88541	188.88100	241.05089	-727.87821	1
122	O	75.62210	74.87039	82.09202	531.88613	-49.19943	427.07960	1
123	N	76.54459	74.60785	80.01242	708.14833	26.93417	-179.73509	1
124	H	76.12309	74.61110	79.08315	-2232.69501	-1179.09831	1023.94816	1
125	C	77.62307	73.71248	80.44832	-738.32412	259.92548	104.42456	1
126	H	77.36930	73.51299	81.51728	2028.89123	1260.02983	1311.33324	1
127	C	77.62923	72.48023	79.57361	-258.65678	-345.52513	661.28459	1
128	H	77.68592	72.81012	78.51188	-1826.06090	-1801.46097	-918.64554	1
129	C	78.83429	71.59925	79.85598	-541.23400	531.92970	-218.41428	1
130	H	78.84191	70.68061	79.20788	1311.73218	-2219.18200	882.19023	1
131	H	79.79878	72.14460	79.66921	-1048.71298	1223.58118	-2196.97971	1
132	H	78.85417	71.25580	80.92651	419.06414	1903.92898	1903.44670	1
133	C	76.35621	71.66698	79.73400	-423.86431	152.66566	-648.55262	1
134	H	76.33193	70.78775	79.03326	105.68386	-2342.50080	1387.51238	1
135	H	76.25499	71.26323	80.77885	-1695.63603	-1484.73621	-1531.02793	1
136	H	75.44263	72.28864	79.52915	-1853.57121	-487.39031	1936.59343	1
137	C	79.09460	74.48482	80.30210	539.71428	-510.58232	267.58633	1
138	O	79.90596	74.34249	81.18784	-15.93758	-278.34085	-624.49402	1
139	N	79.26509	75.05064	79.11226	-676.81886	12.05292	276.17960	1
140	H	78.40381	75.02164	78.56834	-1694.44250	-373.84189	-2100.66098	1
141	C	80.27486	76.01913	78.86113	412.33078	-664.70360	108.35451	1
142	H	79.95765	76.47104	77.89720	1765.77476	1294.44366	1621.76594	1
143	C	80.22564	77.05264	80.05911	-179.66635	-721.95667	-264.73915	1
144	H	79.18520	77.42312	80.20531	-607.34922	2587.87032	-598.10018	1
145	H	80.49693	76.54398	81.01395	-359.69332	-1479.13954	-2259.74260	1
146	C	81.19811	78.24280	79.76738	-240.01076	616.02425	431.85322	1
147	H	82.24134	77.87390	79.61143	-1359.17131	782.54425	2227.99181	1
148	H	80.91412	78.76324	78.82109	-820.36667	85.81767	-2596.78715	1
149	C	81.15006	79.23821	80.99545	-513.07015	236.18570	-551.87280	1
150	H	80.12906	79.66451	81.12511	1816.11944	-1183.11722	-1650.94321	1
151	H	81.38084	78.70816	81.94807	-1800.04429	-1361.53473	1526.34643	1
152	C	82.18990	80.34883	80.71807	726.08972	-253.19732	-179.64713	1
153	H	83.23846	79.99355	80.66451	1224.27271	-456.51798	-2390.90304	1
154	H	81.96240	80.98594	79.84032	1206.40339	-1150.93514	-2154.90344	1
155	N	82.17507	81.33070	81.93775	329.70796	-633.68968	-155.67358	1
156	H	82.86325	82.13618	81.88308	1348.31305	1938.76845	1359.00643	1
157	H	81.26808	81.84471	82.13708	2096.92035	1446.54551	-966.48890	1
158	H	82.41051	80.92188	82.88866	-1197.07217	-2303.53719	827.28733	1
159	C	81.78264	75.38662	78.76940	-378.01186	-556.17301	-413.96481	1
160	O	82.70366	76.12622	78.49260	-409.44433	-307.55053	-453.30833	1
161	N	81.83683	74.07846	78.99515	-429.02477	524.70884	274.08502	1
162	H	80.95176	73.65790	79.27217	1706.34263	-1425.96036	1574.38926	1
163	C	83.12716	73.50259	79.26962	-45.25864	-626.22952	478.93267	1
164	H	83.64500	74.24587	79.91558	1988.63164	570.90773	1772.87287	1
165	C	82.87370	72.09907	79.93482	551.77128	-20.49526	-564.54996	1
166	H	82.30644	72.19647	80.88853	1434.61535	-1753.10253	1513.99471	1
167	H	82.24206	71.46802	79.26917	-714.67738	1819.09770	1898.36494	1
168	C	84.27434	71.43378	80.16721	446.99263	-555.77305	338.97221	1
169	H	84.88196	71.48069	79.23566	1953.68466	1892.25957	-161.67766	1
170	H	84.85915	71.98103	80.93964	-403.03785	2688.07032	-188.43591	1
171	C	84.03258	69.93050	80.59062	567.86262	335.74681	434.04421	1
172	H	83.52388	69.87242	81.58034	-1080.02275	1568.26081	-1948.78900	1

173	H	83.35077	69.42385	79.86947	-919.54108	2111.34692	1456.13463	1
174	C	85.40380	69.21558	80.62763	195.81897	173.33862	-745.11536	1
175	H	85.93110	69.17869	79.65337	1405.67949	-2301.21089	-390.08113	1
176	H	86.09373	69.57563	81.41658	-940.37328	-1118.32446	2299.72133	1
177	N	85.13793	67.71381	80.98316	319.26422	656.36007	-42.02424	1
178	H	85.99863	67.09526	81.02438	1961.03633	619.91968	1787.09422	1
179	H	84.68989	67.50988	81.92358	854.14343	-2156.80752	1429.08711	1
180	H	84.51855	67.16251	80.32030	1237.02905	-1378.50857	-1998.28500	1
181	C	83.90079	73.26330	77.84595	532.53319	-268.57236	517.55729	1
182	O	83.51041	72.43035	77.03247	266.16714	-290.73804	-558.88002	1
183	N	84.97948	74.01009	77.83846	-226.25352	640.49678	-270.32839	1
184	H	85.07999	74.64083	78.63377	2007.69063	-1035.27229	1523.50231	1
185	C	85.95837	74.03550	76.81767	-540.76542	-573.33303	49.50000	1
186	H	86.76857	74.66261	77.25215	-2374.20950	-1036.76023	843.75774	1
187	C	86.42353	72.53946	76.47689	-77.09082	666.87422	-415.84136	1
188	H	85.52131	71.93549	76.17447	-985.81834	617.19825	2463.91927	1
189	O	87.04821	71.80684	77.54270	293.29899	-391.65602	-477.80926	1
190	H	86.43560	71.04739	77.63188	2528.72714	-681.76262	-751.27122	1
191	C	87.30096	72.82890	75.20415	252.47363	-605.14473	440.05134	1
192	H	87.60026	71.88897	74.68495	-2052.65063	1456.49051	-1043.51830	1
193	H	86.74773	73.46389	74.46406	-2152.98800	-1661.97574	-161.70652	1
194	H	88.23673	73.37355	75.47035	-473.12726	-1584.27339	2165.61725	1
195	C	85.36129	74.69470	75.43566	360.36307	488.46713	505.10056	1
196	O	85.98894	75.57589	74.89859	-200.08817	-528.03552	-385.82850	1
197	N	84.27849	74.05970	75.00032	-597.54095	-226.44775	355.20479	1
198	H	83.83157	73.29639	75.56800	2179.23655	-1300.70981	-991.33835	1
199	C	83.61621	74.62533	73.88761	-687.68921	297.39807	-249.45179	1
200	H	84.20726	75.51152	73.55445	-349.16256	-2467.37713	-1101.72831	1
201	C	83.45551	73.47623	72.77404	672.47345	361.54328	-201.62880	1
202	H	83.03019	72.55308	73.22920	1541.41502	582.18425	2169.97026	1
203	H	82.73911	73.81883	71.99176	-2534.67717	60.25153	997.72295	1
204	C	84.82785	73.19646	72.15306	574.26774	-389.43119	-377.02542	1
205	C	85.36930	74.11971	71.20730	688.82679	-287.33580	-257.96133	1
206	H	84.81621	75.03623	70.92995	331.14182	1470.38163	2269.80013	1
207	C	85.55639	72.02411	72.52032	-383.52382	-675.04808	144.24917	1
208	H	85.14766	71.31831	73.26566	4.09847	1517.59662	2262.86397	1
209	C	86.60841	73.83643	70.63560	-134.76730	428.45285	-649.50303	1
210	H	87.02461	74.54716	69.89989	-903.23433	1600.49020	2011.53387	1
211	C	86.79165	71.78333	71.91491	-335.53281	-615.00040	-364.39058	1
212	H	87.34162	70.86831	72.19623	1596.45398	-1369.33862	1732.02659	1
213	C	87.36123	72.66813	70.95285	585.48547	-340.24194	-406.23938	1
214	O	88.61306	72.42999	70.32870	-419.15649	-173.04408	-511.94141	1
215	H	88.84050	71.56155	70.73757	-1071.84350	1559.71507	-1960.13012	1
216	C	82.07118	74.92754	74.33446	291.41878	-183.13091	710.72246	1
217	O	81.48180	74.24895	75.14421	379.87695	523.47396	-222.23622	1
218	N	81.59448	75.90789	73.57329	564.30591	373.09380	277.24371	1
219	H	82.19442	76.38543	72.90207	-120.59931	-2436.07824	-1214.35098	1
220	C	80.25739	76.34328	73.84392	404.07514	-299.37480	608.84009	1
221	H	79.79581	75.37126	74.18891	-1071.07882	-841.69025	2359.66467	1
222	C	80.35280	77.37492	75.04534	-683.12807	68.71770	-390.13096	1
223	H	81.14712	77.06097	75.76039	2068.88918	1596.58590	770.89603	1
224	H	80.65761	78.38518	74.69137	1379.86429	2342.49779	-179.85638	1
225	C	78.96060	77.40514	75.75069	-176.39967	537.49466	550.97268	1
226	H	78.13787	77.60427	75.02662	-396.28051	1942.22168	1869.33314	1
227	H	78.72454	76.41168	76.19747	-94.44700	586.00678	-2659.20016	1
228	C	79.02144	78.54930	76.86526	-291.69381	-718.18079	-150.72929	1
229	H	79.86855	78.48675	77.59924	-2303.38776	1089.76242	964.62032	1
230	H	78.98608	79.59798	76.47417	884.16729	2568.80533	-207.74283	1
231	N	77.83458	78.30109	77.56808	-594.49522	-252.81478	342.29276	1
232	H	77.20247	77.62298	77.17049	-1735.17426	2084.05705	-263.71605	1
233	C	77.50121	78.87252	78.65728	595.23177	-271.52487	442.22352	1
234	N	78.37377	79.82511	79.20271	585.53813	-424.79750	-105.81303	1

235	H	79.26103	80.16810	78.83881	959.88797	1327.56823	-2177.11905	1
236	H	78.19963	80.36121	80.05250	1578.48647	16.27378	-2220.76233	1
237	N	76.26486	78.40482	79.10455	-452.17763	-390.33541	-421.51853	1
238	H	75.64223	77.69162	78.64530	470.26107	1974.25629	-1817.92087	1
239	H	75.82850	78.74651	79.96721	1856.67307	-1573.97321	-1224.35416	1
240	C	79.64946	76.88867	72.43129	-531.47271	-581.45780	-55.06206	1
241	O	79.65177	76.19475	71.44369	-243.00837	192.73507	609.52485	1
242	N	79.22687	78.19584	72.50229	343.49288	-644.25607	38.09164	1
243	H	79.19505	78.37363	73.50773	-1691.16043	-1535.97525	-1484.73099	1
244	C	78.06317	78.57310	71.65606	542.66492	350.14337	454.42563	1
245	H	77.32099	77.75906	71.81704	1209.57979	-2396.95920	463.86744	1
246	C	77.56989	79.92325	72.11569	-737.14309	145.93010	242.71942	1
247	H	78.45171	80.59760	72.20105	-1050.18303	159.36419	-2509.06125	1
248	C	76.60789	80.53274	71.11019	-706.77696	-252.88343	-245.16230	1
249	H	76.31359	81.58062	71.39292	-1624.64039	-1665.49085	1417.86935	1
250	H	77.06234	80.57379	70.07905	2566.10521	598.51109	693.22305	1
251	H	75.66250	79.92994	71.02607	-1972.69758	107.10018	-1876.34312	1
252	C	76.90333	79.85539	73.47913	412.85148	672.58832	-27.69222	1
253	H	76.49737	80.85570	73.79360	1447.02277	1762.76533	-1490.78944	1
254	H	76.04277	79.13091	73.48082	1320.77379	-145.20455	2378.68491	1
255	H	77.61738	79.52138	74.27983	-1512.10848	1470.52031	1724.75147	1
256	C	78.58297	78.63963	70.10121	-607.11113	499.56689	73.73769	1
257	O	77.77270	78.58667	69.20086	357.97126	460.81534	356.68785	1
258	N	79.88632	78.90277	70.01409	536.55407	-368.62270	332.76306	1
259	H	80.39901	78.87962	70.89663	524.38866	2297.69985	1367.20941	1
260	C	80.52635	78.53703	68.79578	46.50277	-774.29190	-147.97904	1
261	H	79.74915	77.97857	68.22630	1676.51875	1883.29066	1032.55549	1
262	C	81.01112	79.88043	68.04472	-559.41456	-34.19198	-556.30433	1
263	H	81.82907	80.35266	68.63936	-64.66664	395.18769	2695.05373	1
264	H	81.46021	79.62978	67.05411	-2703.44278	-60.40056	333.79418	1
265	C	79.86090	80.84080	67.89183	-519.76435	377.31045	459.42366	1
266	H	79.39514	80.98610	68.89341	-1746.74323	1667.50644	-1261.73691	1
267	C	80.35941	82.19117	67.39186	570.95554	16.46261	-545.27700	1
268	H	79.52272	82.92981	67.29266	2391.58273	28.05277	-1305.07271	1
269	H	81.11487	82.63664	68.08926	175.75588	917.63458	2559.43867	1
270	H	80.84625	82.10444	66.38666	-1063.97851	-2155.34650	1283.00462	1
271	C	78.79791	80.30005	66.94759	193.76014	2.62946	-765.53141	1
272	H	78.02249	81.07403	66.71123	507.39394	-846.55087	2539.60089	1
273	H	79.23671	79.96117	65.97362	1337.57841	1818.19054	1526.01994	1
274	H	78.25672	79.41947	67.41004	1100.88635	-1172.91350	-2199.08909	1
275	C	81.84955	77.70133	69.18582	-549.21115	475.64486	-309.38218	1
276	O	82.47732	77.89247	70.19468	556.06106	-390.37755	-78.24250	1
277	O	82.34668	76.83877	68.18037	-572.27940	-310.19032	-209.75862	1
278	H	81.60410	76.92425	67.52080	-1380.08193	2212.14486	790.85944	1

Listing 122: C00122.xmolout

1		276								
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.6442	2577	
		0.2500	300.00	0.00	0.00	0.00	-1293.3647	0.0000	300.0000	
3	H	61.30083	77.04047	67.81352	-2043.14101	-1757.64893	399.89339		1	
4	N	61.22278	77.75775	67.09405	426.75047	490.45733	-334.42467		1	
5	H	60.44387	78.33244	67.42896	442.25559	-1110.30854	-2448.52907		1	
6	C	62.39217	78.52976	66.91454	415.32972	-666.39213	83.73172		1	
7	H	63.25829	77.90794	67.23176	879.32219	2491.00447	667.35213		1	
8	C	62.46676	78.96842	65.36111	31.35357	477.41777	628.23362		1	
9	H	61.57051	79.58627	65.11522	1168.38489	2240.25337	-1019.71136		1	
10	H	63.35239	79.62334	65.18041	-360.43770	2534.90498	931.67112		1	
11	C	62.51278	77.74219	64.49006	463.18208	512.70242	-382.34388		1	
12	H	61.71364	77.04595	64.83251	1725.29117	1863.52247	-987.07854		1	
13	C	62.24358	78.10984	63.03585	710.42801	-144.27427	-313.15367		1	
14	H	62.24947	77.20649	62.37292	364.20195	-1033.13725	2494.72524		1	

15	H	61.24695	78.60671	62.91146	2567.61904	335.80679	847.48802	1
16	H	63.01778	78.81609	62.63937	-2587.99029	680.92867	-512.16411	1
17	C	63.85693	77.03376	64.59199	268.17616	741.64379	-40.42634	1
18	H	63.89486	76.12537	63.93680	1283.54314	-1945.37420	-1411.27812	1
19	H	64.69997	77.70244	64.27943	-1258.57796	1317.15249	-2026.02085	1
20	H	64.07040	76.69631	65.63859	-2502.84526	909.80597	575.92391	1
21	C	62.14612	79.85292	67.81884	619.36578	-458.64843	-172.09273	1
22	O	61.00040	80.19918	68.14803	-81.40433	433.87611	522.34594	1
23	N	63.28817	80.47416	67.97225	175.23996	-622.20190	341.55523	1
24	H	64.06588	79.99633	67.51730	-876.57256	-303.22879	-2561.90213	1
25	C	63.58777	81.38621	69.03506	-571.88214	-534.10783	-106.15033	1
26	H	64.18169	82.18758	68.54752	-2713.20841	-16.25800	-248.80809	1
27	C	62.26768	81.90824	69.75169	166.60354	288.16399	-716.09568	1
28	H	61.73078	80.99777	70.14789	-2097.85574	1636.78449	-586.18044	1
29	O	61.32881	82.58048	68.91514	-317.80580	-363.38227	484.43082	1
30	H	60.81288	81.75521	68.56227	1863.74748	-1451.84923	1357.29467	1
31	C	62.85632	82.73902	70.95099	503.80731	517.99032	318.51606	1
32	H	62.05008	83.09843	71.63185	640.61020	-2157.10410	-1536.29104	1
33	H	63.57059	82.13965	71.56876	1687.88455	465.60692	2087.56452	1
34	H	63.40899	83.63842	70.59217	-1293.07895	-1899.88581	-1463.57452	1
35	C	64.46045	80.53476	70.12289	-153.07550	-733.68902	248.70981	1
36	O	63.94780	79.62636	70.72165	186.15459	-480.78787	-449.34387	1
37	N	65.71377	81.01201	70.21115	-487.53139	543.18517	42.03850	1
38	C	66.56027	80.68393	71.31265	-699.35871	69.34393	360.10701	1
39	H	66.07903	79.80257	71.79900	2.81126	-221.99807	-2715.58072	1
40	C	67.91101	80.39504	70.51720	-507.46439	-592.59194	122.07761	1
41	H	68.81235	80.32789	71.16641	-1975.08116	525.87560	-1801.71556	1
42	H	67.85331	79.43507	69.95840	1588.27743	-1913.22100	1113.83566	1
43	C	67.92144	81.61302	69.54481	-613.62442	-457.55993	-194.14490	1
44	H	68.23664	82.54212	70.07081	1707.54637	-721.27992	1996.92523	1
45	H	68.61455	81.48804	68.68341	758.23357	2100.81767	1560.55011	1
46	C	66.39333	81.68680	69.11270	-352.41524	704.96076	49.21465	1
47	H	65.98586	82.72292	69.04524	1714.76886	-2070.42778	443.35792	1
48	H	66.13176	81.12130	68.18775	1224.15040	1801.50881	1636.97633	1
49	C	66.61818	82.00093	72.28895	566.85117	537.05831	117.62814	1
50	O	65.57083	82.60342	72.53275	-550.26779	-406.08867	4.21666	1
51	N	67.82712	82.21444	72.71456	566.34832	-425.77725	180.18749	1
52	H	68.52623	81.57279	72.34693	644.44502	2646.80550	-52.73430	1
53	C	68.25068	83.15549	73.70363	612.34801	-281.48662	411.56221	1
54	H	68.98916	83.81075	73.19274	1667.23498	-1490.75142	1556.16753	1
55	C	67.01768	83.96222	74.29136	-714.45746	-175.43074	286.98927	1
56	H	66.24750	83.20863	74.62420	-787.09484	1763.03619	-1922.46060	1
57	O	66.35108	84.83013	73.37188	-429.46514	516.51932	-128.40526	1
58	H	65.67176	84.15796	72.98532	1981.82785	436.16847	-1818.18182	1
59	C	67.65219	84.67057	75.54339	630.79189	-468.94448	76.03230	1
60	H	66.90115	85.29818	76.07759	-1775.71861	2062.30353	131.89849	1
61	H	68.05778	83.93266	76.29037	-1855.14608	88.94118	1993.53760	1
62	H	68.49065	85.34413	75.24908	-1504.82350	-780.94249	-2132.90992	1
63	C	68.98966	82.21090	74.82815	288.57638	618.62814	-397.00270	1
64	O	68.46666	81.20433	75.24118	321.70495	-185.26452	574.37218	1
65	N	70.18394	82.73141	75.10424	-447.05792	-446.53431	367.76425	1
66	H	70.41894	83.58381	74.59405	350.31316	1975.63644	-1843.31522	1
67	C	70.85214	82.50665	76.34340	-511.23061	374.03917	-471.51480	1
68	H	71.85932	82.91095	76.09741	2234.79579	-898.70890	-1273.45190	1
69	C	70.16976	83.38423	77.49064	529.53781	-159.34528	563.72604	1
70	H	70.86220	83.34267	78.37284	654.59388	2347.94251	1217.51488	1
71	H	70.13370	84.45467	77.15969	-1526.55661	2103.42026	817.87394	1
72	O	68.82639	82.98349	77.92466	-554.84278	14.12789	399.58769	1
73	H	69.03206	82.07424	78.21874	1297.06236	2061.84854	1220.68812	1
74	C	70.89187	80.93852	76.76800	-662.15484	-412.13544	123.62687	1
75	O	70.74613	80.59949	77.91788	-540.01537	-317.05804	274.91456	1
76	N	71.30901	80.17454	75.73151	-202.76299	-690.00100	-131.49145	1

77	H	71.26721	80.72718	74.87431	-702.62132	-2617.37191	281.70413	1
78	C	71.07840	78.71952	75.76288	-491.73914	576.34187	222.73509	1
79	H	70.14745	78.58288	76.36044	1977.17978	-1823.58850	-434.68928	1
80	C	70.98410	78.24551	74.33085	-649.50797	-328.66843	306.11224	1
81	H	71.86377	78.65287	73.78324	2075.07803	1452.16490	-1004.45904	1
82	C	71.03126	76.73017	74.24134	-615.18735	-489.99689	-70.96352	1
83	H	71.02396	76.37461	73.17460	-1226.32661	-1724.38906	-1716.47170	1
84	H	71.95925	76.31712	74.72627	2381.64273	-969.84735	900.46860	1
85	H	70.15114	76.25691	74.75711	2122.74991	1702.23946	-141.36228	1
86	C	69.72860	78.76227	73.65003	-501.86074	-479.61276	-376.42482	1
87	H	69.72869	78.54191	72.54735	993.79261	-2246.95401	-1177.81305	1
88	H	68.80278	78.29394	74.08328	42.71279	-626.15391	-2651.37258	1
89	H	69.61431	79.87612	73.77585	-2026.39012	-1590.33709	-887.82922	1
90	C	72.41652	78.07664	76.49574	-672.89153	382.57394	-156.34072	1
91	O	73.53857	78.27844	76.07571	410.04627	221.86223	500.35950	1
92	N	72.04897	77.28234	77.48195	-378.11782	-443.79414	-441.10984	1
93	H	71.05510	77.19308	77.67993	2404.15973	-568.14894	1149.30085	1
94	C	73.06740	76.85409	78.39405	-544.54484	466.16019	331.29119	1
95	H	73.88989	77.58597	78.22597	-1409.80988	-170.17955	2325.32679	1
96	C	72.42291	76.87558	79.84356	-184.48284	116.78282	-758.89137	1
97	H	71.98981	77.87648	80.06887	1893.78641	1861.14652	611.04528	1
98	H	71.57656	76.15439	79.90627	-2170.79665	-974.19311	1327.50117	1
99	C	73.54965	76.49929	80.85469	389.51668	672.81878	-138.49152	1
100	H	74.06215	75.56743	80.53024	510.64577	1933.03327	1851.02484	1
101	H	74.35133	77.27035	80.83757	-2302.30869	-1105.72939	-948.89774	1
102	C	73.01015	76.31462	82.32638	-559.93427	-126.34590	542.30857	1
103	O	73.68698	75.73990	83.13919	-670.36003	-111.83166	76.36448	1
104	N	71.80222	76.87799	82.54193	-216.06729	-537.07037	446.51379	1
105	H	71.21116	77.41940	81.90030	-1251.96487	1074.12894	-2168.52500	1
106	H	71.33751	76.90706	83.45597	-2451.83023	-720.73851	944.84612	1
107	C	73.46429	75.32059	78.01631	546.24052	-563.88337	-85.11809	1
108	O	72.71365	74.40165	78.31943	71.70702	-307.40463	606.69673	1
109	N	74.65168	75.26633	77.42298	479.90863	-504.50129	222.86849	1
110	C	75.07162	74.11587	76.66485	75.51268	-600.91904	506.73700	1
111	H	74.14681	73.75357	76.15894	-2033.61562	1795.30103	254.89480	1
112	C	76.19253	74.71460	75.71450	523.79067	517.99274	284.45581	1
113	H	76.91454	73.94378	75.36240	1599.61665	-1127.00911	1895.98173	1
114	H	75.75223	75.18198	74.80557	-1881.83093	1275.82488	-1501.55016	1
115	C	76.84226	75.78580	76.64569	-600.05639	-404.05026	316.64485	1
116	H	77.52005	75.30816	77.39195	-2597.05260	496.36221	657.73249	1
117	H	77.45203	76.54373	76.10368	-1666.24518	1294.38985	-1723.90591	1
118	C	75.56008	76.40325	77.34851	493.57570	-129.95376	-602.56394	1
119	H	75.72854	76.78870	78.38273	-1469.08415	-637.84797	2204.22581	1
120	H	75.00323	77.18140	76.73552	-1038.97840	1068.88701	-2280.71789	1
121	C	75.69598	72.99952	77.67048	188.88100	241.05089	-727.87821	1
122	O	76.83622	72.64857	77.56781	531.88613	-49.19943	427.07960	1
123	N	74.72339	72.51915	78.46819	708.14833	26.93417	-179.73509	1
124	H	73.79825	73.01421	78.43812	-2232.69501	-1179.09831	1023.94816	1
125	C	75.12115	71.77671	79.68472	-738.32412	259.92548	104.42456	1
126	H	75.94488	72.38367	80.12727	2028.89123	1260.02983	1311.33324	1
127	C	73.91961	71.62829	80.59017	-258.65678	-345.52513	661.28459	1
128	H	73.10488	71.15462	79.99628	-1826.06090	-1801.46097	-918.64554	1
129	C	74.22629	70.72516	81.77281	-541.23400	531.92970	-218.41428	1
130	H	73.32354	70.56664	82.42417	1311.73218	-2219.18200	882.19023	1
131	H	74.58207	69.71051	81.43594	-1048.71298	1223.58118	-2196.97971	1
132	H	75.03569	71.15751	82.42269	419.06414	1903.92898	1903.44670	1
133	C	73.39702	72.96076	81.09587	-423.86431	152.66566	-648.55262	1
134	H	72.50566	72.83082	81.76940	105.68386	-2342.50080	1387.51238	1
135	H	74.17611	73.51754	81.68694	-1695.63603	-1484.73621	-1531.02793	1
136	H	73.07768	73.63029	80.24265	-1853.57121	-487.39031	1936.59343	1
137	C	75.65175	70.29102	79.20897	539.71428	-510.58232	267.58633	1
138	O	76.32446	69.62270	79.95784	-15.93758	-278.34085	-624.49402	1

139	N	75.13973	69.92257	78.03253	-676.81886	12.05292	276.17960	1
140	H	74.60434	70.63967	77.54374	-1694.44250	-373.84189	-2100.66098	1
141	C	75.91095	68.95088	77.31040	412.33078	-664.70360	108.35451	1
142	H	76.89430	68.89858	77.83754	1765.77476	1294.44366	1621.76594	1
143	C	75.10230	67.59886	77.42902	-179.66635	-721.95667	-264.73915	1
144	H	74.82471	67.41487	78.49150	-607.34922	2587.87032	-598.10018	1
145	H	74.14043	67.65764	76.87174	-359.69332	-1479.13954	-2259.74260	1
146	C	76.00793	66.44544	76.88253	-240.01076	616.02425	431.85322	1
147	H	76.15322	66.53939	75.78257	-1359.17131	782.54425	2227.99181	1
148	H	77.02548	66.49285	77.33126	-820.36667	85.81767	-2596.78715	1
149	C	75.29768	65.08276	77.25777	-513.07015	236.18570	-551.87280	1
150	H	75.16562	64.99996	78.36121	1816.11944	-1183.11722	-1650.94321	1
151	H	74.27103	65.03987	76.82702	-1800.04429	-1361.53473	1526.34643	1
152	C	76.16295	63.91671	76.72682	726.08972	-253.19732	-179.64713	1
153	H	76.21510	63.84536	75.62210	1224.27271	-456.51798	-2390.90304	1
154	H	77.18256	63.86334	77.15794	1206.40339	-1150.93514	-2154.90344	1
155	N	75.47409	62.58556	77.18275	329.70796	-633.68968	-155.67358	1
156	H	75.95516	61.69100	76.87728	1348.31305	1938.76845	1359.00643	1
157	H	75.38111	62.42449	78.22787	2096.92035	1446.54551	-966.48890	1
158	H	74.48223	62.41426	76.84598	-1197.07217	-2303.53719	827.28733	1
159	C	75.96952	69.45063	75.75135	-378.01186	-556.17301	-413.96481	1
160	O	75.00280	69.87326	75.16259	-409.44433	-307.55053	-453.30833	1
161	N	77.19430	69.23216	75.29174	-429.02477	524.70884	274.08502	1
162	H	77.91016	68.83450	75.89705	1706.34263	-1425.96036	1574.38926	1
163	C	77.50689	69.65160	73.95591	-45.25864	-626.22952	478.93267	1
164	H	76.63332	69.24216	73.40030	1988.63164	570.90773	1772.87287	1
165	C	77.50011	71.23370	73.91707	551.77128	-20.49526	-564.54996	1
166	H	76.70436	71.63963	74.58231	1434.61535	-1753.10253	1513.99471	1
167	H	78.45863	71.63814	74.31345	-714.67738	1819.09770	1898.36494	1
168	C	77.26776	71.67692	72.43394	446.99263	-555.77305	338.97221	1
169	H	77.88564	71.06512	71.73612	1953.68466	1892.25957	-161.67766	1
170	H	76.21140	71.50501	72.12849	-403.03785	2688.07032	-188.43591	1
171	C	77.65534	73.20514	72.31096	567.86262	335.74681	434.04421	1
172	H	76.94840	73.84478	72.88758	-1080.02275	1568.26081	-1948.78900	1
173	H	78.66298	73.39518	72.74733	-919.54108	2111.34692	1456.13463	1
174	C	77.64115	73.57003	70.80819	195.81897	173.33862	-745.11536	1
175	H	78.41217	73.05309	70.20237	1405.67949	-2301.21089	-390.08113	1
176	H	76.65139	73.47753	70.31844	-940.37328	-1118.32446	2299.72133	1
177	N	78.00232	75.08931	70.68732	319.26422	656.36007	-42.02424	1
178	H	78.04999	75.47291	69.69937	1961.03633	619.91968	1787.09422	1
179	H	77.34285	75.78222	71.14747	854.14343	-2156.80752	1429.08711	1
180	H	78.94377	75.39247	71.07256	1237.02905	-1378.50857	-1998.28500	1
181	C	78.93351	68.95643	73.59517	532.53319	-268.57236	517.55729	1
182	O	79.21597	67.85518	74.00990	266.16714	-290.73804	-558.88002	1
183	N	79.65769	69.74739	72.80612	-226.25352	640.49678	-270.32839	1
184	H	79.32410	70.67596	72.54994	2007.69063	-1035.27229	1523.50231	1
185	C	80.86753	69.25266	72.26932	-540.76542	-573.33303	49.50000	1
186	H	81.00191	68.22261	72.67619	-2374.20950	-1036.76023	843.75774	1
187	C	80.74584	69.33512	70.67095	-77.09082	666.87422	-415.84136	1
188	H	80.68536	70.41966	70.37921	-985.81834	617.19825	2463.91927	1
189	O	79.59653	68.70292	70.08498	293.29899	-391.65602	-477.80926	1
190	H	79.14146	69.47114	69.68359	2528.72714	-681.76262	-751.27122	1
191	C	82.13594	68.74685	70.23038	252.47363	-605.14473	440.05134	1
192	H	82.28622	68.83153	69.12936	-2052.65063	1456.49051	-1043.51830	1
193	H	82.98767	69.27327	70.72095	-2152.98800	-1661.97574	-161.70652	1
194	H	82.21994	67.66684	70.49256	-473.12726	-1584.27339	2165.61725	1
195	C	82.02591	70.35203	72.68275	360.36307	488.46713	505.10056	1
196	O	81.84146	71.54159	72.56184	-200.08817	-528.03552	-385.82850	1
197	N	83.12498	69.68216	72.98573	-597.54095	-226.44775	355.20479	1
198	H	83.06749	68.66431	72.98977	2179.23655	-1300.70981	-991.33835	1
199	C	84.27232	70.31970	73.51822	-687.68921	297.39807	-249.45179	1
200	H	85.04489	69.52315	73.45137	-349.16256	-2467.37713	-1101.72831	1

201	C	84.62775	71.62569	72.66802	672.47345	361.54328	-201.62880	1
202	H	83.77002	72.34701	72.67677	1541.41502	582.18425	2169.97026	1
203	H	85.50522	72.14350	73.12016	-2534.67717	60.25153	997.72295	1
204	C	84.92600	71.20265	71.22200	574.26774	-389.43119	-377.02542	1
205	C	86.18606	70.64133	70.85839	688.82679	-287.33580	-257.96133	1
206	H	86.98734	70.51241	71.60859	331.14182	1470.38163	2269.80013	1
207	C	83.89079	71.36454	70.25327	-383.52382	-675.04808	144.24917	1
208	H	82.90841	71.78045	70.55388	4.09847	1517.59662	2262.86397	1
209	C	86.37834	70.25756	69.53150	-134.76730	428.45285	-649.50303	1
210	H	87.35194	69.82418	69.24342	-903.23433	1600.49020	2011.53387	1
211	C	84.13358	70.96472	68.93699	-335.53281	-615.00040	-364.39058	1
212	H	83.32641	71.08967	68.19431	1596.45398	-1369.33862	1732.02659	1
213	C	85.37685	70.39990	68.52780	585.48547	-340.24194	-406.23938	1
214	O	85.63451	69.98398	67.19530	-419.15649	-173.04408	-511.94141	1
215	H	84.77877	70.23509	66.77447	-1071.84350	1559.71507	-1960.13012	1
216	C	83.93501	70.66714	75.08417	291.41878	-183.13091	710.72246	1
217	O	84.03140	69.78269	75.90257	379.87695	523.47396	-222.23622	1
218	N	83.50652	71.91876	75.26783	564.30591	373.09380	277.24371	1
219	H	83.45515	72.51279	74.44163	-120.59931	-2436.07824	-1214.35098	1
220	C	83.79267	72.49987	76.55450	404.07514	-299.37480	608.84009	1
221	H	84.76557	72.06673	76.87718	-1071.07882	-841.69025	2359.66467	1
222	C	83.78757	74.06624	76.36574	-683.12807	68.71770	-390.13096	1
223	H	84.60892	74.39969	75.69175	2068.88918	1596.58590	770.89603	1
224	H	82.84376	74.38746	75.86982	1379.86429	2342.49779	-179.85638	1
225	C	83.91229	74.71784	77.78006	-176.39967	537.49466	550.97268	1
226	H	83.25824	74.19619	78.51697	-396.28051	1942.22168	1869.33314	1
227	H	84.94612	74.62877	78.18143	-94.44700	586.00678	-2659.20016	1
228	C	83.46977	76.24239	77.61017	-291.69381	-718.18079	-150.72929	1
229	H	84.11564	76.87116	76.94590	-2303.38776	1089.76242	964.62032	1
230	H	82.40322	76.39456	77.30164	884.16729	2568.80533	-207.74283	1
231	N	83.59183	76.71953	78.92314	-594.49522	-252.81478	342.29276	1
232	H	83.79207	76.03588	79.63566	-1735.17426	2084.05705	-263.71605	1
233	C	83.44955	77.93526	79.26715	595.23177	-271.52487	442.22352	1
234	N	83.17491	78.86726	78.26101	585.53813	-424.79750	-105.81303	1
235	H	83.03926	78.71731	77.26192	959.88797	1327.56823	-2177.11905	1
236	H	83.02164	79.86497	78.41080	1578.48647	16.27378	-2220.76233	1
237	N	83.61241	78.07753	80.65187	-452.17763	-390.33541	-421.51853	1
238	H	83.79484	77.38770	81.37947	470.26107	1974.25629	-1817.92087	1
239	H	83.51976	78.97301	81.13310	1856.67307	-1573.97321	-1224.35416	1
240	C	82.59445	72.11280	77.59589	-531.47271	-581.45780	-55.06206	1
241	O	82.88759	71.95463	78.76634	-243.00837	192.73507	609.52485	1
242	N	81.39282	72.20891	77.03849	343.49288	-644.25607	38.09164	1
243	H	81.43013	72.36566	76.03043	-1691.16043	-1535.97525	-1484.73099	1
244	C	80.25651	71.59301	77.64143	542.66492	350.14337	454.42563	1
245	H	79.43074	71.81056	76.92647	1209.57979	-2396.95920	463.86744	1
246	C	80.55348	70.03479	77.74323	-737.14309	145.93010	242.71942	1
247	H	81.43844	69.84572	78.39020	-1050.18303	159.36419	-2509.06125	1
248	C	79.27168	69.34330	78.31861	-706.77696	-252.88343	-245.16230	1
249	H	79.37049	68.23177	78.33595	-1624.64039	-1665.49085	1417.86935	1
250	H	79.06297	69.68127	79.37002	2566.10521	598.51109	693.22305	1
251	H	78.36605	69.59450	77.71177	-1972.69758	107.10018	-1876.34312	1
252	C	80.81114	69.49455	76.29441	412.85148	672.58832	-27.69222	1
253	H	80.91608	68.38421	76.27562	1447.02277	1762.76533	-1490.78944	1
254	H	79.97808	69.75908	75.60119	1320.77379	-145.20455	2378.68491	1
255	H	81.74977	69.92253	75.86253	-1512.10848	1470.52031	1724.75147	1
256	C	80.01502	72.25652	79.11154	-607.11113	499.56689	73.73769	1
257	O	79.59405	71.60721	80.04818	357.97126	460.81534	356.68785	1
258	N	80.26699	73.55817	79.05884	536.55407	-368.62270	332.76306	1
259	H	80.61880	73.94334	78.18285	524.38866	2297.69985	1367.20941	1
260	C	79.96514	74.36291	80.18198	46.50277	-774.29190	-147.97904	1
261	H	79.35504	73.71259	80.85029	1676.51875	1883.29066	1032.55549	1
262	C	81.34669	74.84731	80.86821	-559.41456	-34.19198	-556.30433	1

263	H	81.88641	75.52254	80.16322	-64.66664	395.18769	2695.05373	1
264	H	81.13393	75.46230	81.77461	-2703.44278	-60.40056	333.79418	1
265	C	82.19278	73.65379	81.21312	-519.76435	377.31045	459.42366	1
266	H	82.35963	73.04022	80.27463	-1746.74323	1667.50644	-1261.73691	1
267	C	83.54947	74.08830	81.75252	570.95554	16.46261	-545.27700	1
268	H	84.18134	73.20581	82.03121	2391.58273	28.05277	-1305.07271	1
269	H	84.12899	74.67911	80.99866	175.75588	917.63458	2559.43867	1
270	H	83.44681	74.72629	82.66762	-1063.97851	-2155.34650	1283.00462	1
271	C	81.50345	72.75445	82.22879	193.76014	2.62946	-765.53141	1
272	H	82.18220	71.93369	82.57828	507.39394	-846.55087	2539.60089	1
273	H	81.17328	73.32333	83.13609	1337.57841	1818.19054	1526.01994	1
274	H	80.59339	72.25947	81.77834	1100.88635	-1172.91350	-2199.08909	1
275	C	79.20946	75.67327	79.61626	-549.21115	475.64486	-309.38218	1
276	O	79.36153	76.09252	78.49806	556.06106	-390.37755	-78.24250	1
277	O	78.41945	76.38227	80.55063	-572.27940	-310.19032	-209.75862	1
278	H	78.54944	75.78959	81.34325	-1380.08193	2212.14486	790.85944	1

Listing 123: C00123.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.2750	1100
		0.2500	300.00	0.00	0.00	0.00	-1293.3643	0.0000	300.0000
3	H	60.13081	71.47686	78.20793	-2043.14101	-1757.64893	399.89339		1
4	N	60.17649	72.38795	78.66443	426.75047	490.45733	-334.42467		1
5	H	60.25831	72.15748	79.66654	442.25559	-1110.30854	-2448.52907		1
6	C	61.25370	73.19089	78.23322	415.32972	-666.39213	83.73172		1
7	H	61.62843	72.78465	77.26839	879.32219	2491.00447	667.35213		1
8	C	60.77171	74.72692	78.13166	31.35357	477.41777	628.23362		1
9	H	60.44642	75.07205	79.14210	1168.38489	2240.25337	-1019.71136		1
10	H	61.62914	75.38152	77.84380	-360.43770	2534.90498	931.67112		1
11	C	59.63826	74.86111	77.14905	463.18208	512.70242	-382.34388		1
12	H	58.83971	74.14119	77.43938	1725.29117	1863.52247	-987.07854		1
13	C	59.06827	76.27344	77.20480	710.42801	-144.27427	-313.15367		1
14	H	58.20624	76.40132	76.50070	364.20195	-1033.13725	2494.72524		1
15	H	58.70045	76.53102	78.23147	2567.61904	335.80679	847.48802		1
16	H	59.83846	77.03872	76.92763	-2587.99029	680.92867	-512.16411		1
17	C	60.08313	74.54529	75.72787	268.17616	741.64379	-40.42634		1
18	H	59.24928	74.68951	74.99299	1283.54314	-1945.37420	-1411.27812		1
19	H	60.92869	75.20528	75.40358	-1258.57796	1317.15249	-2026.02085		1
20	H	60.43115	73.48496	75.62871	-2502.84526	909.80597	575.92391		1
21	C	62.28385	73.07340	79.48372	619.36578	-458.64843	-172.09273		1
22	O	61.91075	72.62404	80.55497	-81.40433	433.87611	522.34594		1
23	N	63.45047	73.61325	79.15768	175.23996	-622.20190	341.55523		1
24	H	63.57449	73.97359	78.21183	-876.57256	-303.22879	-2561.90213		1
25	C	64.50263	73.63774	80.10659	-571.88214	-534.10783	-106.15033		1
26	H	64.04306	73.23029	81.03654	-2713.20841	-16.25800	-248.80809		1
27	C	65.68478	72.72967	79.51228	166.60354	288.16399	-716.09568		1
28	H	65.98158	73.15852	78.51673	-2097.85574	1636.78449	-586.18044		1
29	O	65.34363	71.35389	79.27423	-317.80580	-363.38227	484.43082		1
30	H	65.39618	71.31010	78.29870	1863.74748	-1451.84923	1357.29467		1
31	C	66.84444	72.97034	80.54550	503.80731	517.99032	318.51606		1
32	H	67.77431	72.43709	80.23957	640.61020	-2157.10410	-1536.29104		1
33	H	67.10059	74.05315	80.63865	1687.88455	465.60692	2087.56452		1
34	H	66.57031	72.60160	81.56098	-1293.07895	-1899.88581	-1463.57452		1
35	C	64.99480	75.19797	80.18822	-153.07550	-733.68902	248.70981		1
36	O	65.87056	75.56995	79.45127	186.15459	-480.78787	-449.34387		1
37	N	64.30001	75.90354	81.09457	-487.53139	543.18517	42.03850		1
38	C	64.53041	77.30509	81.25333	-699.35871	69.34393	360.10701		1
39	H	64.88995	77.65751	80.25901	2.81126	-221.99807	-2715.58072		1
40	C	63.12825	77.85429	81.74180	-507.46439	-592.59194	122.07761		1
41	H	63.23358	78.78502	82.34747	-1975.08116	525.87560	-1801.71556		1
42	H	62.46184	78.09801	80.88407	1588.27743	-1913.22100	1113.83566		1

43	C	62.57690	76.64965	82.57122	-613.62442	-457.55993	-194.14490	1
44	H	62.99808	76.65661	83.60160	1707.54637	-721.27992	1996.92523	1
45	H	61.46922	76.66130	82.68458	758.23357	2100.81767	1560.55011	1
46	C	63.10175	75.39636	81.75161	-352.41524	704.96076	49.21465	1
47	H	63.38822	74.51794	82.37577	1714.76886	-2070.42778	443.35792	1
48	H	62.42899	75.05362	80.92925	1224.15040	1801.50881	1636.97633	1
49	C	65.60923	77.61922	82.45752	566.85117	537.05831	117.62814	1
50	O	65.33108	78.45124	83.28941	-550.26779	-406.08867	4.21666	1
51	N	66.75273	76.97698	82.26069	566.34832	-425.77725	180.18749	1
52	H	66.77763	76.34288	81.45974	644.44502	2646.80550	-52.73430	1
53	C	67.75793	77.01361	83.26664	612.34801	-281.48662	411.56221	1
54	H	67.32377	77.70124	84.03075	1667.23498	-1490.75142	1556.16753	1
55	C	67.94836	75.52428	83.81505	-714.45746	-175.43074	286.98927	1
56	H	68.34288	74.88439	82.98011	-787.09484	1763.03619	-1922.46060	1
57	O	66.73738	74.89051	84.27275	-429.46514	516.51932	-128.40526	1
58	H	66.63300	74.18239	83.60876	1981.82785	436.16847	-1818.18182	1
59	C	69.05572	75.68984	84.91864	630.79189	-468.94448	76.03230	1
60	H	69.26772	74.72267	85.43113	-1775.71861	2062.30353	131.89849	1
61	H	70.02874	76.05712	84.48815	-1855.14608	88.94118	1993.53760	1
62	H	68.74416	76.41695	85.70471	-1504.82350	-780.94249	-2132.90992	1
63	C	69.10104	77.61093	82.55352	288.57638	618.62814	-397.00270	1
64	O	70.23054	77.18426	82.83437	321.70495	-185.26452	574.37218	1
65	N	68.77007	78.63241	81.80503	-447.05792	-446.53431	367.76425	1
66	H	67.75903	78.76183	81.80883	350.31316	1975.63644	-1843.31522	1
67	C	69.60469	79.32757	80.89654	-511.23061	374.03917	-471.51480	1
68	H	69.05313	80.27917	80.73202	2234.79579	-898.70890	-1273.45190	1
69	C	71.02509	79.55070	81.58922	529.53781	-159.34528	563.72604	1
70	H	71.50022	80.47062	81.14484	654.59388	2347.94251	1217.51488	1
71	H	70.79496	79.78077	82.66541	-1526.55661	2103.42026	817.87394	1
72	O	72.00023	78.50616	81.50276	-554.84278	14.12789	399.58769	1
73	H	71.51974	77.79743	82.08675	1297.06236	2061.84854	1220.68812	1
74	C	69.67876	78.45952	79.51037	-662.15484	-412.13544	123.62687	1
75	O	69.74033	77.25392	79.44193	-540.01537	-317.05804	274.91456	1
76	N	69.67439	79.34307	78.51539	-202.76299	-690.00100	-131.49145	1
77	H	69.64849	80.34210	78.71330	-702.62132	-2617.37191	281.70413	1
78	C	69.68498	78.85308	77.18748	-491.73914	576.34187	222.73509	1
79	H	69.68521	77.73995	77.26148	1977.17978	-1823.58850	-434.68928	1
80	C	68.41205	79.47219	76.45426	-649.50797	-328.66843	306.11224	1
81	H	68.38295	80.57443	76.59246	2075.07803	1452.16490	-1004.45904	1
82	C	68.47854	79.10536	74.93376	-615.18735	-489.99689	-70.96352	1
83	H	67.58676	79.48301	74.37994	-1226.32661	-1724.38906	-1716.47170	1
84	H	69.38175	79.54694	74.44905	2381.64273	-969.84735	900.46860	1
85	H	68.52481	78.00191	74.77896	2122.74991	1702.23946	-141.36228	1
86	C	67.12051	78.81103	77.04443	-501.86074	-479.61276	-376.42482	1
87	H	66.19773	79.18575	76.54170	993.79261	-2246.95401	-1177.81305	1
88	H	67.13711	77.70195	76.92609	42.71279	-626.15391	-2651.37258	1
89	H	67.01728	79.02231	78.13495	-2026.39012	-1590.33709	-887.82922	1
90	C	71.00920	79.49826	76.44921	-672.89153	382.57394	-156.34072	1
91	O	71.19353	80.68993	76.38839	410.04627	221.86223	500.35950	1
92	N	71.69904	78.51664	75.87746	-378.11782	-443.79414	-441.10984	1
93	H	71.41199	77.55154	76.03581	2404.15973	-568.14894	1149.30085	1
94	C	72.98891	78.82458	75.35929	-544.54484	466.16019	331.29119	1
95	H	72.95943	79.92014	75.16180	-1409.80988	-170.17955	2325.32679	1
96	C	74.02828	78.42351	76.49165	-184.48284	116.78282	-758.89137	1
97	H	73.80661	78.97151	77.43561	1893.78641	1861.14652	611.04528	1
98	H	73.93856	77.34182	76.73905	-2170.79665	-974.19311	1327.50117	1
99	C	75.45712	78.76083	75.96312	389.51668	672.81878	-138.49152	1
100	H	75.65030	78.21285	75.01394	510.64577	1933.03327	1851.02484	1
101	H	75.51405	79.83330	75.67245	-2302.30869	-1105.72939	-948.89774	1
102	C	76.59710	78.43499	76.99505	-559.93427	-126.34590	542.30857	1
103	O	77.74894	78.62057	76.68553	-670.36003	-111.83166	76.36448	1
104	N	76.15779	77.94888	78.17367	-216.06729	-537.07037	446.51379	1

105	H	75.19699	77.80810	78.50717	-1251.96487	1074.12894	-2168.52500	1
106	H	76.76778	77.74563	78.97334	-2451.83023	-720.73851	944.84612	1
107	C	73.26897	77.85217	74.06858	546.24052	-563.88337	-85.11809	1
108	O	73.29246	76.65997	74.22135	71.70702	-307.40463	606.69673	1
109	N	73.52915	78.57922	72.97227	479.90863	-504.50129	222.86849	1
110	C	73.46067	78.01256	71.66115	75.51268	-600.91904	506.73700	1
111	H	72.64428	77.25590	71.69032	-2033.61562	1795.30103	254.89480	1
112	C	73.18876	79.27812	70.74561	523.79067	517.99274	284.45581	1
113	H	73.52666	79.12770	69.69557	1599.61665	-1127.00911	1895.98173	1
114	H	72.10452	79.52367	70.69891	-1881.83093	1275.82488	-1501.55016	1
115	C	73.98573	80.39171	71.49491	-600.05639	-404.05026	316.64485	1
116	H	75.07754	80.30479	71.30832	-2597.05260	496.36221	657.73249	1
117	H	73.69303	81.42619	71.20590	-1666.24518	1294.38985	-1723.90591	1
118	C	73.62594	80.03444	73.00012	493.57570	-129.95376	-602.56394	1
119	H	74.39204	80.32765	73.75593	-1469.08415	-637.84797	2204.22581	1
120	H	72.62313	80.40082	73.32627	-1038.97840	1068.88701	-2280.71789	1
121	C	74.87081	77.35073	71.14444	188.88100	241.05089	-727.87821	1
122	O	74.87791	76.72699	70.10649	531.88613	-49.19943	427.07960	1
123	N	75.90163	77.65994	71.92160	708.14833	26.93417	-179.73509	1
124	H	75.68997	78.19852	72.75981	-2232.69501	-1179.09831	1023.94816	1
125	C	77.18090	77.12744	71.60473	-738.32412	259.92548	104.42456	1
126	H	77.05134	76.72878	70.57248	2028.89123	1260.02983	1311.33324	1
127	C	78.22047	78.32416	71.69421	-258.65678	-345.52513	661.28459	1
128	H	78.20059	78.76583	72.71495	-1826.06090	-1801.46097	-918.64554	1
129	C	79.65976	77.83847	71.30414	-541.23400	531.92970	-218.41428	1
130	H	80.42178	78.64723	71.44489	1311.73218	-2219.18200	882.19023	1
131	H	79.98031	76.95741	71.92923	-1048.71298	1223.58118	-2196.97971	1
132	H	79.71447	77.52584	70.23493	419.06414	1903.92898	1903.44670	1
133	C	77.85496	79.40538	70.62039	-423.86431	152.66566	-648.55262	1
134	H	78.56050	80.26877	70.64907	105.68386	-2342.50080	1387.51238	1
135	H	77.88490	78.98073	69.58897	-1695.63603	-1484.73621	-1531.02793	1
136	H	76.82903	79.80618	70.78223	-1853.57121	-487.39031	1936.59343	1
137	C	77.55395	75.94613	72.68068	539.71428	-510.58232	267.58633	1
138	O	78.71018	75.65853	72.90966	-15.93758	-278.34085	-624.49402	1
139	N	76.45788	75.38600	73.16315	-676.81886	12.05292	276.17960	1
140	H	75.57296	75.73172	72.79696	-1694.44250	-373.84189	-2100.66098	1
141	C	76.54014	74.25405	74.02964	412.33078	-664.70360	108.35451	1
142	H	77.36790	74.47237	74.73700	1765.77476	1294.44366	1621.76594	1
143	C	75.10237	74.12542	74.66397	-179.66635	-721.95667	-264.73915	1
144	H	74.77544	75.08744	75.12670	-607.34922	2587.87032	-598.10018	1
145	H	74.34640	73.91075	73.87403	-359.69332	-1479.13954	-2259.74260	1
146	C	75.16413	72.96271	75.71098	-240.01076	616.02425	431.85322	1
147	H	75.47329	72.01327	75.21827	-1359.17131	782.54425	2227.99181	1
148	H	75.93039	73.16723	76.49163	-820.36667	85.81767	-2596.78715	1
149	C	73.72762	72.81570	76.35462	-513.07015	236.18570	-551.87280	1
150	H	73.43304	73.74821	76.88908	1816.11944	-1183.11722	-1650.94321	1
151	H	72.95428	72.66106	75.56716	-1800.04429	-1361.53473	1526.34643	1
152	C	73.77260	71.61064	77.32327	726.08972	-253.19732	-179.64713	1
153	H	73.91830	70.62851	76.83070	1224.27271	-456.51798	-2390.90304	1
154	H	74.48534	71.72095	78.16463	1206.40339	-1150.93514	-2154.90344	1
155	N	72.36927	71.50476	78.00987	329.70796	-633.68968	-155.67358	1
156	H	72.25765	70.70977	78.70331	1348.31305	1938.76845	1359.00643	1
157	H	72.05302	72.33493	78.59105	2096.92035	1446.54551	-966.48890	1
158	H	71.53189	71.34822	77.37679	-1197.07217	-2303.53719	827.28733	1
159	C	76.85103	72.91811	73.11744	-378.01186	-556.17301	-413.96481	1
160	O	76.03599	72.49435	72.33010	-409.44433	-307.55053	-453.30833	1
161	N	78.04708	72.43274	73.41862	-429.02477	524.70884	274.08502	1
162	H	78.59993	72.91445	74.12449	1706.34263	-1425.96036	1574.38926	1
163	C	78.42498	71.17480	72.83665	-45.25864	-626.22952	478.93267	1
164	H	77.59120	70.49061	73.10786	1988.63164	570.90773	1772.87287	1
165	C	78.50061	71.37928	71.27235	551.77128	-20.49526	-564.54996	1
166	H	77.53361	71.77555	70.87927	1434.61535	-1753.10253	1513.99471	1

167	H	79.26973	72.14130	71.01366	-714.67738	1819.09770	1898.36494	1
168	C	78.84559	69.99132	70.63425	446.99263	-555.77305	338.97221	1
169	H	79.80059	69.60021	71.04841	1953.68466	1892.25957	-161.67766	1
170	H	78.06906	69.23493	70.88746	-403.03785	2688.07032	-188.43591	1
171	C	78.96692	70.17431	69.07013	567.86262	335.74681	434.04421	1
172	H	78.01199	70.55429	68.63985	-1080.02275	1568.26081	-1948.78900	1
173	H	79.74166	70.93482	68.81822	-919.54108	2111.34692	1456.13463	1
174	C	79.33184	68.79366	68.47258	195.81897	173.33862	-745.11536	1
175	H	80.32937	68.40419	68.77195	1405.67949	-2301.21089	-390.08113	1
176	H	78.56246	68.00768	68.61306	-940.37328	-1118.32446	2299.72133	1
177	N	79.43360	68.98650	66.92476	319.26422	656.36007	-42.02424	1
178	H	79.72282	68.13138	66.36761	1961.03633	619.91968	1787.09422	1
179	H	78.55028	69.28161	66.41463	854.14343	-2156.80752	1429.08711	1
180	H	80.13678	69.70473	66.58575	1237.02905	-1378.50857	-1998.28500	1
181	C	79.89071	70.66069	73.34156	532.53319	-268.57236	517.55729	1
182	O	80.09984	69.45741	73.30677	266.16714	-290.73804	-558.88002	1
183	N	80.73506	71.64447	73.59681	-226.25352	640.49678	-270.32839	1
184	H	80.33265	72.57677	73.51550	2007.69063	-1035.27229	1523.50231	1
185	C	82.05411	71.46455	74.08341	-540.76542	-573.33303	49.50000	1
186	H	82.32258	72.45995	74.50058	-2374.20950	-1036.76023	843.75774	1
187	C	82.06484	70.31379	75.19586	-77.09082	666.87422	-415.84136	1
188	H	81.63052	69.37309	74.74256	-985.81834	617.19825	2463.91927	1
189	O	81.28825	70.60867	76.37176	293.29899	-391.65602	-477.80926	1
190	H	80.60553	69.90928	76.31984	2528.72714	-681.76262	-751.27122	1
191	C	83.60028	70.08203	75.44009	252.47363	-605.14473	440.05134	1
192	H	83.77652	69.28732	76.20222	-2052.65063	1456.49051	-1043.51830	1
193	H	84.12683	69.76660	74.50684	-2152.98800	-1661.97574	-161.70652	1
194	H	84.10076	71.00862	75.80558	-473.12726	-1584.27339	2165.61725	1
195	C	83.04814	71.07257	72.84556	360.36307	488.46713	505.10056	1
196	O	84.21337	71.39203	72.90452	-200.08817	-528.03552	-385.82850	1
197	N	82.43668	70.36932	71.89556	-597.54095	-226.44775	355.20479	1
198	H	81.44522	70.12727	72.02043	2179.23655	-1300.70981	-991.33835	1
199	C	83.20345	70.08803	70.72833	-687.68921	297.39807	-249.45179	1
200	H	84.22483	69.89169	71.12687	-349.16256	-2467.37713	-1101.72831	1
201	C	82.56087	68.90366	69.86979	672.47345	361.54328	-201.62880	1
202	H	81.53768	69.20006	69.53219	1541.41502	582.18425	2169.97026	1
203	H	83.17469	68.76530	68.94900	-2534.67717	60.25153	997.72295	1
204	C	82.49933	67.58596	70.65467	574.26774	-389.43119	-377.02542	1
205	C	83.67413	66.78695	70.79286	688.82679	-287.33580	-257.96133	1
206	H	84.63736	67.12101	70.36624	331.14182	1470.38163	2269.80013	1
207	C	81.26019	67.14527	71.20982	-383.52382	-675.04808	144.24917	1
208	H	80.34738	67.75804	71.11245	4.09847	1517.59662	2262.86397	1
209	C	83.57921	65.57052	71.46866	-134.76730	428.45285	-649.50303	1
210	H	84.48656	64.94993	71.57058	-903.23433	1600.49020	2011.53387	1
211	C	81.21547	65.91974	71.87731	-335.53281	-615.00040	-364.39058	1
212	H	80.24904	65.59176	72.29840	1596.45398	-1369.33862	1732.02659	1
213	C	82.36233	65.08774	72.03199	585.48547	-340.24194	-406.23938	1
214	O	82.32423	63.83992	72.70644	-419.15649	-173.04408	-511.94141	1
215	H	81.36964	63.81319	72.95388	-1071.84350	1559.71507	-1960.13012	1
216	C	83.19071	71.35696	69.70718	291.41878	-183.13091	710.72246	1
217	O	83.74439	71.25919	68.63197	379.87695	523.47396	-222.23622	1
218	N	82.49802	72.39406	70.17607	564.30591	373.09380	277.24371	1
219	H	82.08516	72.30945	71.10424	-120.59931	-2436.07824	-1214.35098	1
220	C	82.45766	73.56493	69.37412	404.07514	-299.37480	608.84009	1
221	H	82.80661	73.22092	68.37063	-1071.07882	-841.69025	2359.66467	1
222	C	80.96157	74.07832	69.42954	-683.12807	68.71770	-390.13096	1
223	H	80.25663	73.24661	69.20520	2068.88918	1596.58590	770.89603	1
224	H	80.69904	74.42649	70.45440	1379.86429	2342.49779	-179.85638	1
225	C	80.80490	75.23625	68.39606	-176.39967	537.49466	550.97268	1
226	H	81.44168	76.10910	68.66656	-396.28051	1942.22168	1869.33314	1
227	H	81.13797	74.92371	67.38098	-94.44700	586.00678	-2659.20016	1
228	C	79.25000	75.60313	68.41385	-291.69381	-718.18079	-150.72929	1

229	H	78.56367	74.78681	68.07242	-2303.38776	1089.76242	964.62032	1
230	H	78.85286	75.98797	69.38628	884.16729	2568.80533	-207.74283	1
231	N	79.17714	76.63727	67.47036	-594.49522	-252.81478	342.29276	1
232	H	80.03264	76.88305	66.99632	-1735.17426	2084.05705	-263.71605	1
233	C	78.11304	77.26497	67.17070	595.23177	-271.52487	442.22352	1
234	N	76.93924	76.90639	67.84196	585.53813	-424.79750	-105.81303	1
235	H	76.77715	76.19833	68.55689	959.88797	1327.56823	-2177.11905	1
236	H	76.02345	77.33282	67.69955	1578.48647	16.27378	-2220.76233	1
237	N	78.35795	78.22719	66.18063	-452.17763	-390.33541	-421.51853	1
238	H	79.21096	78.46645	65.67712	470.26107	1974.25629	-1817.92087	1
239	H	77.62515	78.81316	65.77881	1856.67307	-1573.97321	-1224.35416	1
240	C	83.41191	74.77678	69.97345	-531.47271	-581.45780	-55.06206	1
241	O	83.96870	75.49050	69.16572	-243.00837	192.73507	609.52485	1
242	N	83.37090	74.86264	71.28611	343.49288	-644.25607	38.09164	1
243	H	82.84426	74.11170	71.72792	-1691.16043	-1535.97525	-1484.73099	1
244	C	84.08159	75.81697	72.06896	542.66492	350.14337	454.42563	1
245	H	84.49988	75.22210	72.90984	1209.57979	-2396.95920	463.86744	1
246	C	85.17176	76.59838	71.22245	-737.14309	145.93010	242.71942	1
247	H	84.72491	77.02656	70.28847	-1050.18303	159.36419	-2509.06125	1
248	C	85.78496	77.74528	72.09984	-706.77696	-252.88343	-245.16230	1
249	H	86.59508	78.28921	71.55965	-1624.64039	-1665.49085	1417.86935	1
250	H	85.01226	78.50034	72.38082	2566.10521	598.51109	693.22305	1
251	H	86.22004	77.35578	73.04977	-1972.69758	107.10018	-1876.34312	1
252	C	86.30581	75.57320	70.87238	412.85148	672.58832	-27.69222	1
253	H	87.15256	76.05897	70.33357	1447.02277	1762.76533	-1490.78944	1
254	H	86.72240	75.08928	71.78693	1320.77379	-145.20455	2378.68491	1
255	H	85.90689	74.76493	70.21121	-1512.10848	1470.52031	1724.75147	1
256	C	83.01016	76.93475	72.60900	-607.11113	499.56689	73.73769	1
257	O	82.19720	77.49591	71.90887	357.97126	460.81534	356.68785	1
258	N	83.28971	77.13896	73.88939	536.55407	-368.62270	332.76306	1
259	H	84.03893	76.61394	74.33883	524.38866	2297.69985	1367.20941	1
260	C	82.65873	78.21233	74.57302	46.50277	-774.29190	-147.97904	1
261	H	82.10702	78.78783	73.79226	1676.51875	1883.29066	1032.55549	1
262	C	81.71855	77.56896	75.69265	-559.41456	-34.19198	-556.30433	1
263	H	82.27656	76.80391	76.27587	-64.66664	395.18769	2695.05373	1
264	H	81.37617	78.33210	76.42625	-2703.44278	-60.40056	333.79418	1
265	C	80.50014	76.92573	74.95483	-519.76435	377.31045	459.42366	1
266	H	80.84167	76.27789	74.11608	-1746.74323	1667.50644	-1261.73691	1
267	C	79.60755	76.11337	75.96247	570.95554	16.46261	-545.27700	1
268	H	78.78617	75.58626	75.42509	2391.58273	28.05277	-1305.07271	1
269	H	80.19585	75.34134	76.51174	175.75588	917.63458	2559.43867	1
270	H	79.13021	76.78681	76.71777	-1063.97851	-2155.34650	1283.00462	1
271	C	79.58560	78.09538	74.43859	193.76014	2.62946	-765.53141	1
272	H	78.66428	77.69306	73.94830	507.39394	-846.55087	2539.60089	1
273	H	79.25358	78.75612	75.28367	1337.57841	1818.19054	1526.01994	1
274	H	80.11104	78.73766	73.69475	1100.88635	-1172.91350	-2199.08909	1
275	C	83.81363	79.04452	75.35789	-549.21115	475.64486	-309.38218	1
276	O	84.86315	78.55929	75.68740	556.06106	-390.37755	-78.24250	1
277	O	83.46758	80.35787	75.74495	-572.27940	-310.19032	-209.75862	1
278	H	82.55348	80.40025	75.34253	-1380.08193	2212.14486	790.85944	1

Listing 124: C00124.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.3642	0.0000	300.0000
3	H	79.90597	81.15335	84.89988	-2043.14101	-1757.64893	399.89339		1
4	N	79.88147	81.72474	84.05627	426.75047	490.45733	-334.42467		1
5	H	78.96825	82.16546	84.16326	442.25559	-1110.30854	-2448.52907		1
6	C	80.94199	82.66582	83.99873	415.32972	-666.39213	83.73172		1
7	H	81.14012	82.97356	85.04818	879.32219	2491.00447	667.35213		1
8	C	82.21776	81.95665	83.31623	31.35357	477.41777	628.23362		1

9	H	81.90901	81.50903	82.34100	1168.38489	2240.25337	-1019.71136	1
10	H	82.99785	82.71948	83.07676	-360.43770	2534.90498	931.67112	1
11	C	82.78018	80.89287	84.22414	463.18208	512.70242	-382.34388	1
12	H	81.94929	80.22383	84.54130	1725.29117	1863.52247	-987.07854	1
13	C	83.81046	80.05700	83.47461	710.42801	-144.27427	-313.15367	1
14	H	84.23331	79.24421	84.11991	364.20195	-1033.13725	2494.72524	1
15	H	83.36627	79.56629	82.56988	2567.61904	335.80679	847.48802	1
16	H	84.67147	80.68262	83.12345	-2587.99029	680.92867	-512.16411	1
17	C	83.42432	81.50106	85.46217	268.17616	741.64379	-40.42634	1
18	H	83.87789	80.71561	86.12053	1283.54314	-1945.37420	-1411.27812	1
19	H	84.24249	82.21732	85.19029	-1258.57796	1317.15249	-2026.02085	1
20	H	82.68409	82.06656	86.08448	-2502.84526	909.80597	575.92391	1
21	C	80.48927	83.91397	83.06468	619.36578	-458.64843	-172.09273	1
22	O	80.94676	85.04265	83.28466	-81.40433	433.87611	522.34594	1
23	N	79.76335	83.49483	82.06156	175.23996	-622.20190	341.55523	1
24	H	79.54754	82.49999	82.10726	-876.57256	-303.22879	-2561.90213	1
25	C	79.04817	84.33334	81.14415	-571.88214	-534.10783	-106.15033	1
26	H	78.04881	84.45995	81.61298	-2713.20841	-16.25800	-248.80809	1
27	C	79.79044	85.73756	80.99174	166.60354	288.16399	-716.09568	1
28	H	80.90139	85.54902	81.06235	-2097.85574	1636.78449	-586.18044	1
29	O	79.52459	86.67943	82.03184	-317.80580	-363.38227	484.43082	1
30	H	80.24351	86.37832	82.71518	1863.74748	-1451.84923	1357.29467	1
31	C	79.41045	86.19396	79.53705	503.80731	517.99032	318.51606	1
32	H	79.91757	87.14898	79.26522	640.61020	-2157.10410	-1536.29104	1
33	H	79.69622	85.43503	78.77155	1687.88455	465.60692	2087.56452	1
34	H	78.31267	86.36427	79.44112	-1293.07895	-1899.88581	-1463.57452	1
35	C	78.88689	83.43732	79.79515	-153.07550	-733.68902	248.70981	1
36	O	77.74979	83.31382	79.42026	186.15459	-480.78787	-449.34387	1
37	N	80.01654	82.98683	79.22766	-487.53139	543.18517	42.03850	1
38	C	79.97419	82.24547	78.00677	-699.35871	69.34393	360.10701	1
39	H	79.14200	82.67927	77.40793	2.81126	-221.99807	-2715.58072	1
40	C	81.44125	82.45954	77.44837	-507.46439	-592.59194	122.07761	1
41	H	81.73942	81.68490	76.70669	-1975.08116	525.87560	-1801.71556	1
42	H	81.55111	83.44605	76.94513	1588.27743	-1913.22100	1113.83566	1
43	C	82.27199	82.39942	78.76836	-613.62442	-457.55993	-194.14490	1
44	H	82.34982	81.34923	79.14063	1707.54637	-721.27992	1996.92523	1
45	H	83.31095	82.78685	78.66780	758.23357	2100.81767	1560.55011	1
46	C	81.35630	83.28603	79.71680	-352.41524	704.96076	49.21465	1
47	H	81.40025	83.03086	80.80062	1714.76886	-2070.42778	443.35792	1
48	H	81.49701	84.38492	79.59320	1224.15040	1801.50881	1636.97633	1
49	C	79.74479	80.64536	78.34588	566.85117	537.05831	117.62814	1
50	O	80.66054	79.98472	78.77432	-550.26779	-406.08867	4.21666	1
51	N	78.50582	80.29165	78.05233	566.34832	-425.77725	180.18749	1
52	H	77.88736	81.02202	77.70135	644.44502	2646.80550	-52.73430	1
53	C	78.06255	78.94301	78.13487	612.34801	-281.48662	411.56221	1
54	H	77.01281	79.01719	77.77421	1667.23498	-1490.75142	1556.16753	1
55	C	78.98428	78.06457	77.18050	-714.45746	-175.43074	286.98927	1
56	H	80.04394	78.16511	77.54106	-787.09484	1763.03619	-1922.46060	1
57	O	79.00070	78.48170	75.77630	-429.46514	516.51932	-128.40526	1
58	H	79.91593	78.80260	75.70699	1981.82785	436.16847	-1818.18182	1
59	C	78.48015	76.59853	77.40000	630.79189	-468.94448	76.03230	1
60	H	79.01394	75.88302	76.73067	-1775.71861	2062.30353	131.89849	1
61	H	78.64481	76.24844	78.45787	-1855.14608	88.94118	1993.53760	1
62	H	77.38684	76.50449	77.18130	-1504.82350	-780.94249	-2132.90992	1
63	C	78.14806	78.47607	79.70263	288.57638	618.62814	-397.00270	1
64	O	78.73384	77.46799	80.04579	321.70495	-185.26452	574.37218	1
65	N	77.41777	79.28002	80.46435	-447.05792	-446.53431	367.76425	1
66	H	76.98141	80.09688	80.03928	350.31316	1975.63644	-1843.31522	1
67	C	77.41532	78.96669	81.85502	-511.23061	374.03917	-471.51480	1
68	H	78.43976	78.56357	82.03136	2234.79579	-898.70890	-1273.45190	1
69	C	77.07034	80.32138	82.62942	529.53781	-159.34528	563.72604	1
70	H	77.23667	80.11668	83.72221	654.59388	2347.94251	1217.51488	1

71	H	77.83071	81.08517	82.31867	-1526.55661	2103.42026	817.87394	1
72	O	75.72038	80.83077	82.47495	-554.84278	14.12789	399.58769	1
73	H	75.85198	81.42108	81.71076	1297.06236	2061.84854	1220.68812	1
74	C	76.30126	77.79487	82.12704	-662.15484	-412.13544	123.62687	1
75	O	76.47193	77.02194	83.04393	-540.01537	-317.05804	274.91456	1
76	N	75.25838	77.90758	81.31763	-202.76299	-690.00100	-131.49145	1
77	H	75.29680	78.66870	80.64172	-702.62132	-2617.37191	281.70413	1
78	C	74.31917	76.83579	81.19746	-491.73914	576.34187	222.73509	1
79	H	74.95429	75.92745	81.29534	1977.17978	-1823.58850	-434.68928	1
80	C	73.25596	76.94414	82.36730	-649.50797	-328.66843	306.11224	1
81	H	72.73299	77.92431	82.32535	2075.07803	1452.16490	-1004.45904	1
82	C	72.24288	75.76320	82.17860	-615.18735	-489.99689	-70.96352	1
83	H	71.46149	75.75922	82.97467	-1226.32661	-1724.38906	-1716.47170	1
84	H	71.71817	75.84236	81.19430	2381.64273	-969.84735	900.46860	1
85	H	72.75366	74.77201	82.20781	2122.74991	1702.23946	-141.36228	1
86	C	73.95310	76.75832	83.76115	-501.86074	-479.61276	-376.42482	1
87	H	73.21009	76.58997	84.57632	993.79261	-2246.95401	-1177.81305	1
88	H	74.65165	75.88517	83.75819	42.71279	-626.15391	-2651.37258	1
89	H	74.55010	77.66128	84.03990	-2026.39012	-1590.33709	-887.82922	1
90	C	73.59643	77.02728	79.74533	-672.89153	382.57394	-156.34072	1
91	O	72.43697	77.36207	79.64428	410.04627	221.86223	500.35950	1
92	N	74.47842	76.82560	78.76427	-378.11782	-443.79414	-441.10984	1
93	H	75.40681	76.48506	79.01451	2404.15973	-568.14894	1149.30085	1
94	C	73.93491	76.72556	77.44440	-544.54484	466.16019	331.29119	1
95	H	73.07862	77.43749	77.45086	-1409.80988	-170.17955	2325.32679	1
96	C	75.13191	77.08171	76.47231	-184.48284	116.78282	-758.89137	1
97	H	75.61499	78.02882	76.79958	1893.78641	1861.14652	611.04528	1
98	H	75.92109	76.29425	76.55331	-2170.79665	-974.19311	1327.50117	1
99	C	74.64520	77.22262	74.99586	389.51668	672.81878	-138.49152	1
100	H	74.36258	76.22450	74.58898	510.64577	1933.03327	1851.02484	1
101	H	73.73162	77.85249	74.93376	-2302.30869	-1105.72939	-948.89774	1
102	C	75.80551	77.89714	74.13918	-559.93427	-126.34590	542.30857	1
103	O	75.65031	78.92342	73.52568	-670.36003	-111.83166	76.36448	1
104	N	77.00101	77.20623	74.25598	-216.06729	-537.07037	446.51379	1
105	H	77.02069	76.48778	74.98399	-1251.96487	1074.12894	-2168.52500	1
106	H	77.86953	77.75791	74.37387	-2451.83023	-720.73851	944.84612	1
107	C	73.49484	75.16596	77.20735	546.24052	-563.88337	-85.11809	1
108	O	74.29547	74.29283	77.41186	71.70702	-307.40463	606.69673	1
109	N	72.26123	75.08544	76.69563	479.90863	-504.50129	222.86849	1
110	C	71.60041	73.81524	76.55999	75.51268	-600.91904	506.73700	1
111	H	71.73599	73.28519	77.52998	-2033.61562	1795.30103	254.89480	1
112	C	70.10177	74.22363	76.23138	523.79067	517.99274	284.45581	1
113	H	69.57993	73.46944	75.60054	1599.61665	-1127.00911	1895.98173	1
114	H	69.49923	74.32128	77.16183	-1881.83093	1275.82488	-1501.55016	1
115	C	70.25664	75.60562	75.52375	-600.05639	-404.05026	316.64485	1
116	H	70.53580	75.48360	74.45271	-2597.05260	496.36221	657.73249	1
117	H	69.32953	76.22221	75.53871	-1666.24518	1294.38985	-1723.90591	1
118	C	71.44273	76.24303	76.37047	493.57570	-129.95376	-602.56394	1
119	H	72.06624	76.98816	75.82418	-1469.08415	-637.84797	2204.22581	1
120	H	71.12809	76.67104	77.35311	-1038.97840	1068.88701	-2280.71789	1
121	C	72.28362	72.98179	75.34531	188.88100	241.05089	-727.87821	1
122	O	72.26400	71.74749	75.33233	531.88613	-49.19943	427.07960	1
123	N	72.74138	73.79302	74.42246	708.14833	26.93417	-179.73509	1
124	H	72.63280	74.78981	74.60110	-2232.69501	-1179.09831	1023.94816	1
125	C	73.25555	73.26532	73.20651	-738.32412	259.92548	104.42456	1
126	H	73.53665	72.20934	73.42210	2028.89123	1260.02983	1311.33324	1
127	C	72.10659	73.39223	72.10685	-258.65678	-345.52513	661.28459	1
128	H	71.78845	74.44640	71.94717	-1826.06090	-1801.46097	-918.64554	1
129	C	72.69421	72.78889	70.78826	-541.23400	531.92970	-218.41428	1
130	H	71.89903	72.67103	70.01852	1311.73218	-2219.18200	882.19023	1
131	H	73.48673	73.44605	70.35481	-1048.71298	1223.58118	-2196.97971	1
132	H	73.14974	71.77629	70.95775	419.06414	1903.92898	1903.44670	1

133	C	70.90095	72.52797	72.60719	-423.86431	152.66566	-648.55262	1
134	H	68.56080	72.19164	70.72275	105.68386	-2342.50080	1387.51238	1
135	H	70.35570	72.05338	71.75300	-1695.63603	-1484.73621	-1531.02793	1
136	H	70.16128	73.14912	73.16816	-1853.57121	-487.39031	1936.59343	1
137	C	74.45972	74.25113	72.70326	539.71428	-510.58232	267.58633	1
138	O	74.28600	75.44357	72.48575	-15.93758	-278.34085	-624.49402	1
139	N	75.54025	73.52335	72.52554	-676.81886	12.05292	276.17960	1
140	H	75.46980	72.51539	72.66041	-1694.44250	-373.84189	-2100.66098	1
141	C	76.77013	74.17571	72.21313	412.33078	-664.70360	108.35451	1
142	H	76.65585	75.18826	72.66742	1765.77476	1294.44366	1621.76594	1
143	C	77.90404	73.26653	72.83311	-179.66635	-721.95667	-264.73915	1
144	H	77.75982	73.16269	73.93205	-607.34922	2587.87032	-598.10018	1
145	H	77.83277	72.23397	72.42257	-359.69332	-1479.13954	-2259.74260	1
146	C	79.31314	73.87336	72.53017	-240.01076	616.02425	431.85322	1
147	H	79.47064	73.97726	71.43038	-1359.17131	782.54425	2227.99181	1
148	H	79.42049	74.89305	72.96410	-820.36667	85.81767	-2596.78715	1
149	C	80.33998	72.85486	73.17310	-513.07015	236.18570	-551.87280	1
150	H	80.13583	72.72664	74.26107	1816.11944	-1183.11722	-1650.94321	1
151	H	80.21705	71.84252	72.72380	-1800.04429	-1361.53473	1526.34643	1
152	C	81.77885	73.37224	72.95042	726.08972	-253.19732	-179.64713	1
153	H	82.09093	73.42818	71.88850	1224.27271	-456.51798	-2390.90304	1
154	H	82.01407	74.32437	73.46644	1206.40339	-1150.93514	-2154.90344	1
155	N	82.74589	72.31920	73.59265	329.70796	-633.68968	-155.67358	1
156	H	83.78045	72.53872	73.51520	1348.31305	1938.76845	1359.00643	1
157	H	82.64838	72.14080	74.63450	2096.92035	1446.54551	-966.48890	1
158	H	82.71365	71.33451	73.19772	-1197.07217	-2303.53719	827.28733	1
159	C	76.82725	74.25186	70.57311	-378.01186	-556.17301	-413.96481	1
160	O	77.74384	73.78351	69.94469	-409.44433	-307.55053	-453.30833	1
161	N	75.73968	74.88470	70.16323	-429.02477	524.70884	274.08502	1
162	H	75.09395	75.29965	70.86736	1706.34263	-1425.96036	1574.38926	1
163	C	75.52469	75.09132	68.75636	-45.25864	-626.22952	478.93267	1
164	H	76.39765	75.73240	68.50404	1988.63164	570.90773	1772.87287	1
165	C	75.61009	73.70883	68.00489	551.77128	-20.49526	-564.54996	1
166	H	76.53341	73.15366	68.30642	1434.61535	-1753.10253	1513.99471	1
167	H	74.76163	73.04106	68.27703	-714.67738	1819.09770	1898.36494	1
168	C	75.63189	74.02294	66.46936	446.99263	-555.77305	338.97221	1
169	H	74.72182	74.58624	66.16609	1953.68466	1892.25957	-161.67766	1
170	H	76.49267	74.68228	66.21864	-403.03785	2688.07032	-188.43591	1
171	C	75.73828	72.65361	65.68737	567.86262	335.74681	434.04421	1
172	H	76.63929	72.08273	66.01061	-1080.02275	1568.26081	-1948.78900	1
173	H	74.86694	71.99615	65.91142	-919.54108	2111.34692	1456.13463	1
174	C	75.81296	72.98075	64.17716	195.81897	173.33862	-745.11536	1
175	H	74.89728	73.44416	63.75891	1405.67949	-2301.21089	-390.08113	1
176	H	76.70387	73.56772	63.87655	-940.37328	-1118.32446	2299.72133	1
177	N	75.96354	71.62678	63.40642	319.26422	656.36007	-42.02424	1
178	H	76.02482	71.70285	62.34994	1961.03633	619.91968	1787.09422	1
179	H	76.83041	71.05492	63.62261	854.14343	-2156.80752	1429.08711	1
180	H	75.19096	70.90788	63.52177	1237.02905	-1378.50857	-1998.28500	1
181	C	74.10336	75.88387	68.64033	532.53319	-268.57236	517.55729	1
182	O	74.03865	77.00900	69.08293	266.16714	-290.73804	-558.88002	1
183	N	73.12392	75.15988	68.09358	-226.25352	640.49678	-270.32839	1
184	H	73.34543	74.22907	67.74366	2007.69063	-1035.27229	1523.50231	1
185	C	71.95931	75.86454	67.68558	-540.76542	-573.33303	49.50000	1
186	H	72.11443	76.90786	68.05312	-2374.20950	-1036.76023	843.75774	1
187	C	71.89438	75.75473	66.08813	-77.09082	666.87422	-415.84136	1
188	H	71.89336	74.66854	65.79670	-985.81834	617.19825	2463.91927	1
189	O	73.00928	76.34527	65.39451	293.29899	-391.65602	-477.80926	1
190	H	73.32841	75.58534	64.86873	2528.72714	-681.76262	-751.27122	1
191	C	70.49039	76.37119	65.74491	252.47363	-605.14473	440.05134	1
192	H	70.34913	76.47212	64.64386	-2052.65063	1456.49051	-1043.51830	1
193	H	69.65169	75.73837	66.12311	-2152.98800	-1661.97574	-161.70652	1
194	H	70.36825	77.38625	66.19082	-473.12726	-1584.27339	2165.61725	1

195	C	70.61830	75.15701	68.30849	360.36307	488.46713	505.10056	1
196	O	69.59681	75.80146	68.39018	-200.08817	-528.03552	-385.82850	1
197	N	70.79902	73.87254	68.58064	-597.54095	-226.44775	355.20479	1
198	H	71.72364	73.49053	68.39523	2179.23655	-1300.70981	-991.33835	1
199	C	69.62477	73.06356	68.86346	-687.68921	297.39807	-249.45179	1
200	H	68.86418	73.54673	68.20570	-349.16256	-2467.37713	-1101.72831	1
201	C	69.96953	71.52620	68.49670	672.47345	361.54328	-201.62880	1
202	H	71.01141	71.26581	68.78738	1541.41502	582.18425	2169.97026	1
203	H	69.29506	70.83719	69.05392	-2534.67717	60.25153	997.72295	1
204	C	69.75941	71.36958	66.98927	574.26774	-389.43119	-377.02542	1
205	C	68.41718	71.30402	66.50469	688.82679	-287.33580	-257.96133	1
206	H	67.56209	71.35891	67.20250	331.14182	1470.38163	2269.80013	1
207	C	70.86383	71.30567	66.08503	-383.52382	-675.04808	144.24917	1
208	H	71.90283	71.35943	66.45744	4.09847	1517.59662	2262.86397	1
209	C	68.21026	71.16874	65.13426	-134.76730	428.45285	-649.50303	1
210	H	67.17306	71.11560	64.75930	-903.23433	1600.49020	2011.53387	1
211	C	70.60177	71.16476	64.72067	-335.53281	-615.00040	-364.39058	1
212	H	71.45959	71.10559	64.02814	1596.45398	-1369.33862	1732.02659	1
213	C	69.27865	71.09170	64.19383	585.48547	-340.24194	-406.23938	1
214	O	69.00071	70.95511	62.80961	-419.15649	-173.04408	-511.94141	1
215	H	69.92084	70.89612	62.45968	-1071.84350	1559.71507	-1960.13012	1
216	C	69.15722	73.08585	70.34395	291.41878	-183.13091	710.72246	1
217	O	69.17528	73.93150	71.19996	379.87695	523.47396	-222.23622	1
218	N	71.18714	69.71035	71.01175	564.30591	373.09380	277.24371	2
219	H	71.96074	69.86517	70.36211	-120.59931	-2436.07824	-1214.35098	2
220	C	71.58321	69.68738	72.17662	404.07514	-299.37480	608.84009	2
221	H	71.23979	71.71174	73.29090	-1071.07882	-841.69025	2359.66467	1
222	C	70.40834	69.36040	73.23410	-683.12807	68.71770	-390.13096	2
223	H	69.62749	70.15351	73.13730	2068.88918	1596.58590	770.89603	2
224	H	69.91030	68.43637	72.85120	1379.86429	2342.49779	-179.85638	2
225	C	70.75905	69.16757	74.67715	-176.39967	537.49466	550.97268	2
226	H	71.56485	68.40848	74.76041	-396.28051	1942.22168	1869.33314	2
227	H	71.19811	70.11322	75.09457	-94.44700	586.00678	-2659.20016	2
228	C	69.59022	68.75040	75.52956	-291.69381	-718.18079	-150.72929	2
229	H	68.69824	69.41752	75.43716	-2303.38776	1089.76242	964.62032	2
230	H	69.26207	67.69249	75.38393	884.16729	2568.80533	-207.74283	2
231	N	69.98047	68.86254	76.98027	-594.49522	-252.81478	342.29276	2
232	H	70.80048	69.32816	77.36009	-1735.17426	2084.05705	-263.71605	2
233	C	69.08544	68.51220	77.96559	595.23177	-271.52487	442.22352	2
234	N	67.86829	67.94394	77.63853	585.53813	-424.79750	-105.81303	2
235	H	67.50120	67.72376	76.71016	959.88797	1327.56823	-2177.11905	2
236	H	67.18126	67.66416	78.33894	1578.48647	16.27378	-2220.76233	2
237	N	69.44811	68.74776	79.27865	-452.17763	-390.33541	-421.51853	2
238	H	70.30841	69.13905	79.67386	470.26107	1974.25629	-1817.92087	2
239	H	68.81212	68.48217	80.03077	1856.67307	-1573.97321	-1224.35416	2
240	C	73.09464	69.88807	72.36649	-531.47271	-581.45780	-55.06206	2
241	O	73.87237	69.88898	71.42258	-243.00837	192.73507	609.52485	2
242	N	73.52148	70.08027	73.67154	343.49288	-644.25607	38.09164	2
243	H	72.89359	70.39977	74.45294	-1691.16043	-1535.97525	-1484.73099	2
244	C	74.85942	69.52867	73.95592	542.66492	350.14337	454.42563	2
245	H	75.41731	69.69114	73.00224	1209.57979	-2396.95920	463.86744	2
246	C	75.50796	70.13208	75.17759	-737.14309	145.93010	242.71942	2
247	H	74.87448	69.90389	76.06487	-1050.18303	159.36419	-2509.06125	2
248	C	76.87353	69.50291	75.40523	-706.77696	-252.88343	-245.16230	2
249	H	77.39472	69.94046	76.29941	-1624.64039	-1665.49085	1417.86935	2
250	H	76.78692	68.39339	75.57944	2566.10521	598.51109	693.22305	2
251	H	77.54963	69.64704	74.51812	-1972.69758	107.10018	-1876.34312	2
252	C	75.64146	71.64214	75.10073	412.85148	672.58832	-27.69222	2
253	H	76.22639	72.05540	75.96806	1447.02277	1762.76533	-1490.78944	2
254	H	76.17201	71.95700	74.16171	1320.77379	-145.20455	2378.68491	2
255	H	74.63546	72.14816	75.10919	-1512.10848	1470.52031	1724.75147	2
256	C	74.63899	67.90973	74.28028	-607.11113	499.56689	73.73769	2

257	O	75.37751	67.09057	73.78660	357.97126	460.81534	356.68785	2
258	N	73.61999	67.74523	75.10613	536.55407	-368.62270	332.76306	2
259	H	73.18162	68.61874	75.39404	524.38866	2297.69985	1367.20941	2
260	C	73.31814	66.51900	75.74908	46.50277	-774.29190	-147.97904	2
261	H	72.23802	66.61281	75.99699	1676.51875	1883.29066	1032.55549	2
262	C	73.66441	65.26200	74.80400	-559.41456	-34.19198	-556.30433	2
263	H	74.77717	65.19235	74.69122	-64.66664	395.18769	2695.05373	2
264	H	73.34513	64.30708	75.28716	-2703.44278	-60.40056	333.79418	2
265	C	73.02490	65.42547	73.44874	-519.76435	377.31045	459.42366	2
266	H	73.31751	66.42716	73.05246	-1746.74323	1667.50644	-1261.73691	2
267	C	73.54914	64.36525	72.48851	570.95554	16.46261	-545.27700	2
268	H	73.10208	64.47406	71.46670	2391.58273	28.05277	-1305.07271	2
269	H	74.66217	64.43351	72.37167	175.75588	917.63458	2559.43867	2
270	H	73.31495	63.32929	72.84569	-1063.97851	-2155.34650	1283.00462	2
271	C	71.50713	65.35179	73.52818	193.76014	2.62946	-765.53141	2
272	H	71.03596	65.46471	72.51751	507.39394	-846.55087	2539.60089	2
273	H	71.16345	64.37082	73.94721	1337.57841	1818.19054	1526.01994	2
274	H	71.08663	66.15928	74.18131	1100.88635	-1172.91350	-2199.08909	2
275	C	74.21213	66.43101	77.08590	-549.21115	475.64486	-309.38218	2
276	O	75.14761	67.14627	77.33175	556.06106	-390.37755	-78.24250	2
277	O	73.85037	65.39050	77.97840	-572.27940	-310.19032	-209.75862	2
278	H	73.05550	65.04047	77.49125	-1380.08193	2212.14486	790.85944	2

Listing 125: C00125.xmolout

1	276								
2	initial	150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	
		11100	0.2500	300.00	0.00	0.00	-1293.3602	0.0000 300.0000	
3	H	83.59154	68.91789	73.47310	-2043.14101	-1757.64893	399.89339	1	
4	N	83.44817	69.65839	72.78952	426.75047	490.45733	-334.42467	1	
5	H	82.75274	70.23744	73.25665	442.25559	-1110.30854	-2448.52907	1	
6	C	84.63373	70.34215	72.43735	415.32972	-666.39213	83.73172	1	
7	H	85.39422	69.53448	72.40980	879.32219	2491.00447	667.35213	1	
8	C	84.41065	71.03743	71.00430	31.35357	477.41777	628.23362	1	
9	H	83.49291	71.67341	71.02379	1168.38489	2240.25337	-1019.71136	1	
10	H	85.26201	71.72108	70.76726	-360.43770	2534.90498	931.67112	1	
11	C	84.27085	69.96948	69.94782	463.18208	512.70242	-382.34388	1	
12	H	83.49171	69.24899	70.28480	1725.29117	1863.52247	-987.07854	1	
13	C	83.82327	70.58853	68.62957	710.42801	-144.27427	-313.15367	1	
14	H	83.68523	69.81210	67.83325	364.20195	-1033.13725	2494.72524	1	
15	H	82.84958	71.13297	68.73566	2567.61904	335.80679	847.48802	1	
16	H	84.57519	71.32552	68.24548	-2587.99029	680.92867	-512.16411	1	
17	C	85.57348	69.21248	69.73132	268.17616	741.64379	-40.42634	1	
18	H	85.48056	68.46026	68.90548	1283.54314	-1945.37420	-1411.27812	1	
19	H	86.41138	69.90429	69.45653	-1258.57796	1317.15249	-2026.02085	1	
20	H	85.89066	68.65500	70.64984	-2502.84526	909.80597	575.92391	1	
21	C	84.93250	71.39475	73.65117	619.36578	-458.64843	-172.09273	1	
22	O	85.49990	71.01372	74.66113	-81.40433	433.87611	522.34594	1	
23	N	84.46737	72.60007	73.38024	175.23996	-622.20190	341.55523	1	
24	H	83.95346	72.74931	72.51571	-876.57256	-303.22879	-2561.90213	1	
25	C	84.64705	73.64585	74.33606	-571.88214	-534.10783	-106.15033	1	
26	H	85.63240	73.45215	74.81399	-2713.20841	-16.25800	-248.80809	1	
27	C	84.51607	75.03300	73.54285	166.60354	288.16399	-716.09568	1	
28	H	83.55773	75.01643	72.95349	-2097.85574	1636.78449	-586.18044	1	
29	O	85.55745	75.31973	72.59774	-317.80580	-363.38227	484.43082	1	
30	H	85.04983	75.37641	71.76181	1863.74748	-1451.84923	1357.29467	1	
31	C	84.35002	76.01959	74.75634	503.80731	517.99032	318.51606	1	
32	H	84.09912	77.05225	74.41874	640.61020	-2157.10410	-1536.29104	1	
33	H	83.52973	75.67579	75.43990	1687.88455	465.60692	2087.56452	1	
34	H	85.28357	76.08647	75.36194	-1293.07895	-1899.88581	-1463.57452	1	
35	C	83.39486	73.58270	75.37692	-153.07550	-733.68902	248.70981	1	
36	O	82.28006	73.82097	74.96716	186.15459	-480.78787	-449.34387	1	

37	N	83.78639	73.32126	76.63141	-487.53139	543.18517	42.03850	1
38	C	82.78138	73.09933	77.62935	-699.35871	69.34393	360.10701	1
39	H	81.91005	72.70944	77.05666	2.81126	-221.99807	-2715.58072	1
40	C	83.48156	72.04940	78.59356	-507.46439	-592.59194	122.07761	1
41	H	83.07773	72.08808	79.63081	-1975.08116	525.87560	-1801.71556	1
42	H	83.32113	71.00894	78.23277	1588.27743	-1913.22100	1113.83566	1
43	C	84.99014	72.44143	78.50439	-613.62442	-457.55993	-194.14490	1
44	H	85.22782	73.27815	79.19907	1707.54637	-721.27992	1996.92523	1
45	H	85.67721	71.60913	78.77666	758.23357	2100.81767	1560.55011	1
46	C	85.12882	72.88321	76.98634	-352.41524	704.96076	49.21465	1
47	H	85.82912	73.73333	76.80810	1714.76886	-2070.42778	443.35792	1
48	H	85.36045	72.04330	76.25202	1224.15040	1801.50881	1636.97633	1
49	C	82.39933	74.46820	78.43715	566.85117	537.05831	117.62814	1
50	O	81.21136	74.62459	78.73897	-550.26779	-406.08867	4.21666	1
51	N	83.42332	75.22674	78.72610	566.34832	-425.77725	180.18749	1
52	H	84.30268	74.88375	78.34220	644.44502	2646.80550	-52.73430	1
53	C	83.34082	76.36525	79.56877	612.34801	-281.48662	411.56221	1
54	H	84.36383	76.79848	79.52066	1667.23498	-1490.75142	1556.16753	1
55	C	82.22374	77.34248	78.96953	-714.45746	-175.43074	286.98927	1
56	H	81.25000	76.77896	78.88139	-787.09484	1763.03619	-1922.46060	1
57	O	82.50417	77.85836	77.65531	-429.46514	516.51932	-128.40526	1
58	H	81.76007	77.48131	77.14400	1981.82785	436.16847	-1818.18182	1
59	C	82.08888	78.40986	80.11582	630.79189	-468.94448	76.03230	1
60	H	81.28396	79.14800	79.89220	-1775.71861	2062.30353	131.89849	1
61	H	81.84243	77.93780	81.09614	-1855.14608	88.94118	1993.53760	1
62	H	83.03517	78.98285	80.25259	-1504.82350	-780.94249	-2132.90992	1
63	C	82.96362	75.89877	81.09498	288.57638	618.62814	-397.00270	1
64	O	83.76696	76.14558	81.96025	321.70495	-185.26452	574.37218	1
65	N	81.75050	75.37000	81.21378	-447.05792	-446.53431	367.76425	1
66	H	81.15699	75.16430	80.37192	350.31316	1975.63644	-1843.31522	1
67	C	81.45687	74.74949	82.46091	-511.23061	374.03917	-471.51480	1
68	H	82.35527	74.90768	83.10576	2234.79579	-898.70890	-1273.45190	1
69	C	80.14478	75.49974	83.02407	529.53781	-159.34528	563.72604	1
70	H	79.97309	75.10850	84.06430	654.59388	2347.94251	1217.51488	1
71	H	80.42219	76.58220	83.12508	-1526.55661	2103.42026	817.87394	1
72	O	78.91796	75.33038	82.28014	-554.84278	14.12789	399.58769	1
73	H	79.05645	76.01317	81.59298	1297.06236	2061.84854	1220.68812	1
74	C	81.09889	73.19405	82.18550	-662.15484	-412.13544	123.62687	1
75	O	80.64800	72.76615	81.12689	-540.01537	-317.05804	274.91456	1
76	N	81.33786	72.51162	83.29110	-202.76299	-690.00100	-131.49145	1
77	H	81.69196	73.06197	84.06979	-702.62132	-2617.37191	281.70413	1
78	C	81.34429	71.04675	83.28307	-491.73914	576.34187	222.73509	1
79	H	81.72360	70.83129	82.25606	1977.17978	-1823.58850	-434.68928	1
80	C	82.25143	70.56739	84.40187	-649.50797	-328.66843	306.11224	1
81	H	81.89224	71.02142	85.35221	2075.07803	1452.16490	-1004.45904	1
82	C	82.21355	69.05884	84.55948	-615.18735	-489.99689	-70.96352	1
83	H	82.90332	68.70848	85.37654	-1226.32661	-1724.38906	-1716.47170	1
84	H	81.17703	68.69749	84.81836	2381.64273	-969.84735	900.46860	1
85	H	82.52329	68.53443	83.61359	2122.74991	1702.23946	-141.36228	1
86	C	83.68443	71.02061	84.18382	-501.86074	-479.61276	-376.42482	1
87	H	84.35041	70.73106	85.04241	993.79261	-2246.95401	-1177.81305	1
88	H	84.12301	70.56399	83.25422	42.71279	-626.15391	-2651.37258	1
89	H	83.75422	72.13688	84.06569	-2026.39012	-1590.33709	-887.82922	1
90	C	79.75696	70.57247	83.42876	-672.89153	382.57394	-156.34072	1
91	O	79.37934	69.97323	84.40090	410.04627	221.86223	500.35950	1
92	N	79.09402	70.92824	82.34891	-378.11782	-443.79414	-441.10984	1
93	H	79.56982	71.47295	81.59144	2404.15973	-568.14894	1149.30085	1
94	C	77.69093	70.63174	82.24729	-544.54484	466.16019	331.29119	1
95	H	77.69844	69.53306	82.42454	-1409.80988	-170.17955	2325.32679	1
96	C	76.97706	71.33755	83.47127	-184.48284	116.78282	-758.89137	1
97	H	77.48709	71.08164	84.43162	1893.78641	1861.14652	611.04528	1
98	H	77.06941	72.44494	83.38407	-2170.79665	-974.19311	1327.50117	1

99	C	75.48797	70.86344	83.50504	389.51668	672.81878	-138.49152	1
100	H	75.07833	70.78581	82.47307	510.64577	1933.03327	1851.02484	1
101	H	75.42412	69.82282	83.89233	-2302.30869	-1105.72939	-948.89774	1
102	C	74.56836	71.81645	84.35857	-559.93427	-126.34590	542.30857	1
103	O	73.37571	71.65855	84.34289	-670.36003	-111.83166	76.36448	1
104	N	75.24275	72.76060	85.05017	-216.06729	-537.07037	446.51379	1
105	H	76.25461	72.90727	85.14513	-1251.96487	1074.12894	-2168.52500	1
106	H	74.79618	73.43204	85.68402	-2451.83023	-720.73851	944.84612	1
107	C	77.28266	71.01086	80.72188	546.24052	-563.88337	-85.11809	1
108	O	77.91323	70.42556	79.87076	71.70702	-307.40463	606.69673	1
109	N	76.28733	71.89381	80.53213	479.90863	-504.50129	222.86849	1
110	C	75.46610	71.79844	79.36792	75.51268	-600.91904	506.73700	1
111	H	75.35433	70.71217	79.15218	-2033.61562	1795.30103	254.89480	1
112	C	74.15778	72.54769	79.85301	523.79067	517.99274	284.45581	1
113	H	73.51463	72.88434	79.00910	1599.61665	-1127.00911	1895.98173	1
114	H	73.52863	71.88921	80.49289	-1881.83093	1275.82488	-1501.55016	1
115	C	74.75044	73.72934	80.68464	-600.05639	-404.05026	316.64485	1
116	H	75.07871	74.56544	80.02716	-2597.05260	496.36221	657.73249	1
117	H	74.02393	74.16866	81.40431	-1666.24518	1294.38985	-1723.90591	1
118	C	75.97562	73.01940	81.40391	493.57570	-129.95376	-602.56394	1
119	H	76.90078	73.63555	81.51225	-1469.08415	-637.84797	2204.22581	1
120	H	75.70254	72.59974	82.39903	-1038.97840	1068.88701	-2280.71789	1
121	C	76.07888	72.59561	78.05880	188.88100	241.05089	-727.87821	1
122	O	75.79054	72.20547	76.92627	531.88613	-49.19943	427.07960	1
123	N	76.71310	73.69004	78.41831	708.14833	26.93417	-179.73509	1
124	H	76.73602	73.69000	79.43874	-2232.69501	-1179.09831	1023.94816	1
125	C	77.63108	74.46746	77.67283	-738.32412	259.92548	104.42456	1
126	H	77.98950	75.19729	78.43346	2028.89123	1260.02983	1311.33324	1
127	C	78.79219	73.51269	77.14479	-258.65678	-345.52513	661.28459	1
128	H	78.41738	72.76739	76.41018	-1826.06090	-1801.46097	-918.64554	1
129	C	79.75187	74.53537	76.44722	-541.23400	531.92970	-218.41428	1
130	H	80.73022	74.07337	76.10712	1311.73218	-2219.18200	882.19023	1
131	H	79.26949	74.98155	75.54280	-1048.71298	1223.58118	-2196.97971	1
132	H	79.99769	75.39409	77.12084	419.06414	1903.92898	1903.44670	1
133	C	79.38671	72.76856	78.38858	-423.86431	152.66566	-648.55262	1
134	H	80.38543	72.32292	78.17340	105.68386	-2342.50080	1387.51238	1
135	H	79.51449	73.45498	79.26945	-1695.63603	-1484.73621	-1531.02793	1
136	H	78.71584	71.92992	78.72973	-1853.57121	-487.39031	1936.59343	1
137	C	77.06488	75.20545	76.31985	539.71428	-510.58232	267.58633	1
138	O	77.41417	76.34674	76.13019	-15.93758	-278.34085	-624.49402	1
139	N	76.40262	74.39660	75.50680	-676.81886	12.05292	276.17960	1
140	H	76.14844	73.41282	75.79222	-1694.44250	-373.84189	-2100.66098	1
141	C	76.09142	74.93198	74.22422	412.33078	-664.70360	108.35451	1
142	H	76.61727	75.91813	74.18134	1765.77476	1294.44366	1621.76594	1
143	C	76.56669	73.88446	73.12965	-179.66635	-721.95667	-264.73915	1
144	H	77.67609	73.79953	73.11694	-607.34922	2587.87032	-598.10018	1
145	H	76.19684	72.86161	73.36269	-359.69332	-1479.13954	-2259.74260	1
146	C	76.02105	74.37290	71.74864	-240.01076	616.02425	431.85322	1
147	H	74.91030	74.45911	71.78220	-1359.17131	782.54425	2227.99181	1
148	H	76.39833	75.39328	71.51412	-820.36667	85.81767	-2596.78715	1
149	C	76.45182	73.34585	70.62504	-513.07015	236.18570	-551.87280	1
150	H	77.55995	73.30285	70.51659	1816.11944	-1183.11722	-1650.94321	1
151	H	76.12896	72.31104	70.88285	-1800.04429	-1361.53473	1526.34643	1
152	C	75.77419	73.82502	69.31987	726.08972	-253.19732	-179.64713	1
153	H	74.65313	73.84895	69.36984	1224.27271	-456.51798	-2390.90304	1
154	H	76.15609	74.79005	68.92969	1206.40339	-1150.93514	-2154.90344	1
155	N	76.10329	72.79100	68.19419	329.70796	-633.68968	-155.67358	1
156	H	75.69780	73.01533	67.23988	1348.31305	1938.76845	1359.00643	1
157	H	77.12662	72.64057	67.95424	2096.92035	1446.54551	-966.48890	1
158	H	75.75985	71.79647	68.33500	-1197.07217	-2303.53719	827.28733	1
159	C	74.45883	75.09531	74.10324	-378.01186	-556.17301	-413.96481	1
160	O	74.00537	76.21129	73.85677	-409.44433	-307.55053	-453.30833	1

161	N	73.85126	73.94026	74.21868	-429.02477	524.70884	274.08502	1
162	H	74.48755	73.16957	74.41938	1706.34263	-1425.96036	1574.38926	1
163	C	72.44886	73.77649	74.35498	-45.25864	-626.22952	478.93267	1
164	H	72.34814	72.71468	74.67258	1988.63164	570.90773	1772.87287	1
165	C	71.98396	74.80778	75.46105	551.77128	-20.49526	-564.54996	1
166	H	72.60971	74.69903	76.37575	1434.61535	-1753.10253	1513.99471	1
167	H	72.13666	75.86013	75.12307	-714.67738	1819.09770	1898.36494	1
168	C	70.47663	74.52060	75.76619	446.99263	-555.77305	338.97221	1
169	H	69.82962	74.85966	74.92552	1953.68466	1892.25957	-161.67766	1
170	H	70.28864	73.42942	75.88077	-403.03785	2688.07032	-188.43591	1
171	C	70.14331	75.29031	77.10604	567.86262	335.74681	434.04421	1
172	H	70.74284	74.88592	77.95459	-1080.02275	1568.26081	-1948.78900	1
173	H	70.43572	76.36856	77.01726	-919.54108	2111.34692	1456.13463	1
174	C	68.62972	75.16331	77.39531	195.81897	173.33862	-745.11536	1
175	H	67.98098	75.73672	76.70337	1405.67949	-2301.21089	-390.08113	1
176	H	68.25724	74.12361	77.49059	-940.37328	-1118.32446	2299.72133	1
177	N	68.39037	75.80107	78.80525	319.26422	656.36007	-42.02424	1
178	H	67.37883	75.90923	79.10626	1961.03633	619.91968	1787.09422	1
179	H	68.80022	75.27654	79.63079	854.14343	-2156.80752	1429.08711	1
180	H	68.76935	76.77847	78.97065	1237.02905	-1378.50857	-1998.28500	1
181	C	71.65191	74.05479	72.93640	532.53319	-268.57236	517.55729	1
182	O	70.90892	73.18610	72.55659	266.16714	-290.73804	-558.88002	1
183	N	71.91535	75.24649	72.44415	-226.25352	640.49678	-270.32839	1
184	H	72.59939	75.86331	72.95428	2007.69063	-1035.27229	1523.50231	1
185	C	71.45439	75.68228	71.17298	-540.76542	-573.33303	49.50000	1
186	H	72.19270	76.47883	70.93106	-2374.20950	-1036.76023	843.75774	1
187	C	71.45636	74.48522	70.12696	-77.09082	666.87422	-415.84136	1
188	H	70.75639	73.68250	70.49874	-985.81834	617.19825	2463.91927	1
189	O	72.75102	73.84819	69.91519	293.29899	-391.65602	-477.80926	1
190	H	72.59320	73.00093	70.37469	2528.72714	-681.76262	-751.27122	1
191	C	70.83339	75.16042	68.85511	252.47363	-605.14473	440.05134	1
192	H	70.72210	74.43059	68.01979	-2052.65063	1456.49051	-1043.51830	1
193	H	69.82008	75.57731	69.06688	-2152.98800	-1661.97574	-161.70652	1
194	H	71.46953	75.99660	68.48220	-473.12726	-1584.27339	2165.61725	1
195	C	69.94744	76.31552	71.37328	360.36307	488.46713	505.10056	1
196	O	68.93035	75.68073	71.17010	-200.08817	-528.03552	-385.82850	1
197	N	70.07660	77.58922	71.70627	-597.54095	-226.44775	355.20479	1
198	H	71.01560	77.96824	71.81386	2179.23655	-1300.70981	-991.33835	1
199	C	68.92179	78.36271	72.00616	-687.68921	297.39807	-249.45179	1
200	H	68.21784	77.62420	72.45045	-349.16256	-2467.37713	-1101.72831	1
201	C	69.32792	79.59010	72.93989	672.47345	361.54328	-201.62880	1
202	H	70.04239	80.25231	72.39948	1541.41502	582.18425	2169.97026	1
203	H	68.42077	80.20211	73.15150	-2534.67717	60.25153	997.72295	1
204	C	69.95830	79.09322	74.25041	574.26774	-389.43119	-377.02542	1
205	C	69.11597	78.63737	75.30845	688.82679	-287.33580	-257.96133	1
206	H	68.01962	78.59081	75.17728	331.14182	1470.38163	2269.80013	1
207	C	71.37583	79.11981	74.41807	-383.52382	-675.04808	144.24917	1
208	H	72.03390	79.45175	73.59496	4.09847	1517.59662	2262.86397	1
209	C	69.70542	78.27512	76.52195	-134.76730	428.45285	-649.50303	1
210	H	69.04451	77.95027	77.34362	-903.23433	1600.49020	2011.53387	1
211	C	71.91931	78.73769	75.64846	-335.53281	-615.00040	-364.39058	1
212	H	73.01701	78.77069	75.76548	1596.45398	-1369.33862	1732.02659	1
213	C	71.11448	78.31952	76.74920	585.48547	-340.24194	-406.23938	1
214	O	71.66095	77.94597	78.01021	-419.15649	-173.04408	-511.94141	1
215	H	72.61485	78.11789	77.83189	-1071.84350	1559.71507	-1960.13012	1
216	C	68.33747	79.01799	70.62793	291.41878	-183.13091	710.72246	1
217	O	67.87201	80.13112	70.59583	379.87695	523.47396	-222.23622	1
218	N	68.40519	78.11123	69.65637	564.30591	373.09380	277.24371	1
219	H	68.75709	77.17189	69.89067	-120.59931	-2436.07824	-1214.35098	1
220	C	68.01594	78.49068	68.33791	404.07514	-299.37480	608.84009	1
221	H	68.27230	79.57176	68.25940	-1071.07882	-841.69025	2359.66467	1
222	C	68.80753	77.53554	67.35544	-683.12807	68.71770	-390.13096	1

223	H	69.89242	77.52917	67.60436	2068.88918	1596.58590	770.89603	1
224	H	68.46525	76.48451	67.48855	1379.86429	2342.49779	-179.85638	1
225	C	68.58216	77.99749	65.88225	-176.39967	537.49466	550.97268	1
226	H	67.49514	78.09364	65.65292	-396.28051	1942.22168	1869.33314	1
227	H	69.01903	79.00491	65.70187	-94.44700	586.00678	-2659.20016	1
228	C	69.26833	76.88569	64.96277	-291.69381	-718.18079	-150.72929	1
229	H	70.37587	76.77419	65.08459	-2303.38776	1089.76242	964.62032	1
230	H	68.81582	75.86323	65.02612	884.16729	2568.80533	-207.74283	1
231	N	69.02670	77.37653	63.67162	-594.49522	-252.81478	342.29276	1
232	H	68.51590	78.24303	63.60266	-1735.17426	2084.05705	-263.71605	1
233	C	69.40377	76.80584	62.60023	595.23177	-271.52487	442.22352	1
234	N	70.10950	75.60311	62.71677	585.53813	-424.79750	-105.81303	1
235	H	70.37619	75.08835	63.55500	959.88797	1327.56823	-2177.11905	1
236	H	70.45995	75.05290	61.93209	1578.48647	16.27378	-2220.76233	1
237	N	69.01333	77.54085	61.47193	-452.17763	-390.33541	-421.51853	1
238	H	68.49577	78.41470	61.39036	470.26107	1974.25629	-1817.92087	1
239	H	69.21973	77.24853	60.51601	1856.67307	-1573.97321	-1224.35416	1
240	C	66.41039	78.24791	68.11925	-531.47271	-581.45780	-55.06206	1
241	O	65.87322	78.66720	67.12106	-243.00837	192.73507	609.52485	1
242	N	65.87115	77.53013	69.10147	343.49288	-644.25607	38.09164	1
243	H	66.52775	77.28564	69.84040	-1691.16043	-1535.97525	-1484.73099	1
244	C	64.45471	77.17469	69.13241	542.66492	350.14337	454.42563	1
245	H	64.24611	76.72228	68.13398	1209.57979	-2396.95920	463.86744	1
246	C	64.25234	76.24122	70.31004	-737.14309	145.93010	242.71942	1
247	H	64.75894	76.69277	71.19370	-1050.18303	159.36419	-2509.06125	1
248	C	62.78381	76.08750	70.65818	-706.77696	-252.88343	-245.16230	1
249	H	62.62839	75.37103	71.51128	-1624.64039	-1665.49085	1417.86935	1
250	H	62.33138	77.07686	70.96510	2566.10521	598.51109	693.22305	1
251	H	62.18742	75.70512	69.78422	-1972.69758	107.10018	-1876.34312	1
252	C	64.89081	74.88625	70.06492	412.85148	672.58832	-27.69222	1
253	H	64.79571	74.21121	70.95940	1447.02277	1762.76533	-1490.78944	1
254	H	64.41590	74.35618	69.19405	1320.77379	-145.20455	2378.68491	1
255	H	65.98845	74.98410	69.83587	-1512.10848	1470.52031	1724.75147	1
256	C	63.55885	78.56311	69.34922	-607.11113	499.56689	73.73769	1
257	O	62.43199	78.60226	68.91545	357.97126	460.81534	356.68785	1
258	N	64.22168	79.45727	70.06275	536.55407	-368.62270	332.76306	1
259	H	65.18156	79.20066	70.28835	524.38866	2297.69985	1367.20941	1
260	C	63.58211	80.58288	70.63779	46.50277	-774.29190	-147.97904	1
261	H	64.42461	81.19241	71.03228	1676.51875	1883.29066	1032.55549	1
262	C	62.72388	81.33596	69.49654	-559.41456	-34.19198	-556.30433	1
263	H	61.90410	80.65335	69.14837	-64.66664	395.18769	2695.05373	1
264	H	62.22176	82.24777	69.89909	-2703.44278	-60.40056	333.79418	1
265	C	63.63550	81.67923	68.34965	-519.76435	377.31045	459.42366	1
266	H	64.18527	80.75505	68.05408	-1746.74323	1667.50644	-1261.73691	1
267	C	62.82558	82.15942	67.15170	570.95554	16.46261	-545.27700	1
268	H	63.48457	82.40484	66.27924	2391.58273	28.05277	-1305.07271	1
269	H	62.09724	81.37970	66.80821	175.75588	917.63458	2559.43867	1
270	H	62.23669	83.08158	67.39323	-1063.97851	-2155.34650	1283.00462	1
271	C	64.65041	82.74316	68.74523	193.76014	2.62946	-765.53141	1
272	H	65.29712	83.03855	67.87921	507.39394	-846.55087	2539.60089	1
273	H	64.14986	83.67333	69.11937	1337.57841	1818.19054	1526.01994	1
274	H	65.33343	82.38164	69.55680	1100.88635	-1172.91350	-2199.08909	1
275	C	62.61240	80.06927	71.81495	-549.21115	475.64486	-309.38218	1
276	O	62.61718	78.94706	72.25182	556.06106	-390.37755	-78.24250	1
277	O	61.78754	81.05940	72.40447	-572.27940	-310.19032	-209.75862	1
278	H	62.08474	81.84388	71.86862	-1380.08193	2212.14486	790.85944	1

Listing 126: C00126.xmolout

1	276								
2	150.0000	150.0000	150.0000	0.0000	0.0000	0.0000	*****	2.7750	11100
	0.2500	300.00	0.00	0.00	0.00	-1293.3533	0.0000	300.0000	

3	H	67.54065	81.67793	77.02445	-2043.14101	-1757.64893	399.89339	1
4	N	67.38016	82.65722	77.25269	426.75047	490.45733	-334.42467	1
5	H	66.96686	82.57773	78.18035	442.25559	-1110.30854	-2448.52907	1
6	C	68.55632	83.44540	77.23464	415.32972	-666.39213	83.73172	1
7	H	69.09067	83.07757	76.33081	879.32219	2491.00447	667.35213	1
8	C	68.15199	85.00302	77.12028	31.35357	477.41777	628.23362	1
9	H	67.76463	85.35796	78.10495	1168.38489	2240.25337	-1019.71136	1
10	H	69.05130	85.62858	76.90247	-360.43770	2534.90498	931.67112	1
11	C	67.10607	85.18286	76.05237	463.18208	512.70242	-382.34388	1
12	H	66.25190	84.50422	76.27903	1725.29117	1863.52247	-987.07854	1
13	C	66.59071	86.61711	76.05496	710.42801	-144.27427	-313.15367	1
14	H	65.79901	86.77411	75.27794	364.20195	-1033.13725	2494.72524	1
15	H	66.14297	86.89358	77.04422	2567.61904	335.80679	847.48802	1
16	H	67.41161	87.35020	75.84597	-2587.99029	680.92867	-512.16411	1
17	C	67.64962	84.82241	74.67929	268.17616	741.64379	-40.42634	1
18	H	66.95791	85.14971	73.86082	1283.54314	-1945.37420	-1411.27812	1
19	H	68.66969	85.30067	74.48098	-1258.57796	1317.15249	-2026.02085	1
20	H	67.78668	83.71508	74.57400	-2502.84526	909.80597	575.92391	1
21	C	69.32444	83.09067	78.60812	619.36578	-458.64843	-172.09273	1
22	O	69.13264	82.01547	79.19148	-81.40433	433.87611	522.34594	1
23	N	70.22262	84.00516	78.86816	175.23996	-622.20190	341.55523	1
24	H	70.26615	84.80126	78.23252	-876.57256	-303.22879	-2561.90213	1
25	C	70.82327	84.18593	80.16304	-571.88214	-534.10783	-106.15033	1
26	H	70.16113	84.90089	80.69999	-2713.20841	-16.25800	-248.80809	1
27	C	70.93041	82.79802	80.94390	166.60354	288.16399	-716.09568	1
28	H	71.18732	82.00723	80.18024	-2097.85574	1636.78449	-586.18044	1
29	O	69.73706	82.32933	81.57102	-317.80580	-363.38227	484.43082	1
30	H	69.32818	81.80495	80.77710	1863.74748	-1451.84923	1357.29467	1
31	C	72.14504	83.04364	81.91153	503.80731	517.99032	318.51606	1
32	H	72.44271	82.10967	82.44212	640.61020	-2157.10410	-1536.29104	1
33	H	73.04412	83.42595	81.37031	1687.88455	465.60692	2087.56452	1
34	H	71.88966	83.79939	82.69067	-1293.07895	-1899.88581	-1463.57452	1
35	C	72.25087	84.88083	79.83713	-153.07550	-733.68902	248.70981	1
36	O	72.71432	85.58576	80.69567	186.15459	-480.78787	-449.34387	1
37	N	72.83772	84.42045	78.71944	-487.53139	543.18517	42.03850	1
38	C	73.72993	85.22994	77.95271	-699.35871	69.34393	360.10701	1
39	H	74.09216	86.00920	78.66282	2.81126	-221.99807	-2715.58072	1
40	C	74.80751	84.15559	77.50225	-507.46439	-592.59194	122.07761	1
41	H	75.43645	84.48991	76.64692	-1975.08116	525.87560	-1801.71556	1
42	H	75.50802	83.91286	78.33182	1588.27743	-1913.22100	1113.83566	1
43	C	73.88623	82.93861	77.17439	-613.62442	-457.55993	-194.14490	1
44	H	73.37499	83.07270	76.19403	1707.54637	-721.27992	1996.92523	1
45	H	74.43219	81.96996	77.12316	758.23357	2100.81767	1560.55011	1
46	C	72.84735	83.00231	78.37161	-352.41524	704.96076	49.21465	1
47	H	71.80484	82.71119	78.10264	1714.76886	-2070.42778	443.35792	1
48	H	73.15710	82.45756	79.29381	1224.15040	1801.50881	1636.97633	1
49	C	72.85125	85.88015	76.72141	566.85117	537.05831	117.62814	1
50	O	71.92902	86.60627	77.00296	-550.26779	-406.08867	4.21666	1
51	N	73.27788	85.50356	75.52271	566.34832	-425.77725	180.18749	1
52	H	74.08390	84.88562	75.45890	644.44502	2646.80550	-52.73430	1
53	C	72.83473	86.24174	74.38586	612.34801	-281.48662	411.56221	1
54	H	72.40384	87.16548	74.83760	1667.23498	-1490.75142	1556.16753	1
55	C	74.12495	86.47719	73.47580	-714.45746	-175.43074	286.98927	1
56	H	74.53965	85.48301	73.14667	-787.09484	1763.03619	-1922.46060	1
57	O	75.23914	87.13077	74.11699	-429.46514	516.51932	-128.40526	1
58	H	75.93546	86.45093	74.02752	1981.82785	436.16847	-1818.18182	1
59	C	73.50635	87.22910	72.24123	630.79189	-468.94448	76.03230	1
60	H	74.26108	87.37401	71.43380	-1775.71861	2062.30353	131.89849	1
61	H	72.64856	86.67069	71.79879	-1855.14608	88.94118	1993.53760	1
62	H	73.13281	88.23919	72.52864	-1504.82350	-780.94249	-2132.90992	1
63	C	71.67470	85.33891	73.65853	288.57638	618.62814	-397.00270	1
64	O	70.52191	85.47310	74.01644	321.70495	-185.26452	574.37218	1

65	N	72.17265	84.52444	72.74460	-447.05792	-446.53431	367.76425	1
66	H	73.17355	84.51744	72.55507	350.31316	1975.63644	-1843.31522	1
67	C	71.30193	83.69624	72.00037	-511.23061	374.03917	-471.51480	1
68	H	70.27742	83.96093	72.35158	2234.79579	-898.70890	-1273.45190	1
69	C	71.57570	84.03996	70.45470	529.53781	-159.34528	563.72604	1
70	H	70.86752	83.39975	69.86167	654.59388	2347.94251	1217.51488	1
71	H	71.26405	85.10557	70.29470	-1526.55661	2103.42026	817.87394	1
72	O	72.91961	83.80326	69.97026	-554.84278	14.12789	399.58769	1
73	H	73.30592	84.68578	70.12657	1297.06236	2061.84854	1220.68812	1
74	C	71.67229	82.11613	72.21535	-662.15484	-412.13544	123.62687	1
75	O	71.13018	81.27720	71.52866	-540.01537	-317.05804	274.91456	1
76	N	72.45646	81.94167	73.28242	-202.76299	-690.00100	-131.49145	1
77	H	72.75797	82.83962	73.66134	-702.62132	-2617.37191	281.70413	1
78	C	73.36455	80.81977	73.34218	-491.73914	576.34187	222.73509	1
79	H	73.94080	80.82722	72.39193	1977.17978	-1823.58850	-434.68928	1
80	C	74.20850	81.13216	74.63928	-649.50797	-328.66843	306.11224	1
81	H	73.50125	81.50806	75.40844	2075.07803	1452.16490	-1004.45904	1
82	C	74.95586	79.86365	75.17781	-615.18735	-489.99689	-70.96352	1
83	H	75.45646	80.06145	76.15468	-1226.32661	-1724.38906	-1716.47170	1
84	H	74.24674	79.01313	75.33487	2381.64273	-969.84735	900.46860	1
85	H	75.74437	79.52756	74.46853	2122.74991	1702.23946	-141.36228	1
86	C	75.32959	82.18812	74.33503	-501.86074	-479.61276	-376.42482	1
87	H	75.90172	82.45286	75.25483	993.79261	-2246.95401	-1177.81305	1
88	H	76.06385	81.80094	73.59068	42.71279	-626.15391	-2651.37258	1
89	H	74.90749	83.13390	73.92348	-2026.39012	-1590.33709	-887.82922	1
90	C	72.49800	79.46361	73.55470	-672.89153	382.57394	-156.34072	1
91	O	72.07329	79.15934	74.64657	410.04627	221.86223	500.35950	1
92	N	72.45632	78.72577	72.41330	-378.11782	-443.79414	-441.10984	1
93	H	72.74734	79.28894	71.61076	2404.15973	-568.14894	1149.30085	1
94	C	71.25648	77.92118	72.30644	-544.54484	466.16019	331.29119	1
95	H	70.68621	78.16653	73.23313	-1409.80988	-170.17955	2325.32679	1
96	C	70.51051	78.37804	70.99154	-184.48284	116.78282	-758.89137	1
97	H	70.25281	79.46992	71.04858	1893.78641	1861.14652	611.04528	1
98	H	71.16699	78.28510	70.09658	-2170.79665	-974.19311	1327.50117	1
99	C	69.23733	77.48455	70.84735	389.51668	672.81878	-138.49152	1
100	H	69.51509	76.40982	70.93098	510.64577	1933.03327	1851.02484	1
101	H	68.55372	77.64770	71.70951	-2302.30869	-1105.72939	-948.89774	1
102	C	68.45465	77.70984	69.50003	-559.93427	-126.34590	542.30857	1
103	O	67.49326	77.02844	69.25130	-670.36003	-111.83166	76.36448	1
104	N	68.95944	78.69051	68.71983	-216.06729	-537.07037	446.51379	1
105	H	69.74397	79.32945	68.89315	-1251.96487	1074.12894	-2168.52500	1
106	H	68.54627	78.97822	67.82572	-2451.83023	-720.73851	944.84612	1
107	C	71.65791	76.34243	72.30714	546.24052	-563.88337	-85.11809	1
108	O	71.05812	75.68953	73.12071	71.70702	-307.40463	606.69673	1
109	N	72.53216	75.92411	71.38125	479.90863	-504.50129	222.86849	1
110	C	73.03649	74.58340	71.40354	75.51268	-600.91904	506.73700	1
111	H	72.28067	73.96633	71.95167	-2033.61562	1795.30103	254.89480	1
112	C	73.21234	74.27420	69.85261	523.79067	517.99274	284.45581	1
113	H	73.90565	73.42561	69.65871	1599.61665	-1127.00911	1895.98173	1
114	H	72.24252	74.01891	69.37047	-1881.83093	1275.82488	-1501.55016	1
115	C	73.75390	75.64748	69.35000	-600.05639	-404.05026	316.64485	1
116	H	74.81754	75.79355	69.64447	-2597.05260	496.36221	657.73249	1
117	H	73.70672	75.77153	68.24470	-1666.24518	1294.38985	-1723.90591	1
118	C	72.78701	76.63569	70.13394	493.57570	-129.95376	-602.56394	1
119	H	73.22091	77.63223	70.37975	-1469.08415	-637.84797	2204.22581	1
120	H	71.78655	76.77101	69.65690	-1038.97840	1068.88701	-2280.71789	1
121	C	74.53244	74.51935	72.05313	188.88100	241.05089	-727.87821	1
122	O	75.27085	73.56731	71.81345	531.88613	-49.19943	427.07960	1
123	N	74.76578	75.55786	72.82790	708.14833	26.93417	-179.73509	1
124	H	74.00328	76.23105	72.89068	-2232.69501	-1179.09831	1023.94816	1
125	C	76.13853	75.92002	73.06440	-738.32412	259.92548	104.42456	1
126	H	76.64105	75.64961	72.10885	2028.89123	1260.02983	1311.33324	1

127	C	76.16531	77.46185	73.42303	-258.65678	-345.52513	661.28459	1
128	H	75.40861	77.66800	74.20931	-1826.06090	-1801.46097	-918.64554	1
129	C	77.60422	77.86402	73.90044	-541.23400	531.92970	-218.41428	1
130	H	77.70658	78.96640	74.03288	1311.73218	-2219.18200	882.19023	1
131	H	77.85367	77.39019	74.88156	-1048.71298	1223.58118	-2196.97971	1
132	H	78.38348	77.54417	73.17007	419.06414	1903.92898	1903.44670	1
133	C	75.86236	78.28771	72.12445	-423.86431	152.66566	-648.55262	1
134	H	75.89999	79.38589	72.31376	105.68386	-2342.50080	1387.51238	1
135	H	76.59998	78.06542	71.31833	-1695.63603	-1484.73621	-1531.02793	1
136	H	74.84901	78.05439	71.72316	-1853.57121	-487.39031	1936.59343	1
137	C	76.69043	75.01584	74.29783	539.71428	-510.58232	267.58633	1
138	O	76.84863	75.44696	75.41108	-15.93758	-278.34085	-624.49402	1
139	N	77.03455	73.81009	73.80535	-676.81886	12.05292	276.17960	1
140	H	76.65133	73.52681	72.86540	-1694.44250	-373.84189	-2100.66098	1
141	C	77.20407	72.80558	74.82677	412.33078	-664.70360	108.35451	1
142	H	77.55582	73.37861	75.71838	1765.77476	1294.44366	1621.76594	1
143	C	75.76508	72.18325	75.07272	-179.66635	-721.95667	-264.73915	1
144	H	74.98550	72.97428	75.15039	-607.34922	2587.87032	-598.10018	1
145	H	75.45485	71.53914	74.21906	-359.69332	-1479.13954	-2259.74260	1
146	C	75.90258	71.37189	76.40118	-240.01076	616.02425	431.85322	1
147	H	76.83435	70.74800	76.33719	-1359.17131	782.54425	2227.99181	1
148	H	76.05060	72.05808	77.26540	-820.36667	85.81767	-2596.78715	1
149	C	74.65772	70.43097	76.64523	-513.07015	236.18570	-551.87280	1
150	H	73.84655	70.94804	77.20696	1816.11944	-1183.11722	-1650.94321	1
151	H	74.20471	70.09346	75.68794	-1800.04429	-1361.53473	1526.34643	1
152	C	75.25891	69.23787	77.43328	726.08972	-253.19732	-179.64713	1
153	H	75.96414	68.60662	76.85305	1224.27271	-456.51798	-2390.90304	1
154	H	75.73163	69.52474	78.39878	1206.40339	-1150.93514	-2154.90344	1
155	N	74.15336	68.24749	77.86567	329.70796	-633.68968	-155.67358	1
156	H	74.60055	67.40503	78.46017	1348.31305	1938.76845	1359.00643	1
157	H	73.37906	68.62003	78.48658	2096.92035	1446.54551	-966.48890	1
158	H	73.60088	67.76564	77.10040	-1197.07217	-2303.53719	827.28733	1
159	C	78.25111	71.67324	74.32973	-378.01186	-556.17301	-413.96481	1
160	O	78.26326	70.57831	74.89783	-409.44433	-307.55053	-453.30833	1
161	N	79.00750	72.09382	73.34186	-429.02477	524.70884	274.08502	1
162	H	78.83278	73.05551	73.05161	1706.34263	-1425.96036	1574.38926	1
163	C	80.03773	71.30387	72.76912	-45.25864	-626.22952	478.93267	1
164	H	80.52604	71.99743	72.04804	1988.63164	570.90773	1772.87287	1
165	C	81.00487	70.80833	73.92098	551.77128	-20.49526	-564.54996	1
166	H	81.31643	71.65515	74.57255	1434.61535	-1753.10253	1513.99471	1
167	H	80.47364	70.09147	74.59020	-714.67738	1819.09770	1898.36494	1
168	C	82.23817	70.14464	73.22337	446.99263	-555.77305	338.97221	1
169	H	81.90186	69.28199	72.59437	1953.68466	1892.25957	-161.67766	1
170	H	82.72378	70.86337	72.52534	-403.03785	2688.07032	-188.43591	1
171	C	83.27472	69.65528	74.31194	567.86262	335.74681	434.04421	1
172	H	83.62761	70.50238	74.94389	-1080.02275	1568.26081	-1948.78900	1
173	H	82.80688	68.92682	75.01242	-919.54108	2111.34692	1456.13463	1
174	C	84.44827	69.01489	73.53294	195.81897	173.33862	-745.11536	1
175	H	84.17121	68.12327	72.93622	1405.67949	-2301.21089	-390.08113	1
176	H	85.02064	69.72370	72.90170	-940.37328	-1118.32446	2299.72133	1
177	N	85.49510	68.49618	74.57359	319.26422	656.36007	-42.02424	1
178	H	86.36182	68.04093	74.16415	1961.03633	619.91968	1787.09422	1
179	H	85.92727	69.22575	75.21033	854.14343	-2156.80752	1429.08711	1
180	H	85.18149	67.75682	75.26817	1237.02905	-1378.50857	-1998.28500	1
181	C	79.35984	69.99260	72.03956	532.53319	-268.57236	517.55729	1
182	O	79.89538	68.90688	72.07494	266.16714	-290.73804	-558.88002	1
183	N	78.28523	70.38459	71.37460	-226.25352	640.49678	-270.32839	1
184	H	78.05437	71.37346	71.46493	2007.69063	-1035.27229	1523.50231	1
185	C	77.41104	69.47886	70.72027	-540.76542	-573.33303	49.50000	1
186	H	76.70135	70.16142	70.20172	-2374.20950	-1036.76023	843.75774	1
187	C	78.28705	68.63343	69.68582	-77.09082	666.87422	-415.84136	1
188	H	78.96362	67.95813	70.28158	-985.81834	617.19825	2463.91927	1

189	O	79.14436	69.41374	68.82482	293.29899	-391.65602	-477.80926	1
190	H	80.02130	69.18390	69.18891	2528.72714	-681.76262	-751.27122	1
191	C	77.23028	67.76328	68.91372	252.47363	-605.14473	440.05134	1
192	H	77.72552	67.04910	68.21478	-2052.65063	1456.49051	-1043.51830	1
193	H	76.58662	67.15857	69.61587	-2152.98800	-1661.97574	-161.70652	1
194	H	76.54964	68.40075	68.30246	-473.12726	-1584.27339	2165.61725	1
195	C	76.64056	68.56812	71.84047	360.36307	488.46713	505.10056	1
196	O	76.11036	67.52778	71.50138	-200.08817	-528.03552	-385.82850	1
197	N	76.57661	69.18700	73.00514	-597.54095	-226.44775	355.20479	1
198	H	77.09768	70.06453	73.05982	2179.23655	-1300.70981	-991.33835	1
199	C	75.89142	68.71861	74.14681	-687.68921	297.39807	-249.45179	1
200	H	75.86431	69.62775	74.78209	-349.16256	-2467.37713	-1101.72831	1
201	C	74.46645	68.08943	73.77177	672.47345	361.54328	-201.62880	1
202	H	74.62076	67.27708	73.01547	1541.41502	582.18425	2169.97026	1
203	H	74.01285	67.61717	74.67359	-2534.67717	60.25153	997.72295	1
204	C	73.55187	69.18776	73.20920	574.26774	-389.43119	-377.02542	1
205	C	72.61187	69.86490	74.04267	688.82679	-287.33580	-257.96133	1
206	H	72.50906	69.60332	75.11140	331.14182	1470.38163	2269.80013	1
207	C	73.66030	69.52393	71.82670	-383.52382	-675.04808	144.24917	1
208	H	74.39114	68.99882	71.18190	4.09847	1517.59662	2262.86397	1
209	C	71.81084	70.85690	73.47540	-134.76730	428.45285	-649.50303	1
210	H	71.08587	71.38436	74.12006	-903.23433	1600.49020	2011.53387	1
211	C	72.82962	70.51674	71.30108	-335.53281	-615.00040	-364.39058	1
212	H	72.92036	70.76463	70.22898	1596.45398	-1369.33862	1732.02659	1
213	C	71.87528	71.21244	72.09730	585.48547	-340.24194	-406.23938	1
214	O	71.01837	72.21659	71.56668	-419.15649	-173.04408	-511.94141	1
215	H	71.26359	72.15527	70.61397	-1071.84350	1559.71507	-1960.13012	1
216	C	76.69388	67.49099	74.86128	291.41878	-183.13091	710.72246	1
217	O	76.18493	66.39496	74.91365	379.87695	523.47396	-222.23622	1
218	N	77.82852	67.91736	75.41423	564.30591	373.09380	277.24371	1
219	H	78.16413	68.90933	75.31776	-120.59931	-2436.07824	-1214.35098	1
220	C	78.66672	66.89238	75.93394	404.07514	-299.37480	608.84009	1
221	H	78.19814	65.94485	75.57410	-1071.07882	-841.69025	2359.66467	1
222	C	80.11406	67.18111	75.35866	-683.12807	68.71770	-390.13096	1
223	H	80.06208	67.47721	74.28482	2068.88918	1596.58590	770.89603	1
224	H	80.58834	68.03850	75.88746	1379.86429	2342.49779	-179.85638	1
225	C	80.93985	65.87105	75.54556	-176.39967	537.49466	550.97268	1
226	H	80.95759	65.57084	76.61549	-396.28051	1942.22168	1869.33314	1
227	H	80.46035	65.02335	75.00728	-94.44700	586.00678	-2659.20016	1
228	C	82.42101	66.11917	75.00180	-291.69381	-718.18079	-150.72929	1
229	H	82.51939	66.31255	73.90323	-2303.38776	1089.76242	964.62032	1
230	H	83.00989	66.89946	75.54709	884.16729	2568.80533	-207.74283	1
231	N	82.99341	64.86895	75.28980	-594.49522	-252.81478	342.29276	1
232	H	82.42661	64.22165	75.81615	-1735.17426	2084.05705	-263.71605	1
233	C	84.16221	64.50339	74.94762	595.23177	-271.52487	442.22352	1
234	N	84.94505	65.40884	74.22458	585.53813	-424.79750	-105.81303	1
235	H	84.72330	66.35554	73.92063	959.88797	1327.56823	-2177.11905	1
236	H	85.89406	65.23012	73.89514	1578.48647	16.27378	-2220.76233	1
237	N	84.43223	63.20250	75.39599	-452.17763	-390.33541	-421.51853	1
238	H	83.86009	62.54272	75.92075	470.26107	1974.25629	-1817.92087	1
239	H	85.31680	62.72419	75.22173	1856.67307	-1573.97321	-1224.35416	1
240	C	78.71107	67.01185	77.58347	-531.47271	-581.45780	-55.06206	1
241	O	79.16444	67.96157	78.17154	-243.00837	192.73507	609.52485	1
242	N	78.28568	65.84386	78.06951	343.49288	-644.25607	38.09164	1
243	H	77.90856	65.22034	77.35629	-1691.16043	-1535.97525	-1484.73099	1
244	C	78.01061	65.59202	79.48803	542.66492	350.14337	454.42563	1
245	H	77.54696	64.58099	79.40369	1209.57979	-2396.95920	463.86744	1
246	C	79.30860	65.56073	80.27611	-737.14309	145.93010	242.71942	1
247	H	79.60520	66.61328	80.48437	-1050.18303	159.36419	-2509.06125	1
248	C	79.14137	64.82302	81.59365	-706.77696	-252.88343	-245.16230	1
249	H	80.05492	64.91987	82.24076	-1624.64039	-1665.49085	1417.86935	1
250	H	78.26723	65.19870	82.19190	2566.10521	598.51109	693.22305	1

251	H	78.96944	63.72506	81.42858	-1972.69758	107.10018	-1876.34312	1
252	C	80.45156	64.92664	79.50196	412.85148	672.58832	-27.69222	1
253	H	81.40056	64.90262	80.10402	1447.02277	1762.76533	-1490.78944	1
254	H	80.21465	63.86807	79.20741	1320.77379	-145.20455	2378.68491	1
255	H	80.66730	65.49640	78.55874	-1512.10848	1470.52031	1724.75147	1
256	C	76.89106	66.71079	79.96268	-607.11113	499.56689	73.73769	1
257	O	75.92526	66.92987	79.22178	357.97126	460.81534	356.68785	1
258	N	77.14291	67.18002	81.15431	536.55407	-368.62270	332.76306	1
259	H	78.01564	66.83189	81.54299	524.38866	2297.69985	1367.20941	1
260	C	76.45142	68.21566	81.82077	46.50277	-774.29190	-147.97904	1
261	H	77.12871	68.45315	82.66926	1676.51875	1883.29066	1032.55549	1
262	C	76.24687	69.45367	80.80964	-559.41456	-34.19198	-556.30433	1
263	H	75.68111	69.08909	79.90996	-64.66664	395.18769	2695.05373	1
264	H	75.61361	70.24411	81.28085	-2703.44278	-60.40056	333.79418	1
265	C	77.59351	70.00315	80.42071	-519.76435	377.31045	459.42366	1
266	H	78.21196	69.16996	80.00978	-1746.74323	1667.50644	-1261.73691	1
267	C	77.46956	71.07367	79.34361	570.95554	16.46261	-545.27700	1
268	H	78.44333	71.60071	79.17063	2391.58273	28.05277	-1305.07271	1
269	H	77.16318	70.63428	78.36187	175.75588	917.63458	2559.43867	1
270	H	76.71322	71.85450	79.61735	-1063.97851	-2155.34650	1283.00462	1
271	C	78.30781	70.60462	81.62464	193.76014	2.62946	-765.53141	1
272	H	79.28166	71.07583	81.33274	507.39394	-846.55087	2539.60089	1
273	H	77.68905	71.40015	82.11485	1337.57841	1818.19054	1526.01994	1
274	H	78.53678	69.83370	82.40389	1100.88635	-1172.91350	-2199.08909	1
275	C	74.99981	67.73127	82.34442	-549.21115	475.64486	-309.38218	1
276	O	74.25763	67.00122	81.74400	556.06106	-390.37755	-78.24250	1
277	O	74.57337	68.35663	83.54231	-572.27940	-310.19032	-209.75862	1
278	H	75.39740	68.87730	83.74659	-1380.08193	2212.14486	790.85944	1

Listing 127: C00127.xmolout

1		276							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100
		0.2500	300.00	0.00	0.00	0.00	-1293.3463	0.0000	300.0000
3	H	75.73027	63.25027	70.97825	-2043.14101	-1757.64893	399.89339		1
4	N	75.62271	64.24232	70.77120	426.75047	490.45733	-334.42467		1
5	H	74.97905	64.51543	71.51272	442.25559	-1110.30854	-2448.52907		1
6	C	76.84908	64.95225	70.79158	415.32972	-666.39213	83.73172		1
7	H	77.53357	64.37321	71.44830	879.32219	2491.00447	667.35213		1
8	C	77.39714	65.05031	69.28065	31.35357	477.41777	628.23362		1
9	H	76.61193	65.51642	68.63815	1168.38489	2240.25337	-1019.71136		1
10	H	78.28266	65.72950	69.23054	-360.43770	2534.90498	931.67112		1
11	C	77.74793	63.67334	68.77555	463.18208	512.70242	-382.34388		1
12	H	76.91614	62.98114	69.03592	1725.29117	1863.52247	-987.07854		1
13	C	77.90269	63.68330	67.26011	710.42801	-144.27427	-313.15367		1
14	H	78.15501	62.66584	66.86359	364.20195	-1033.13725	2494.72524		1
15	H	76.96174	64.01487	66.74958	2567.61904	335.80679	847.48802		1
16	H	78.71959	64.37769	66.93407	-2587.99029	680.92867	-512.16411		1
17	C	79.03246	63.16320	69.41407	268.17616	741.64379	-40.42634		1
18	H	79.30376	62.14256	69.03896	1283.54314	-1945.37420	-1411.27812		1
19	H	79.89849	63.83866	69.19058	-1258.57796	1317.15249	-2026.02085		1
20	H	78.94633	63.09467	70.52891	-2502.84526	909.80597	575.92391		1
21	C	76.55957	66.44887	71.35524	619.36578	-458.64843	-172.09273		1
22	O	77.40983	67.03873	71.99584	-81.40433	433.87611	522.34594		1
23	N	75.37703	66.89585	70.94491	175.23996	-622.20190	341.55523		1
24	H	74.79215	66.25048	70.41613	-876.57256	-303.22879	-2561.90213		1
25	C	74.91872	68.15831	71.40566	-571.88214	-534.10783	-106.15033		1
26	H	75.83208	68.67379	71.77858	-2713.20841	-16.25800	-248.80809		1
27	C	74.17182	68.88372	70.18625	166.60354	288.16399	-716.09568		1
28	H	73.36382	68.19797	69.81008	-2097.85574	1636.78449	-586.18044		1
29	O	74.99115	69.19550	69.04823	-317.80580	-363.38227	484.43082		1
30	H	74.57661	68.63950	68.35703	1863.74748	-1451.84923	1357.29467		1

31	C	73.50891	70.10424	70.92386	503.80731	517.99032	318.51606	1
32	H	72.88496	70.71241	70.22863	640.61020	-2157.10410	-1536.29104	1
33	H	72.84413	69.76289	71.75436	1687.88455	465.60692	2087.56452	1
34	H	74.27476	70.78415	71.36384	-1293.07895	-1899.88581	-1463.57452	1
35	C	73.79025	67.85145	72.55477	-153.07550	-733.68902	248.70981	1
36	O	72.68510	67.52729	72.20813	186.15459	-480.78787	-449.34387	1
37	N	74.27075	68.04887	73.79356	-487.53139	543.18517	42.03850	1
38	C	73.47661	67.76183	74.94453	-699.35871	69.34393	360.10701	1
39	H	72.76410	66.95329	74.66190	2.81126	-221.99807	-2715.58072	1
40	C	74.58260	67.36705	76.01432	-507.46439	-592.59194	122.07761	1
41	H	74.21851	67.45248	77.06283	-1975.08116	525.87560	-1801.71556	1
42	H	74.92534	66.31727	75.87802	1588.27743	-1913.22100	1113.83566	1
43	C	75.71514	68.38375	75.66663	-613.62442	-457.55993	-194.14490	1
44	H	75.49705	69.38458	76.10287	1707.54637	-721.27992	1996.92523	1
45	H	76.71561	68.08349	76.05227	758.23357	2100.81767	1560.55011	1
46	C	75.64815	68.42971	74.08162	-352.41524	704.96076	49.21465	1
47	H	75.82853	69.43721	73.63784	1714.76886	-2070.42778	443.35792	1
48	H	76.29129	67.67432	73.54854	1224.15040	1801.50881	1636.97633	1
49	C	72.70585	69.11905	75.45716	566.85117	537.05831	117.62814	1
50	O	71.99127	69.05391	76.42888	-550.26779	-406.08867	4.21666	1
51	N	72.98234	70.17466	74.70125	566.34832	-425.77725	180.18749	1
52	H	73.64459	70.03904	73.94047	644.44502	2646.80550	-52.73430	1
53	C	72.48660	71.45655	75.11177	612.34801	-281.48662	411.56221	1
54	H	72.63677	71.48825	76.21471	1667.23498	-1490.75142	1556.16753	1
55	C	73.30491	72.56502	74.30489	-714.45746	-175.43074	286.98927	1
56	H	73.14572	72.40008	73.20374	-787.09484	1763.03619	-1922.46060	1
57	O	74.73114	72.54849	74.50425	-429.46514	516.51932	-128.40526	1
58	H	75.04671	72.37291	73.59517	1981.82785	436.16847	-1818.18182	1
59	C	72.55389	73.87591	74.74327	630.79189	-468.94448	76.03230	1
60	H	72.94622	74.77137	74.20787	-1775.71861	2062.30353	131.89849	1
61	H	71.45868	73.81184	74.53138	-1855.14608	88.94118	1993.53760	1
62	H	72.67014	74.06593	75.83555	-1504.82350	-780.94249	-2132.90992	1
63	C	70.90191	71.49590	74.74876	288.57638	618.62814	-397.00270	1
64	O	70.16144	72.17852	75.46255	321.70495	-185.26452	574.37218	1
65	N	70.63425	70.83750	73.64988	-447.05792	-446.53431	367.76425	1
66	H	71.42668	70.33827	73.24662	350.31316	1975.63644	-1843.31522	1
67	C	69.31258	70.65517	73.14790	-511.23061	374.03917	-471.51480	1
68	H	69.51896	69.95589	72.30457	2234.79579	-898.70890	-1273.45190	1
69	C	68.46754	69.98106	74.31173	529.53781	-159.34528	563.72604	1
70	H	67.64930	69.35711	73.86852	654.59388	2347.94251	1217.51488	1
71	H	69.14990	69.27027	74.84748	-1526.55661	2103.42026	817.87394	1
72	O	67.86355	70.87522	75.29732	-554.84278	14.12789	399.58769	1
73	H	68.68360	71.46939	75.45968	1297.06236	2061.84854	1220.68812	1
74	C	68.73952	72.08737	72.62491	-662.15484	-412.13544	123.62687	1
75	O	69.37349	72.78497	71.87506	-540.01537	-317.05804	274.91456	1
76	N	67.47844	72.25912	73.03278	-202.76299	-690.00100	-131.49145	1
77	H	67.10238	71.61135	73.74395	-702.62132	-2617.37191	281.70413	1
78	C	66.74443	73.46653	72.66613	-491.73914	576.34187	222.73509	1
79	H	67.16281	73.69648	71.65818	1977.17978	-1823.58850	-434.68928	1
80	C	65.26579	73.14260	72.69890	-649.50797	-328.66843	306.11224	1
81	H	65.03726	72.71011	73.69942	2075.07803	1452.16490	-1004.45904	1
82	C	64.40221	74.37761	72.51662	-615.18735	-489.99689	-70.96352	1
83	H	63.30630	74.12548	72.54324	-1226.32661	-1724.38906	-1716.47170	1
84	H	64.58860	75.13568	73.33048	2381.64273	-969.84735	900.46860	1
85	H	64.60506	74.88543	71.53397	2122.74991	1702.23946	-141.36228	1
86	C	64.89123	72.10613	71.65355	-501.86074	-479.61276	-376.42482	1
87	H	63.80869	71.81036	71.72846	993.79261	-2246.95401	-1177.81305	1
88	H	65.05805	72.49372	70.61107	42.71279	-626.15391	-2651.37258	1
89	H	65.50473	71.16983	71.76086	-2026.39012	-1590.33709	-887.82922	1
90	C	67.13387	74.65582	73.78278	-672.89153	382.57394	-156.34072	1
91	O	66.35554	74.94023	74.65928	410.04627	221.86223	500.35950	1
92	N	68.32735	75.14562	73.51812	-378.11782	-443.79414	-441.10984	1

93	H	68.81537	74.66203	72.75912	2404.15973	-568.14894	1149.30085	1
94	C	68.94409	76.22898	74.21465	-544.54484	466.16019	331.29119	1
95	H	69.99195	75.86268	74.28740	-1409.80988	-170.17955	2325.32679	1
96	C	68.84980	77.52216	73.30081	-184.48284	116.78282	-758.89137	1
97	H	69.03524	77.26805	72.23238	1893.78641	1861.14652	611.04528	1
98	H	67.82715	77.96198	73.34369	-2170.79665	-974.19311	1327.50117	1
99	C	69.91887	78.52971	73.83328	389.51668	672.81878	-138.49152	1
100	H	69.65456	78.83761	74.86998	510.64577	1933.03327	1851.02484	1
101	H	70.90335	78.02478	73.94239	-2302.30869	-1105.72939	-948.89774	1
102	C	70.10023	79.81323	72.94296	-559.93427	-126.34590	542.30857	1
103	O	71.03341	80.54936	73.15473	-670.36003	-111.83166	76.36448	1
104	N	69.13629	79.99074	72.01786	-216.06729	-537.07037	446.51379	1
105	H	68.32634	79.39775	71.80112	-1251.96487	1074.12894	-2168.52500	1
106	H	69.11208	80.77221	71.35328	-2451.83023	-720.73851	944.84612	1
107	C	68.25796	76.59971	75.64302	546.24052	-563.88337	-85.11809	1
108	O	67.87840	77.73322	75.78587	71.70702	-307.40463	606.69673	1
109	N	68.34543	75.61672	76.55097	479.90863	-504.50129	222.86849	1
110	C	67.36218	75.48388	77.58186	75.51268	-600.91904	506.73700	1
111	H	66.41987	75.91010	77.16703	-2033.61562	1795.30103	254.89480	1
112	C	67.34960	73.91747	77.82862	523.79067	517.99274	284.45581	1
113	H	66.97074	73.64119	78.83858	1599.61665	-1127.00911	1895.98173	1
114	H	66.69510	73.40266	77.08892	-1881.83093	1275.82488	-1501.55016	1
115	C	68.84575	73.53713	77.59941	-600.05639	-404.05026	316.64485	1
116	H	69.48283	73.81150	78.46763	-2597.05260	496.36221	657.73249	1
117	H	69.00947	72.44984	77.41521	-1666.24518	1294.38985	-1723.90591	1
118	C	69.17573	74.43626	76.33035	493.57570	-129.95376	-602.56394	1
119	H	70.23945	74.75688	76.23121	-1469.08415	-637.84797	2204.22581	1
120	H	68.82614	74.00850	75.35841	-1038.97840	1068.88701	-2280.71789	1
121	C	67.81985	76.24828	78.95856	188.88100	241.05089	-727.87821	1
122	O	66.98639	76.51350	79.79557	531.88613	-49.19943	427.07960	1
123	N	69.13937	76.40645	79.02583	708.14833	26.93417	-179.73509	1
124	H	69.66475	76.05230	78.22743	-2232.69501	-1179.09831	1023.94816	1
125	C	69.68350	77.00225	80.18937	-738.32412	259.92548	104.42456	1
126	H	68.79364	77.29583	80.79520	2028.89123	1260.02983	1311.33324	1
127	C	70.59511	75.91661	80.91422	-258.65678	-345.52513	661.28459	1
128	H	71.47264	75.66484	80.27987	-1826.06090	-1801.46097	-918.64554	1
129	C	71.04612	76.48775	82.30092	-541.23400	531.92970	-218.41428	1
130	H	71.74265	75.79023	82.82343	1311.73218	-2219.18200	882.19023	1
131	H	71.57908	77.46582	82.18913	-1048.71298	1223.58118	-2196.97971	1
132	H	70.17584	76.66119	82.97674	419.06414	1903.92898	1903.44670	1
133	C	69.75478	74.63288	81.23149	-423.86431	152.66566	-648.55262	1
134	H	70.37751	73.83885	81.70692	105.68386	-2342.50080	1387.51238	1
135	H	68.91278	74.85959	81.92665	-1695.63603	-1484.73621	-1531.02793	1
136	H	69.30559	74.19860	80.30959	-1853.57121	-487.39031	1936.59343	1
137	C	70.65990	78.26655	79.78756	539.71428	-510.58232	267.58633	1
138	O	70.94152	79.04605	80.66604	-15.93758	-278.34085	-624.49402	1
139	N	71.17959	78.15753	78.56802	-676.81886	12.05292	276.17960	1
140	H	70.81437	77.34776	78.06453	-1694.44250	-373.84189	-2100.66098	1
141	C	71.56168	79.27387	77.75647	412.33078	-664.70360	108.35451	1
142	H	72.03290	78.76125	76.88872	1765.77476	1294.44366	1621.76594	1
143	C	70.26286	80.07089	77.34039	-179.66635	-721.95667	-264.73915	1
144	H	69.46809	79.40028	76.93885	-607.34922	2587.87032	-598.10018	1
145	H	69.81388	80.59404	78.21538	-359.69332	-1479.13954	-2259.74260	1
146	C	70.79341	81.08161	76.26777	-240.01076	616.02425	431.85322	1
147	H	71.58803	81.71611	76.72256	-1359.17131	782.54425	2227.99181	1
148	H	71.28408	80.53774	75.42616	-820.36667	85.81767	-2596.78715	1
149	C	69.63700	81.99556	75.70141	-513.07015	236.18570	-551.87280	1
150	H	68.87813	81.39477	75.14822	1816.11944	-1183.11722	-1650.94321	1
151	H	69.08826	82.51760	76.51885	-1800.04429	-1361.53473	1526.34643	1
152	C	70.35742	82.99842	74.76605	726.08972	-253.19732	-179.64713	1
153	H	71.00074	83.73651	75.28740	1224.27271	-456.51798	-2390.90304	1
154	H	70.92383	82.51933	73.93482	1206.40339	-1150.93514	-2154.90344	1

155	N	69.27925	83.85415	74.03019	329.70796	-633.68968	-155.67358	1
156	H	69.65815	84.59048	73.36650	1348.31305	1938.76845	1359.00643	1
157	H	68.62164	83.32000	73.39206	2096.92035	1446.54551	-966.48890	1
158	H	68.60798	84.42530	74.62204	-1197.07217	-2303.53719	827.28733	1
159	C	72.55389	80.34730	78.49375	-378.01186	-556.17301	-413.96481	1
160	O	72.13247	81.28476	79.12469	-409.44433	-307.55053	-453.30833	1
161	N	73.81151	80.08006	78.16897	-429.02477	524.70884	274.08502	1
162	H	74.12915	79.30821	77.56294	1706.34263	-1425.96036	1574.38926	1
163	C	74.83617	80.69904	78.97971	-45.25864	-626.22952	478.93267	1
164	H	74.67518	81.79553	78.87052	1988.63164	570.90773	1772.87287	1
165	C	74.58129	80.24548	80.47563	551.77128	-20.49526	-564.54996	1
166	H	73.50300	80.39935	80.72671	1434.61535	-1753.10253	1513.99471	1
167	H	74.76134	79.15239	80.59300	-714.67738	1819.09770	1898.36494	1
168	C	75.49387	81.06155	81.44828	446.99263	-555.77305	338.97221	1
169	H	76.56801	80.82413	81.27817	1953.68466	1892.25957	-161.67766	1
170	H	75.38395	82.15467	81.26914	-403.03785	2688.07032	-188.43591	1
171	C	75.08442	80.69718	82.93246	567.86262	335.74681	434.04421	1
172	H	74.01946	80.96013	83.12974	-1080.02275	1568.26081	-1948.78900	1
173	H	75.16315	79.59961	83.10938	-919.54108	2111.34692	1456.13463	1
174	C	76.03415	81.48027	83.86849	195.81897	173.33862	-745.11536	1
175	H	77.10366	81.20538	83.77409	1405.67949	-2301.21089	-390.08113	1
176	H	75.92227	82.58189	83.82141	-940.37328	-1118.32446	2299.72133	1
177	N	75.66494	81.11118	85.34516	319.26422	656.36007	-42.02424	1
178	H	76.24761	81.58403	86.09521	1961.03633	619.91968	1787.09422	1
179	H	74.68132	81.34388	85.66897	854.14343	-2156.80752	1429.08711	1
180	H	75.75287	80.09135	85.62592	1237.02905	-1378.50857	-1998.28500	1
181	C	76.14535	80.12239	78.23171	532.53319	-268.57236	517.55729	1
182	O	75.99836	79.44110	77.20703	266.16714	-290.73804	-558.88002	1
183	N	77.25307	80.46001	78.84943	-226.25352	640.49678	-270.32839	1
184	H	77.17627	81.07206	79.66068	2007.69063	-1035.27229	1523.50231	1
185	C	78.51775	80.32263	78.18920	-540.76542	-573.33303	49.50000	1
186	H	78.30467	80.71820	77.17123	-2374.20950	-1036.76023	843.75774	1
187	C	79.55370	81.17792	79.04072	-77.09082	666.87422	-415.84136	1
188	H	79.69215	80.68666	80.04300	-985.81834	617.19825	2463.91927	1
189	O	79.15473	82.53574	79.32170	293.29899	-391.65602	-477.80926	1
190	H	79.18356	82.54626	80.29834	2528.72714	-681.76262	-751.27122	1
191	C	80.86934	81.00231	78.19561	252.47363	-605.14473	440.05134	1
192	H	81.74205	81.48002	78.69866	-2052.65063	1456.49051	-1043.51830	1
193	H	81.12224	79.92467	78.04247	-2152.98800	-1661.97574	-161.70652	1
194	H	80.77259	81.46850	77.18763	-473.12726	-1584.27339	2165.61725	1
195	C	78.91799	78.73832	78.14656	360.36307	488.46713	505.10056	1
196	O	79.76118	78.29417	78.88770	-200.08817	-528.03552	-385.82850	1
197	N	78.21281	78.10753	77.21097	-597.54095	-226.44775	355.20479	1
198	H	77.42206	78.57356	76.70315	2179.23655	-1300.70981	-991.33835	1
199	C	78.56281	76.76223	76.96083	-687.68921	297.39807	-249.45179	1
200	H	79.21145	76.43951	77.80895	-349.16256	-2467.37713	-1101.72831	1
201	C	77.22367	75.91492	76.73389	672.47345	361.54328	-201.62880	1
202	H	76.76555	76.17764	75.75287	1541.41502	582.18425	2169.97026	1
203	H	77.47142	74.82989	76.68072	-2534.67717	60.25153	997.72295	1
204	C	76.22467	76.19818	77.86459	574.26774	-389.43119	-377.02542	1
205	C	76.60658	76.05875	79.23319	688.82679	-287.33580	-257.96133	1
206	H	77.61673	75.70129	79.50326	331.14182	1470.38163	2269.80013	1
207	C	74.91542	76.64589	77.51587	-383.52382	-675.04808	144.24917	1
208	H	74.61373	76.74809	76.45755	4.09847	1517.59662	2262.86397	1
209	C	75.68987	76.42010	80.22017	-134.76730	428.45285	-649.50303	1
210	H	75.99266	76.33260	81.27799	-903.23433	1600.49020	2011.53387	1
211	C	74.03639	76.98868	78.54442	-335.53281	-615.00040	-364.39058	1
212	H	73.03382	77.35230	78.26983	1596.45398	-1369.33862	1732.02659	1
213	C	74.38517	76.91094	79.92242	585.48547	-340.24194	-406.23938	1
214	O	73.49548	77.28776	80.96048	-419.15649	-173.04408	-511.94141	1
215	H	72.77570	77.71319	80.42192	-1071.84350	1559.71507	-1960.13012	1
216	C	79.27369	76.66313	75.47653	291.41878	-183.13091	710.72246	1

217	O	78.82780	77.22461	74.50246	379.87695	523.47396	-222.23622	1
218	N	80.22137	75.74250	75.56284	564.30591	373.09380	277.24371	1
219	H	80.40349	75.35160	76.48604	-120.59931	-2436.07824	-1214.35098	1
220	C	81.12153	75.48736	74.48971	404.07514	-299.37480	608.84009	1
221	H	81.57135	74.49892	74.73563	-1071.07882	-841.69025	2359.66467	1
222	C	80.25886	75.47980	73.15633	-683.12807	68.71770	-390.13096	1
223	H	79.27306	75.00073	73.35466	2068.88918	1596.58590	770.89603	1
224	H	80.01964	76.52422	72.83678	1379.86429	2342.49779	-179.85638	1
225	C	81.02217	74.71765	72.03042	-176.39967	537.49466	550.97268	1
226	H	81.91607	75.28758	71.68692	-396.28051	1942.22168	1869.33314	1
227	H	81.41032	73.74169	72.39786	-94.44700	586.00678	-2659.20016	1
228	C	79.98281	74.49874	70.83585	-291.69381	-718.18079	-150.72929	1
229	H	79.08519	73.87097	71.06828	-2303.38776	1089.76242	964.62032	1
230	H	79.63425	75.44190	70.34254	884.16729	2568.80533	-207.74283	1
231	N	80.78048	73.80508	69.91422	-594.49522	-252.81478	342.29276	1
232	H	81.77708	73.83793	70.06801	-1735.17426	2084.05705	-263.71605	1
233	C	80.34425	73.17191	68.90132	595.23177	-271.52487	442.22352	1
234	N	78.96332	73.15018	68.68298	585.53813	-424.79750	-105.81303	1
235	H	78.21453	73.58899	69.21727	959.88797	1327.56823	-2177.11905	1
236	H	78.50192	72.67983	67.90349	1578.48647	16.27378	-2220.76233	1
237	N	81.40313	72.60200	68.18064	-452.17763	-390.33541	-421.51853	1
238	H	82.41014	72.65751	68.32608	470.26107	1974.25629	-1817.92087	1
239	H	81.27440	72.07787	67.31459	1856.67307	-1573.97321	-1224.35416	1
240	C	82.24645	76.66823	74.46066	-531.47271	-581.45780	-55.06206	1
241	O	82.19012	77.70561	75.07622	-243.00837	192.73507	609.52485	1
242	N	83.22646	76.23771	73.67683	343.49288	-644.25607	38.09164	1
243	H	83.24990	75.34672	73.14721	-1691.16043	-1535.97525	-1484.73099	1
244	C	84.26831	77.16127	73.34396	542.66492	350.14337	454.42563	1
245	H	83.81837	78.17854	73.30083	1209.57979	-2396.95920	463.86744	1
246	C	85.37849	77.04684	74.47781	-737.14309	145.93010	242.71942	1
247	H	85.76609	76.00722	74.53676	-1050.18303	159.36419	-2509.06125	1
248	C	86.53732	78.05761	74.18318	-706.77696	-252.88343	-245.16230	1
249	H	87.30565	78.04512	74.99152	-1624.64039	-1665.49085	1417.86935	1
250	H	87.06062	77.81724	73.22822	2566.10521	598.51109	693.22305	1
251	H	86.15781	79.10318	74.10252	-1972.69758	107.10018	-1876.34312	1
252	C	84.73056	77.46365	75.84392	412.85148	672.58832	-27.69222	1
253	H	85.48705	77.52136	76.66184	1447.02277	1762.76533	-1490.78944	1
254	H	84.23194	78.46097	75.77318	1320.77379	-145.20455	2378.68491	1
255	H	83.94887	76.73207	76.16333	-1512.10848	1470.52031	1724.75147	1
256	C	84.73986	76.50368	71.92650	-607.11113	499.56689	73.73769	1
257	O	84.37236	75.36676	71.66585	357.97126	460.81534	356.68785	1
258	N	85.49617	77.34307	71.24318	536.55407	-368.62270	332.76306	1
259	H	85.68131	78.24545	71.68324	524.38866	2297.69985	1367.20941	1
260	C	86.18157	76.96687	70.06343	46.50277	-774.29190	-147.97904	1
261	H	86.86953	77.82262	69.88428	1676.51875	1883.29066	1032.55549	1
262	C	86.95237	75.56168	70.25812	-559.41456	-34.19198	-556.30433	1
263	H	86.20230	74.76270	70.48217	-64.66664	395.18769	2695.05373	1
264	H	87.43877	75.26796	69.29730	-2703.44278	-60.40056	333.79418	1
265	C	87.96650	75.65392	71.36483	-519.76435	377.31045	459.42366	1
266	H	87.42638	75.84580	72.31933	-1746.74323	1667.50644	-1261.73691	1
267	C	88.72826	74.33909	71.48765	570.95554	16.46261	-545.27700	1
268	H	89.47726	74.37047	72.32028	2391.58273	28.05277	-1305.07271	1
269	H	88.04012	73.47848	71.69003	175.75588	917.63458	2559.43867	1
270	H	89.28955	74.10044	70.54762	-1063.97851	-2155.34650	1283.00462	1
271	C	88.95812	76.78650	71.13311	193.76014	2.62946	-765.53141	1
272	H	89.76600	76.79351	71.90937	507.39394	-846.55087	2539.60089	1
273	H	89.45831	76.69801	70.13437	1337.57841	1818.19054	1526.01994	1
274	H	88.45982	77.78907	71.16821	1100.88635	-1172.91350	-2199.08909	1
275	C	85.09896	76.80009	68.88309	-549.21115	475.64486	-309.38218	1
276	O	85.18885	75.95577	68.03125	556.06106	-390.37755	-78.24250	1
277	O	84.11483	77.81622	68.79577	-572.27940	-310.19032	-209.75862	1
278	H	84.29523	78.27468	69.66457	-1380.08193	2212.14486	790.85944	1

Listing 128: C00128.xmolout

1	276								
2	150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.7750	11100	
	0.2500	300.00	0.00	0.00	0.00	-1293.3450	0.0000	300.0000	
3	H	64.38604	79.26139	81.78076	-2043.14101	-1757.64893	399.89339	1	
4	N	64.65841	80.04452	82.36809	426.75047	490.45733	-334.42467	1	
5	H	64.67693	79.62902	83.29498	442.25559	-1110.30854	-2448.52907	1	
6	C	65.81945	80.74866	81.96694	415.32972	-666.39213	83.73172	1	
7	H	65.70648	80.85711	80.85596	879.32219	2491.00447	667.35213	1	
8	C	65.85710	82.17573	82.74243	31.35357	477.41777	628.23362	1	
9	H	66.07936	81.99742	83.82101	1168.38489	2240.25337	-1019.71136	1	
10	H	66.70004	82.79829	82.36070	-360.43770	2534.90498	931.67112	1	
11	C	64.54320	82.88404	82.59565	463.18208	512.70242	-382.34388	1	
12	H	63.73037	82.16583	82.85082	1725.29117	1863.52247	-987.07854	1	
13	C	64.46118	84.06702	83.55397	710.42801	-144.27427	-313.15367	1	
14	H	63.47770	84.59722	83.47385	364.20195	-1033.13725	2494.72524	1	
15	H	64.57868	83.74561	84.62070	2567.61904	335.80679	847.48802	1	
16	H	65.26206	84.82195	83.34608	-2587.99029	680.92867	-512.16411	1	
17	C	64.33244	83.37027	81.16713	268.17616	741.64379	-40.42634	1	
18	H	63.35502	83.90592	81.05324	1283.54314	-1945.37420	-1411.27812	1	
19	H	65.13945	84.07953	80.84994	-1258.57796	1317.15249	-2026.02085	1	
20	H	64.33235	82.51941	80.43808	-2502.84526	909.80597	575.92391	1	
21	C	67.13395	79.96382	82.36195	619.36578	-458.64843	-172.09273	1	
22	O	68.30738	80.47391	82.23277	-81.40433	433.87611	522.34594	1	
23	N	66.95051	78.74408	82.80402	175.23996	-622.20190	341.55523	1	
24	H	66.00191	78.40045	82.93629	-876.57256	-303.22879	-2561.90213	1	
25	C	68.05103	78.33826	83.63375	-571.88214	-534.10783	-106.15033	1	
26	H	67.88759	78.95413	84.54199	-2713.20841	-16.25800	-248.80809	1	
27	C	67.87192	76.81960	83.98839	166.60354	288.16399	-716.09568	1	
28	H	67.73513	76.20633	83.05148	-2097.85574	1636.78449	-586.18044	1	
29	O	66.68073	76.49472	84.76250	-317.80580	-363.38227	484.43082	1	
30	H	66.24052	75.85702	84.17626	1863.74748	-1451.84923	1357.29467	1	
31	C	69.25625	76.49844	84.66567	503.80731	517.99032	318.51606	1	
32	H	69.36407	75.41023	84.88160	640.61020	-2157.10410	-1536.29104	1	
33	H	70.11552	76.80045	84.02114	1687.88455	465.60692	2087.56452	1	
34	H	69.36817	77.04076	85.63321	-1293.07895	-1899.88581	-1463.57452	1	
35	C	69.43000	78.98028	82.86274	-153.07550	-733.68902	248.70981	1	
36	O	70.31403	79.38573	83.62727	186.15459	-480.78787	-449.34387	1	
37	N	69.73117	78.30771	81.69344	-487.53139	543.18517	42.03850	1	
38	C	70.84958	78.67264	80.92097	-699.35871	69.34393	360.10701	1	
39	H	71.54334	79.22613	81.59968	2.81126	-221.99807	-2715.58072	1	
40	C	71.33705	77.24216	80.39252	-507.46439	-592.59194	122.07761	1	
41	H	72.03712	77.31563	79.53124	-1975.08116	525.87560	-1801.71556	1	
42	H	71.85844	76.66673	81.18901	1588.27743	-1913.22100	1113.83566	1	
43	C	69.96638	76.60454	80.02821	-613.62442	-457.55993	-194.14490	1	
44	H	69.56873	77.01245	79.07170	1707.54637	-721.27992	1996.92523	1	
45	H	70.00498	75.49863	79.91281	758.23357	2100.81767	1560.55011	1	
46	C	69.09082	77.07712	81.27865	-352.41524	704.96076	49.21465	1	
47	H	68.01938	77.30324	81.05773	1714.76886	-2070.42778	443.35792	1	
48	H	69.15583	76.39088	82.15556	1224.15040	1801.50881	1636.97633	1	
49	C	70.49240	79.49802	79.52625	566.85117	537.05831	117.62814	1	
50	O	71.41339	79.69567	78.72909	-550.26779	-406.08867	4.21666	1	
51	N	69.22349	79.75563	79.41061	566.34832	-425.77725	180.18749	1	
52	H	68.74620	79.48315	80.27135	644.44502	2646.80550	-52.73430	1	
53	C	68.59189	80.65232	78.48820	612.34801	-281.48662	411.56221	1	
54	H	68.47419	81.58962	79.07426	1667.23498	-1490.75142	1556.16753	1	
55	C	69.44376	80.86586	77.16847	-714.45746	-175.43074	286.98927	1	
56	H	69.80510	79.85602	76.82173	-787.09484	1763.03619	-1922.46060	1	
57	O	70.64539	81.64063	77.28636	-429.46514	516.51932	-128.40526	1	

58	H	71.26437	80.91966	77.68758	1981.82785	436.16847	-1818.18182	1
59	C	68.37878	81.46627	76.18134	630.79189	-468.94448	76.03230	1
60	H	68.83461	81.73013	75.20006	-1775.71861	2062.30353	131.89849	1
61	H	67.53638	80.75658	75.97189	-1855.14608	88.94118	1993.53760	1
62	H	67.93108	82.40231	76.58883	-1504.82350	-780.94249	-2132.90992	1
63	C	67.13213	79.95798	78.24704	288.57638	618.62814	-397.00270	1
64	O	66.17717	80.36707	78.87042	321.70495	-185.26452	574.37218	1
65	N	67.19631	78.93008	77.40199	-447.05792	-446.53431	367.76425	1
66	H	68.09827	78.73744	76.96754	350.31316	1975.63644	-1843.31522	1
67	C	65.96255	78.54619	76.72941	-511.23061	374.03917	-471.51480	1
68	H	65.36825	78.22019	77.61350	2234.79579	-898.70890	-1273.45190	1
69	C	65.32401	79.80119	76.05913	529.53781	-159.34528	563.72604	1
70	H	64.26696	79.59734	75.77542	654.59388	2347.94251	1217.51488	1
71	H	65.30333	80.64963	76.77828	-1526.55661	2103.42026	817.87394	1
72	O	65.94253	80.33230	74.66295	-554.84278	14.12789	399.58769	1
73	H	65.13563	80.70312	74.33264	1297.06236	2061.84854	1220.68812	1
74	C	66.32763	77.33360	75.71793	-662.15484	-412.13544	123.62687	1
75	O	66.70530	76.27769	76.13868	-540.01537	-317.05804	274.91456	1
76	N	66.05157	77.68022	74.44284	-202.76299	-690.00100	-131.49145	1
77	H	65.81933	78.68499	74.21745	-702.62132	-2617.37191	281.70413	1
78	C	66.48733	76.75091	73.35928	-491.73914	576.34187	222.73509	1
79	H	66.63294	75.78567	73.90694	1977.17978	-1823.58850	-434.68928	1
80	C	65.35848	76.69588	72.33976	-649.50797	-328.66843	306.11224	1
81	H	65.22300	77.71958	71.92548	2075.07803	1452.16490	-1004.45904	1
82	C	65.66753	75.75865	71.18794	-615.18735	-489.99689	-70.96352	1
83	H	64.81338	75.70112	70.45794	-1226.32661	-1724.38906	-1716.47170	1
84	H	66.57770	76.08997	70.61274	2381.64273	-969.84735	900.46860	1
85	H	65.86800	74.71263	71.54993	2122.74991	1702.23946	-141.36228	1
86	C	64.05003	76.28994	72.99491	-501.86074	-479.61276	-376.42482	1
87	H	63.19212	76.30996	72.26833	993.79261	-2246.95401	-1177.81305	1
88	H	64.10735	75.24870	73.41597	42.71279	-626.15391	-2651.37258	1
89	H	63.78786	76.97535	73.84717	-2026.39012	-1590.33709	-887.82922	1
90	C	67.85523	77.29327	72.71656	-672.89153	382.57394	-156.34072	1
91	O	68.44683	76.66743	71.76917	410.04627	221.86223	500.35950	1
92	N	68.32202	78.38508	73.24483	-378.11782	-443.79414	-441.10984	1
93	H	67.74115	78.82686	73.95370	2404.15973	-568.14894	1149.30085	1
94	C	69.31681	79.01478	72.41837	-544.54484	466.16019	331.29119	1
95	H	68.72305	79.69430	71.77708	-1409.80988	-170.17955	2325.32679	1
96	C	70.27433	79.77923	73.37973	-184.48284	116.78282	-758.89137	1
97	H	69.71374	80.51724	73.99572	1893.78641	1861.14652	611.04528	1
98	H	70.74209	79.07004	74.10217	-2170.79665	-974.19311	1327.50117	1
99	C	71.36885	80.48214	72.50385	389.51668	672.81878	-138.49152	1
100	H	71.85317	79.74275	71.82843	510.64577	1933.03327	1851.02484	1
101	H	70.89733	81.21196	71.81048	-2302.30869	-1105.72939	-948.89774	1
102	C	72.46541	81.20178	73.37201	-559.93427	-126.34590	542.30857	1
103	O	73.47730	81.58671	72.84352	-670.36003	-111.83166	76.36448	1
104	N	72.13977	81.35845	74.67530	-216.06729	-537.07037	446.51379	1
105	H	71.28922	81.12372	75.20286	-1251.96487	1074.12894	-2168.52500	1
106	H	72.72777	81.86980	75.34287	-2451.83023	-720.73851	944.84612	1
107	C	70.09003	77.75982	71.57790	546.24052	-563.88337	-85.11809	1
108	O	70.96983	77.10705	72.15377	71.70702	-307.40463	606.69673	1
109	N	70.17884	78.12312	70.24781	479.90863	-504.50129	222.86849	1
110	C	70.78497	77.26072	69.30762	75.51268	-600.91904	506.73700	1
111	H	70.72668	76.22101	69.70871	-2033.61562	1795.30103	254.89480	1
112	C	69.94870	77.56683	67.97523	523.79067	517.99274	284.45581	1
113	H	70.48735	77.26988	67.04817	1599.61665	-1127.00911	1895.98173	1
114	H	68.97515	77.02891	67.96822	-1881.83093	1275.82488	-1501.55016	1
115	C	69.75331	79.10169	68.11176	-600.05639	-404.05026	316.64485	1
116	H	70.69512	79.64616	67.86522	-2597.05260	496.36221	657.73249	1
117	H	68.95507	79.51543	67.45632	-1666.24518	1294.38985	-1723.90591	1
118	C	69.41658	79.20743	69.67334	493.57570	-129.95376	-602.56394	1
119	H	69.73827	80.16074	70.15778	-1469.08415	-637.84797	2204.22581	1

120	H	68.34886	79.00235	69.93234	-1038.97840	1068.88701	-2280.71789	1
121	C	72.33507	77.75430	69.02881	188.88100	241.05089	-727.87821	1
122	O	72.61393	78.91523	68.86919	531.88613	-49.19943	427.07960	1
123	N	73.09978	76.68686	68.92225	708.14833	26.93417	-179.73509	1
124	H	72.79269	75.70156	69.02457	-2232.69501	-1179.09831	1023.94816	1
125	C	74.50954	76.85451	68.73471	-738.32412	259.92548	104.42456	1
126	H	74.66157	77.65405	67.97564	2028.89123	1260.02983	1311.33324	1
127	C	75.14330	77.25031	70.13929	-258.65678	-345.52513	661.28459	1
128	H	74.83779	76.51911	70.92075	-1826.06090	-1801.46097	-918.64554	1
129	C	76.70243	77.27893	69.99599	-541.23400	531.92970	-218.41428	1
130	H	77.19350	77.62960	70.93397	1311.73218	-2219.18200	882.19023	1
131	H	77.10674	76.25978	69.78103	-1048.71298	1223.58118	-2196.97971	1
132	H	77.03152	77.95595	69.17278	419.06414	1903.92898	1903.44670	1
133	C	74.66068	78.68643	70.54412	-423.86431	152.66566	-648.55262	1
134	H	75.28559	79.11998	71.36086	105.68386	-2342.50080	1387.51238	1
135	H	74.69648	79.39456	69.68014	-1695.63603	-1484.73621	-1531.02793	1
136	H	73.60636	78.67049	70.91349	-1853.57121	-487.39031	1936.59343	1
137	C	74.88058	75.33816	68.27053	539.71428	-510.58232	267.58633	1
138	O	74.05276	74.45473	68.45161	-15.93758	-278.34085	-624.49402	1
139	N	76.08446	75.26453	67.73227	-676.81886	12.05292	276.17960	1
140	H	76.64406	76.11462	67.67448	-1694.44250	-373.84189	-2100.66098	1
141	C	76.57574	74.00611	67.28256	412.33078	-664.70360	108.35451	1
142	H	75.64795	73.40679	67.13010	1765.77476	1294.44366	1621.76594	1
143	C	77.40604	74.32449	65.97107	-179.66635	-721.95667	-264.73915	1
144	H	76.75449	74.82264	65.21899	-607.34922	2587.87032	-598.10018	1
145	H	78.21222	75.06052	66.18375	-359.69332	-1479.13954	-2259.74260	1
146	C	78.01523	73.01157	65.37975	-240.01076	616.02425	431.85322	1
147	H	78.66299	72.50119	66.12753	-1359.17131	782.54425	2227.99181	1
148	H	77.21634	72.28423	65.11287	-820.36667	85.81767	-2596.78715	1
149	C	78.84813	73.43651	64.10214	-513.07015	236.18570	-551.87280	1
150	H	78.20164	73.98081	63.37611	1816.11944	-1183.11722	-1650.94321	1
151	H	79.65519	74.15254	64.38020	-1800.04429	-1361.53473	1526.34643	1
152	C	79.44808	72.17295	63.44519	726.08972	-253.19732	-179.64713	1
153	H	80.19447	71.63836	64.06576	1224.27271	-456.51798	-2390.90304	1
154	H	78.69953	71.45668	63.05186	1206.40339	-1150.93514	-2154.90344	1
155	N	80.24719	72.63779	62.17893	329.70796	-633.68968	-155.67358	1
156	H	80.71764	71.86601	61.62386	1348.31305	1938.76845	1359.00643	1
157	H	79.69916	73.13519	61.41814	2096.92035	1446.54551	-966.48890	1
158	H	81.05792	73.30468	62.33526	-1197.07217	-2303.53719	827.28733	1
159	C	77.50460	73.36067	68.46844	-378.01186	-556.17301	-413.96481	1
160	O	77.08482	72.41064	69.12055	-409.44433	-307.55053	-453.30833	1
161	N	78.66589	73.96714	68.57802	-429.02477	524.70884	274.08502	1
162	H	78.85098	74.77536	67.99011	1706.34263	-1425.96036	1574.38926	1
163	C	79.65365	73.32536	69.39291	-45.25864	-626.22952	478.93267	1
164	H	79.39143	72.24930	69.26212	1988.63164	570.90773	1772.87287	1
165	C	81.09378	73.74409	68.89905	551.77128	-20.49526	-564.54996	1
166	H	81.24164	73.50875	67.82092	1434.61535	-1753.10253	1513.99471	1
167	H	81.24048	74.84344	68.99571	-714.67738	1819.09770	1898.36494	1
168	C	82.10144	72.96041	69.80654	446.99263	-555.77305	338.97221	1
169	H	81.87845	73.16315	70.88043	1953.68466	1892.25957	-161.67766	1
170	H	81.98984	71.86109	69.67199	-403.03785	2688.07032	-188.43591	1
171	C	83.57088	73.42578	69.45818	567.86262	335.74681	434.04421	1
172	H	83.85413	73.12747	68.42250	-1080.02275	1568.26081	-1948.78900	1
173	H	83.65480	74.53650	69.49038	-919.54108	2111.34692	1456.13463	1
174	C	84.50281	72.77520	70.50804	195.81897	173.33862	-745.11536	1
175	H	84.31552	73.09945	71.55139	1405.67949	-2301.21089	-390.08113	1
176	H	84.55244	71.66905	70.46027	-940.37328	-1118.32446	2299.72133	1
177	N	85.96101	73.25600	70.20688	319.26422	656.36007	-42.02424	1
178	H	86.70515	72.90496	70.87641	1961.03633	619.91968	1787.09422	1
179	H	86.37791	72.98433	69.26921	854.14343	-2156.80752	1429.08711	1
180	H	86.13692	74.30255	70.23181	1237.02905	-1378.50857	-1998.28500	1
181	C	79.42808	73.80115	70.94996	532.53319	-268.57236	517.55729	1

182	O	80.17960	74.55348	71.51804	266.16714	-290.73804	-558.88002	1
183	N	78.36726	73.14971	71.41526	-226.25352	640.49678	-270.32839	1
184	H	77.78022	72.58667	70.75950	2007.69063	-1035.27229	1523.50231	1
185	C	77.93226	73.49266	72.72869	-540.76542	-573.33303	49.50000	1
186	H	78.55251	74.38360	72.98974	-2374.20950	-1036.76023	843.75774	1
187	C	76.37204	73.82224	72.60016	-77.09082	666.87422	-415.84136	1
188	H	75.82626	72.85694	72.41974	-985.81834	617.19825	2463.91927	1
189	O	76.02399	74.70430	71.51441	293.29899	-391.65602	-477.80926	1
190	H	75.62649	74.07493	70.87908	2528.72714	-681.76262	-751.27122	1
191	C	76.01265	74.37847	74.02472	252.47363	-605.14473	440.05134	1
192	H	74.92038	74.58206	74.12041	-2052.65063	1456.49051	-1043.51830	1
193	H	76.29745	73.65805	74.84347	-2152.98800	-1661.97574	-161.70652	1
194	H	76.54461	75.33729	74.22968	-473.12726	-1584.27339	2165.61725	1
195	C	78.20251	72.24417	73.74554	360.36307	488.46713	505.10056	1
196	O	77.73225	72.26769	74.86673	-200.08817	-528.03552	-385.82850	1
197	N	78.98883	71.31327	73.22202	-597.54095	-226.44775	355.20479	1
198	H	79.31467	71.44622	72.26642	2179.23655	-1300.70981	-991.33835	1
199	C	79.21891	70.13768	73.97400	-687.68921	297.39807	-249.45179	1
200	H	78.76775	70.34027	74.97393	-349.16256	-2467.37713	-1101.72831	1
201	C	78.54473	68.91659	73.18534	672.47345	361.54328	-201.62880	1
202	H	79.01036	68.80396	72.17987	1541.41502	582.18425	2169.97026	1
203	H	78.71882	67.96445	73.73726	-2534.67717	60.25153	997.72295	1
204	C	77.04506	69.21680	73.06290	574.26774	-389.43119	-377.02542	1
205	C	76.17105	68.92022	74.15188	688.82679	-287.33580	-257.96133	1
206	H	76.55592	68.44397	75.07195	331.14182	1470.38163	2269.80013	1
207	C	76.54222	69.85253	71.88707	-383.52382	-675.04808	144.24917	1
208	H	77.21795	70.10076	71.04861	4.09847	1517.59662	2262.86397	1
209	C	74.82294	69.25720	74.03615	-134.76730	428.45285	-649.50303	1
210	H	74.14786	69.03008	74.87979	-903.23433	1600.49020	2011.53387	1
211	C	75.18422	70.17098	71.81918	-335.53281	-615.00040	-364.39058	1
212	H	74.81039	70.66335	70.90405	1596.45398	-1369.33862	1732.02659	1
213	C	74.27572	69.88681	72.88056	585.48547	-340.24194	-406.23938	1
214	O	72.89368	70.20346	72.82241	-419.15649	-173.04408	-511.94141	1
215	H	72.85495	70.61791	71.92820	-1071.84350	1559.71507	-1960.13012	1
216	C	80.84069	69.87078	73.97401	291.41878	-183.13091	710.72246	1
217	O	81.44786	69.53907	72.98398	379.87695	523.47396	-222.23622	1
218	N	81.29490	70.07922	75.20363	564.30591	373.09380	277.24371	1
219	H	80.66104	70.35846	75.95258	-120.59931	-2436.07824	-1214.35098	1
220	C	82.64462	69.75028	75.49570	404.07514	-299.37480	608.84009	1
221	H	83.03088	69.20641	74.60044	-1071.07882	-841.69025	2359.66467	1
222	C	83.39154	71.12773	75.77403	-683.12807	68.71770	-390.13096	1
223	H	83.03569	71.90846	75.06531	2068.88918	1596.58590	770.89603	1
224	H	83.14365	71.50863	76.79005	1379.86429	2342.49779	-179.85638	1
225	C	84.92595	70.90285	75.62467	-176.39967	537.49466	550.97268	1
226	H	85.29455	70.14561	76.35248	-396.28051	1942.22168	1869.33314	1
227	H	85.17418	70.50297	74.61593	-94.44700	586.00678	-2659.20016	1
228	C	85.62891	72.31677	75.87171	-291.69381	-718.18079	-150.72929	1
229	H	85.35703	73.12560	75.14651	-2303.38776	1089.76242	964.62032	1
230	H	85.51656	72.73384	76.90476	884.16729	2568.80533	-207.74283	1
231	N	86.98533	72.01290	75.68271	-594.49522	-252.81478	342.29276	1
232	H	87.21065	71.05389	75.46877	-1735.17426	2084.05705	-263.71605	1
233	C	87.93350	72.85442	75.77061	595.23177	-271.52487	442.22352	1
234	N	87.60083	74.18005	76.07130	585.53813	-424.79750	-105.81303	1
235	H	86.68656	74.59306	76.25084	959.88797	1327.56823	-2177.11905	1
236	H	88.27339	74.93987	76.17921	1578.48647	16.27378	-2220.76233	1
237	N	89.17464	72.24691	75.53174	-452.17763	-390.33541	-421.51853	1
238	H	89.41845	71.27784	75.33291	470.26107	1974.25629	-1817.92087	1
239	H	90.06001	72.75292	75.57606	1856.67307	-1573.97321	-1224.35416	1
240	C	82.61623	68.91518	76.90566	-531.47271	-581.45780	-55.06206	1
241	O	81.73083	69.03591	77.71688	-243.00837	192.73507	609.52485	1
242	N	83.72401	68.17873	76.99514	343.49288	-644.25607	38.09164	1
243	H	84.37847	68.25893	76.21901	-1691.16043	-1535.97525	-1484.73099	1

244	C	83.97736	67.35025	78.17273	542.66492	350.14337	454.42563	1
245	H	82.98192	66.91861	78.43147	1209.57979	-2396.95920	463.86744	1
246	C	85.05468	66.33854	77.83266	-737.14309	145.93010	242.71942	1
247	H	85.96800	66.90429	77.54028	-1050.18303	159.36419	-2509.06125	1
248	C	85.39482	65.48030	79.03818	-706.77696	-252.88343	-245.16230	1
249	H	86.22557	64.75631	78.81435	-1624.64039	-1665.49085	1417.86935	1
250	H	85.72286	66.10848	79.91239	2566.10521	598.51109	693.22305	1
251	H	84.50894	64.87737	79.37987	-1972.69758	107.10018	-1876.34312	1
252	C	84.66436	65.45707	76.66027	412.85148	672.58832	-27.69222	1
253	H	85.49457	64.75559	76.37158	1447.02277	1762.76533	-1490.78944	1
254	H	83.76368	64.82797	76.90003	1320.77379	-145.20455	2378.68491	1
255	H	84.40802	66.06672	75.75074	-1512.10848	1470.52031	1724.75147	1
256	C	84.55911	68.36221	79.36400	-607.11113	499.56689	73.73769	1
257	O	85.60724	68.95010	79.24510	357.97126	460.81534	356.68785	1
258	N	83.73343	68.33324	80.39559	536.55407	-368.62270	332.76306	1
259	H	82.87672	67.78445	80.34008	524.38866	2297.69985	1367.20941	1
260	C	84.14255	68.93244	81.61288	46.50277	-774.29190	-147.97904	1
261	H	85.23980	69.08869	81.49767	1676.51875	1883.29066	1032.55549	1
262	C	83.33748	70.32126	81.81747	-559.41456	-34.19198	-556.30433	1
263	H	82.24249	70.11081	81.86556	-64.66664	395.18769	2695.05373	1
264	H	83.60347	70.78413	82.79730	-2703.44278	-60.40056	333.79418	1
265	C	83.63974	71.25887	80.68179	-519.76435	377.31045	459.42366	1
266	H	83.39588	70.73952	79.72611	-1746.74323	1667.50644	-1261.73691	1
267	C	82.78021	72.51293	80.78891	570.95554	16.46261	-545.27700	1
268	H	82.98112	73.22533	79.94794	2391.58273	28.05277	-1305.07271	1
269	H	81.68721	72.26755	80.76265	175.75588	917.63458	2559.43867	1
270	H	82.97350	73.06486	81.74462	-1063.97851	-2155.34650	1283.00462	1
271	C	85.11123	71.64815	80.65476	193.76014	2.62946	-765.53141	1
272	H	85.31196	72.45829	79.90719	507.39394	-846.55087	2539.60089	1
273	H	85.46120	72.02181	81.65186	1337.57841	1818.19054	1526.01994	1
274	H	85.75929	70.77153	80.37050	1100.88635	-1172.91350	-2199.08909	1
275	C	83.70005	67.93694	82.80077	-549.21115	475.64486	-309.38218	1
276	O	82.98613	66.98260	82.63523	556.06106	-390.37755	-78.24250	1
277	O	84.15028	68.28359	84.09774	-572.27940	-310.19032	-209.75862	1
278	H	84.69402	69.08491	83.86210	-1380.08193	2212.14486	790.85944	1

Listing 129: N1

1		273							
2		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.5000	2000
		0.2500	300.00	0.00	0.00	0.00	-1290.8409	0.0000	
3	N	68.26713	77.54244	77.65881		0.00000	0.00000	0.00000	1
4	C	68.92185	77.51207	76.46485		0.00000	0.00000	0.00000	1
5	C	68.28644	76.18164	75.60507		0.00000	0.00000	0.00000	1
6	O	67.98507	75.13900	76.13196		0.00000	0.00000	0.00000	1
7	C	70.51480	77.12763	76.74818		0.00000	0.00000	0.00000	1
8	C	71.07403	78.06769	77.74538		0.00000	0.00000	0.00000	1
9	C	72.36892	77.50703	78.33085		0.00000	0.00000	0.00000	1
10	C	71.33944	79.44485	77.14382		0.00000	0.00000	0.00000	1
11	H	68.21844	76.65144	78.11918		0.00000	0.00000	0.00000	1
12	H	68.77365	78.52073	75.99851		0.00000	0.00000	0.00000	1
13	H	70.60054	76.06968	77.12272		0.00000	0.00000	0.00000	1
14	H	71.08374	77.15754	75.79363		0.00000	0.00000	0.00000	1
15	H	70.33797	78.17188	78.57763		0.00000	0.00000	0.00000	1
16	H	73.20049	77.50875	77.58137		0.00000	0.00000	0.00000	1
17	H	72.24288	76.44573	78.67837		0.00000	0.00000	0.00000	1
18	H	72.71282	78.10074	79.21594		0.00000	0.00000	0.00000	1
19	H	72.35538	79.82917	77.41672		0.00000	0.00000	0.00000	1
20	H	70.59468	80.20330	77.49718		0.00000	0.00000	0.00000	1
21	H	71.27997	79.42615	76.02622		0.00000	0.00000	0.00000	1
22	N	68.30577	76.49795	74.32284		0.00000	0.00000	0.00000	1
23	C	67.77587	75.60949	73.30994		0.00000	0.00000	0.00000	1

24	C	68.84185	75.42293	72.03741	0.00000	0.00000	0.00000	1
25	O	68.58717	74.61334	71.17749	0.00000	0.00000	0.00000	1
26	C	66.52885	76.18798	72.64731	0.00000	0.00000	0.00000	1
27	C	65.31252	76.08162	73.54561	0.00000	0.00000	0.00000	1
28	C	66.72377	77.61717	72.18353	0.00000	0.00000	0.00000	1
29	H	68.58947	77.46154	74.16930	0.00000	0.00000	0.00000	1
30	H	67.58335	74.66709	73.88022	0.00000	0.00000	0.00000	1
31	H	66.33174	75.56461	71.74456	0.00000	0.00000	0.00000	1
32	H	65.07030	75.00979	73.79192	0.00000	0.00000	0.00000	1
33	H	65.47646	76.61624	74.52330	0.00000	0.00000	0.00000	1
34	H	64.39710	76.53027	73.06631	0.00000	0.00000	0.00000	1
35	H	65.88836	77.95530	71.50805	0.00000	0.00000	0.00000	1
36	H	66.75902	78.33200	73.05272	0.00000	0.00000	0.00000	1
37	H	67.68741	77.73812	71.61240	0.00000	0.00000	0.00000	1
38	N	69.83814	76.29207	72.07467	0.00000	0.00000	0.00000	1
39	C	70.83510	76.23104	71.06385	0.00000	0.00000	0.00000	1
40	C	72.30217	75.84724	71.68734	0.00000	0.00000	0.00000	1
41	O	73.24296	75.72344	70.93682	0.00000	0.00000	0.00000	1
42	C	71.05002	77.70248	70.49699	0.00000	0.00000	0.00000	1
43	C	71.61180	77.54410	69.05420	0.00000	0.00000	0.00000	1
44	C	70.42401	76.91723	68.18475	0.00000	0.00000	0.00000	1
45	N	70.76958	77.21708	66.86227	0.00000	0.00000	0.00000	1
46	C	70.02379	76.98298	65.85924	0.00000	0.00000	0.00000	1
47	N	68.78558	76.37268	66.09232	0.00000	0.00000	0.00000	1
48	N	70.62655	77.41105	64.66710	0.00000	0.00000	0.00000	1
49	H	69.86338	76.91248	72.87855	0.00000	0.00000	0.00000	1
50	H	70.44502	75.49387	70.32234	0.00000	0.00000	0.00000	1
51	H	70.10182	78.28705	70.50276	0.00000	0.00000	0.00000	1
52	H	71.75957	78.27026	71.14237	0.00000	0.00000	0.00000	1
53	H	71.94429	78.52232	68.64152	0.00000	0.00000	0.00000	1
54	H	72.51201	76.88485	69.05428	0.00000	0.00000	0.00000	1
55	H	70.30634	75.80548	68.26207	0.00000	0.00000	0.00000	1
56	H	69.41804	77.37951	68.34547	0.00000	0.00000	0.00000	1
57	H	71.66478	77.64876	66.69697	0.00000	0.00000	0.00000	1
58	H	68.36859	76.06417	66.96965	0.00000	0.00000	0.00000	1
59	H	68.10406	76.14180	65.36740	0.00000	0.00000	0.00000	1
60	H	71.53701	77.83405	64.49172	0.00000	0.00000	0.00000	1
61	H	70.19000	77.29609	63.75176	0.00000	0.00000	0.00000	1
62	N	72.28541	75.82990	73.01611	0.00000	0.00000	0.00000	1
63	C	73.44506	75.39042	73.70789	0.00000	0.00000	0.00000	1
64	C	73.03438	74.03099	74.50287	0.00000	0.00000	0.00000	1
65	O	72.25998	73.23184	74.02415	0.00000	0.00000	0.00000	1
66	C	73.92083	76.55300	74.69945	0.00000	0.00000	0.00000	1
67	C	74.09696	77.87336	73.93145	0.00000	0.00000	0.00000	1
68	C	74.64108	77.87713	72.61069	0.00000	0.00000	0.00000	1
69	C	73.72403	79.10528	74.55020	0.00000	0.00000	0.00000	1
70	C	74.77664	79.08924	71.93202	0.00000	0.00000	0.00000	1
71	C	73.87537	80.29332	73.83431	0.00000	0.00000	0.00000	1
72	C	74.40439	80.33741	72.51090	0.00000	0.00000	0.00000	1
73	O	74.53578	81.56883	71.81877	0.00000	0.00000	0.00000	1
74	H	71.38599	75.94162	73.48017	0.00000	0.00000	0.00000	1
75	H	74.16410	75.20312	72.87463	0.00000	0.00000	0.00000	1
76	H	73.18832	76.69024	75.52891	0.00000	0.00000	0.00000	1
77	H	74.88266	76.26817	75.18440	0.00000	0.00000	0.00000	1
78	H	74.92581	76.93061	72.11360	0.00000	0.00000	0.00000	1
79	H	73.32503	79.11703	75.58043	0.00000	0.00000	0.00000	1
80	H	75.18655	79.07063	70.90683	0.00000	0.00000	0.00000	1
81	H	73.57802	81.24218	74.31508	0.00000	0.00000	0.00000	1
82	H	74.98500	81.25366	70.99886	0.00000	0.00000	0.00000	1
83	N	73.81551	73.86193	75.57387	0.00000	0.00000	0.00000	1
84	C	73.43932	72.82372	76.50108	0.00000	0.00000	0.00000	1
85	C	72.32253	73.38398	77.55340	0.00000	0.00000	0.00000	1

86	O	71.68095	74.39559	77.38562	0.00000	0.00000	0.00000	1
87	C	74.74580	72.28630	77.19233	0.00000	0.00000	0.00000	1
88	O	74.47956	71.05938	78.11366	0.00000	0.00000	0.00000	1
89	C	75.43354	73.47784	77.91201	0.00000	0.00000	0.00000	1
90	H	74.39305	74.64811	75.85438	0.00000	0.00000	0.00000	1
91	H	72.96738	72.07655	75.81792	0.00000	0.00000	0.00000	1
92	H	75.45186	71.87501	76.43027	0.00000	0.00000	0.00000	1
93	H	74.97000	70.40891	77.62208	0.00000	0.00000	0.00000	1
94	H	76.38625	73.14916	78.39870	0.00000	0.00000	0.00000	1
95	H	74.77805	73.91102	78.71490	0.00000	0.00000	0.00000	1
96	H	75.68322	74.31337	77.22020	0.00000	0.00000	0.00000	1
97	N	72.19870	72.47136	78.50778	0.00000	0.00000	0.00000	1
98	C	71.27674	72.71798	79.55793	0.00000	0.00000	0.00000	1
99	C	72.02994	73.42975	80.82815	0.00000	0.00000	0.00000	1
100	O	71.37420	73.91502	81.72121	0.00000	0.00000	0.00000	1
101	C	70.82844	71.32535	80.18206	0.00000	0.00000	0.00000	1
102	C	69.89063	70.52173	79.22805	0.00000	0.00000	0.00000	1
103	C	68.39473	70.99573	79.42370	0.00000	0.00000	0.00000	1
104	C	68.12556	72.28549	78.61302	0.00000	0.00000	0.00000	1
105	N	66.57373	72.48817	78.57950	0.00000	0.00000	0.00000	1
106	H	72.83478	71.65081	78.54026	0.00000	0.00000	0.00000	1
107	H	70.47567	73.35235	79.11622	0.00000	0.00000	0.00000	1
108	H	71.74016	70.72383	80.39554	0.00000	0.00000	0.00000	1
109	H	70.32895	71.48502	81.16382	0.00000	0.00000	0.00000	1
110	H	70.21147	70.62673	78.16740	0.00000	0.00000	0.00000	1
111	H	69.96642	69.43521	79.46014	0.00000	0.00000	0.00000	1
112	H	67.69825	70.19346	79.08617	0.00000	0.00000	0.00000	1
113	H	68.17069	71.14861	80.50541	0.00000	0.00000	0.00000	1
114	H	68.52175	73.21935	79.05901	0.00000	0.00000	0.00000	1
115	H	68.41335	72.22129	77.54465	0.00000	0.00000	0.00000	1
116	H	65.96010	71.62399	78.60452	0.00000	0.00000	0.00000	1
117	H	66.21202	72.98077	77.71474	0.00000	0.00000	0.00000	1
118	H	66.14850	73.08267	79.34667	0.00000	0.00000	0.00000	1
119	N	73.34509	73.20306	80.79718	0.00000	0.00000	0.00000	1
120	C	74.16425	74.00303	81.66336	0.00000	0.00000	0.00000	1
121	C	74.58732	75.35824	80.87291	0.00000	0.00000	0.00000	1
122	O	74.05278	75.73722	79.85925	0.00000	0.00000	0.00000	1
123	C	75.43732	73.13606	82.03169	0.00000	0.00000	0.00000	1
124	C	75.64170	73.16643	83.58144	0.00000	0.00000	0.00000	1
125	C	74.92398	71.90884	84.21663	0.00000	0.00000	0.00000	1
126	C	73.38592	72.03413	84.12175	0.00000	0.00000	0.00000	1
127	N	72.79616	70.74746	84.79713	0.00000	0.00000	0.00000	1
128	H	73.71006	72.78625	79.94533	0.00000	0.00000	0.00000	1
129	H	73.46968	74.20459	82.51284	0.00000	0.00000	0.00000	1
130	H	75.32908	72.08939	81.66788	0.00000	0.00000	0.00000	1
131	H	76.33655	73.54276	81.51660	0.00000	0.00000	0.00000	1
132	H	76.72624	73.14005	83.82387	0.00000	0.00000	0.00000	1
133	H	75.25578	74.11253	84.02258	0.00000	0.00000	0.00000	1
134	H	75.26773	70.97632	83.71277	0.00000	0.00000	0.00000	1
135	H	75.22412	71.79811	85.28384	0.00000	0.00000	0.00000	1
136	H	72.95551	72.87517	84.70305	0.00000	0.00000	0.00000	1
137	H	72.97362	72.02972	83.09118	0.00000	0.00000	0.00000	1
138	H	73.18817	70.47893	85.74675	0.00000	0.00000	0.00000	1
139	H	72.88626	69.83648	84.25934	0.00000	0.00000	0.00000	1
140	H	71.75534	70.76840	85.00009	0.00000	0.00000	0.00000	1
141	N	75.54026	75.98092	81.57231	0.00000	0.00000	0.00000	1
142	C	76.10002	77.26554	81.10951	0.00000	0.00000	0.00000	1
143	C	76.87086	76.98856	79.68705	0.00000	0.00000	0.00000	1
144	O	77.65180	76.06137	79.56897	0.00000	0.00000	0.00000	1
145	C	77.07447	77.75180	82.16414	0.00000	0.00000	0.00000	1
146	C	77.78031	79.02347	81.72913	0.00000	0.00000	0.00000	1
147	C	76.39264	77.97325	83.50265	0.00000	0.00000	0.00000	1

148	H	75.87187	75.49802	82.40730	0.00000	0.00000	0.00000	1
149	H	75.20113	77.91179	80.99171	0.00000	0.00000	0.00000	1
150	H	77.85161	76.96501	82.29931	0.00000	0.00000	0.00000	1
151	H	78.58317	79.32545	82.45829	0.00000	0.00000	0.00000	1
152	H	78.28857	78.89523	80.72976	0.00000	0.00000	0.00000	1
153	H	77.06636	79.89047	81.64117	0.00000	0.00000	0.00000	1
154	H	75.93120	77.02629	83.89738	0.00000	0.00000	0.00000	1
155	H	77.11133	78.34522	84.28249	0.00000	0.00000	0.00000	1
156	H	75.56544	78.73247	83.42155	0.00000	0.00000	0.00000	1
157	N	76.57342	77.93652	78.79782	0.00000	0.00000	0.00000	1
158	C	77.13709	77.89574	77.47568	0.00000	0.00000	0.00000	1
159	C	78.69859	78.38625	77.59745	0.00000	0.00000	0.00000	1
160	O	79.03222	79.50979	77.31611	0.00000	0.00000	0.00000	1
161	C	76.21086	78.88377	76.65685	0.00000	0.00000	0.00000	1
162	C	75.82404	79.93640	77.74464	0.00000	0.00000	0.00000	1
163	C	75.60910	79.00669	79.01377	0.00000	0.00000	0.00000	1
164	H	77.06773	76.82221	77.19931	0.00000	0.00000	0.00000	1
165	H	76.72828	79.32815	75.77373	0.00000	0.00000	0.00000	1
166	H	75.31121	78.35787	76.26557	0.00000	0.00000	0.00000	1
167	H	76.65728	80.65894	77.90715	0.00000	0.00000	0.00000	1
168	H	74.92383	80.53972	77.48449	0.00000	0.00000	0.00000	1
169	H	75.81758	79.48825	79.99738	0.00000	0.00000	0.00000	1
170	H	74.61494	78.50097	79.05520	0.00000	0.00000	0.00000	1
171	N	79.41761	77.36837	78.06035	0.00000	0.00000	0.00000	1
172	C	80.83524	77.52302	78.08743	0.00000	0.00000	0.00000	1
173	C	81.42377	77.00423	76.65698	0.00000	0.00000	0.00000	1
174	O	80.75838	76.99272	75.64910	0.00000	0.00000	0.00000	1
175	C	81.35844	76.66113	79.31281	0.00000	0.00000	0.00000	1
176	C	82.45963	77.45754	80.07745	0.00000	0.00000	0.00000	1
177	C	81.70839	78.35456	81.13851	0.00000	0.00000	0.00000	1
178	O	80.52464	78.26715	81.34898	0.00000	0.00000	0.00000	1
179	N	82.58628	79.16322	81.76657	0.00000	0.00000	0.00000	1
180	H	78.94924	76.49256	78.37521	0.00000	0.00000	0.00000	1
181	H	80.94169	78.62716	78.20366	0.00000	0.00000	0.00000	1
182	H	80.51630	76.41444	80.00375	0.00000	0.00000	0.00000	1
183	H	81.75383	75.68381	78.95532	0.00000	0.00000	0.00000	1
184	H	83.17070	76.76754	80.58384	0.00000	0.00000	0.00000	1
185	H	83.09249	78.06686	79.39401	0.00000	0.00000	0.00000	1
186	H	83.60111	79.23186	81.62456	0.00000	0.00000	0.00000	1
187	H	82.34842	79.80406	82.53088	0.00000	0.00000	0.00000	1
188	N	82.71190	76.67558	76.77952	0.00000	0.00000	0.00000	1
189	C	83.51876	76.28862	75.61888	0.00000	0.00000	0.00000	1
190	C	83.19745	74.72978	75.14166	0.00000	0.00000	0.00000	1
191	O	83.72934	74.30524	74.14312	0.00000	0.00000	0.00000	1
192	C	84.99609	76.27283	75.95662	0.00000	0.00000	0.00000	1
193	C	85.59068	77.66772	76.00329	0.00000	0.00000	0.00000	1
194	C	85.28671	75.52556	77.24427	0.00000	0.00000	0.00000	1
195	H	83.11042	76.78740	77.70876	0.00000	0.00000	0.00000	1
196	H	83.23033	77.02306	74.82896	0.00000	0.00000	0.00000	1
197	H	85.50205	75.72320	75.12720	0.00000	0.00000	0.00000	1
198	H	85.08375	78.30527	76.77954	0.00000	0.00000	0.00000	1
199	H	86.68835	77.64544	76.25049	0.00000	0.00000	0.00000	1
200	H	85.48072	78.19770	75.01636	0.00000	0.00000	0.00000	1
201	H	84.49899	74.74883	77.45393	0.00000	0.00000	0.00000	1
202	H	86.27678	74.99233	77.20328	0.00000	0.00000	0.00000	1
203	H	85.31646	76.21698	78.13100	0.00000	0.00000	0.00000	1
204	N	82.47056	74.06205	76.03047	0.00000	0.00000	0.00000	1
205	C	81.92664	72.81697	75.62180	0.00000	0.00000	0.00000	1
206	C	80.29826	72.98146	75.65540	0.00000	0.00000	0.00000	1
207	O	79.69622	73.25746	76.66638	0.00000	0.00000	0.00000	1
208	C	82.40172	71.78782	76.75487	0.00000	0.00000	0.00000	1
209	O	81.98946	70.41206	76.57326	0.00000	0.00000	0.00000	1

210	H	82.09984	74.61649	76.79917	0.00000	0.00000	0.00000	1
211	H	82.35688	72.61028	74.61290	0.00000	0.00000	0.00000	1
212	H	83.51220	71.90319	76.86750	0.00000	0.00000	0.00000	1
213	H	81.94802	72.16444	77.71279	0.00000	0.00000	0.00000	1
214	H	82.79127	70.05472	76.14799	0.00000	0.00000	0.00000	1
215	N	79.82900	72.77177	74.43965	0.00000	0.00000	0.00000	1
216	C	78.41000	72.83290	74.24721	0.00000	0.00000	0.00000	1
217	C	78.28059	72.03541	72.85629	0.00000	0.00000	0.00000	1
218	O	79.29695	71.79749	72.23221	0.00000	0.00000	0.00000	1
219	C	77.91755	74.36887	74.09438	0.00000	0.00000	0.00000	1
220	O	78.62667	75.18378	73.15749	0.00000	0.00000	0.00000	1
221	C	77.88247	74.87374	75.58117	0.00000	0.00000	0.00000	1
222	H	80.37556	72.53756	73.59145	0.00000	0.00000	0.00000	1
223	H	77.94438	72.34593	75.13412	0.00000	0.00000	0.00000	1
224	H	76.85797	74.32430	73.71720	0.00000	0.00000	0.00000	1
225	H	77.93024	75.35700	72.48998	0.00000	0.00000	0.00000	1
226	H	78.88778	75.24468	75.90467	0.00000	0.00000	0.00000	1
227	H	77.59486	74.06571	76.29442	0.00000	0.00000	0.00000	1
228	H	77.14835	75.70679	75.70052	0.00000	0.00000	0.00000	1
229	N	77.01173	71.70978	72.59819	0.00000	0.00000	0.00000	1
230	C	76.62706	71.10915	71.35397	0.00000	0.00000	0.00000	1
231	C	76.53376	72.26306	70.19307	0.00000	0.00000	0.00000	1
232	O	75.98036	73.32051	70.36416	0.00000	0.00000	0.00000	1
233	C	75.18267	70.54871	71.68300	0.00000	0.00000	0.00000	1
234	C	74.65245	71.58910	72.72148	0.00000	0.00000	0.00000	1
235	C	75.95620	71.80183	73.60105	0.00000	0.00000	0.00000	1
236	H	77.39641	70.34245	71.11574	0.00000	0.00000	0.00000	1
237	H	74.53840	70.46563	70.77670	0.00000	0.00000	0.00000	1
238	H	75.23766	69.52713	72.12465	0.00000	0.00000	0.00000	1
239	H	74.34141	72.53748	72.22332	0.00000	0.00000	0.00000	1
240	H	73.77439	71.23749	73.31224	0.00000	0.00000	0.00000	1
241	H	76.01705	72.78650	74.12101	0.00000	0.00000	0.00000	1
242	H	76.15475	70.98727	74.34026	0.00000	0.00000	0.00000	1
243	N	77.06509	71.76252	69.08373	0.00000	0.00000	0.00000	1
244	C	76.96996	72.49325	67.87658	0.00000	0.00000	0.00000	1
245	C	75.83691	71.75127	66.94561	0.00000	0.00000	0.00000	1
246	O	76.11966	71.05213	66.00526	0.00000	0.00000	0.00000	1
247	C	78.42741	72.40612	67.19193	0.00000	0.00000	0.00000	1
248	O	79.02580	71.10100	67.15093	0.00000	0.00000	0.00000	1
249	C	79.19524	73.49440	68.02284	0.00000	0.00000	0.00000	1
250	H	77.52277	70.85061	69.07824	0.00000	0.00000	0.00000	1
251	H	76.64636	73.50904	68.19957	0.00000	0.00000	0.00000	1
252	H	78.33002	72.75650	66.12990	0.00000	0.00000	0.00000	1
253	H	78.94619	70.88433	66.19771	0.00000	0.00000	0.00000	1
254	H	78.69336	74.48886	67.98068	0.00000	0.00000	0.00000	1
255	H	80.23774	73.63212	67.65000	0.00000	0.00000	0.00000	1
256	H	79.26293	73.19806	69.09782	0.00000	0.00000	0.00000	1
257	N	74.63096	71.99635	67.45103	0.00000	0.00000	0.00000	1
258	C	73.51103	72.05175	66.33032	0.00000	0.00000	0.00000	1
259	C	73.67935	73.11496	65.35835	0.00000	0.00000	0.00000	1
260	O	73.81538	73.98198	64.56507	0.00000	0.00000	0.00000	1
261	C	72.12306	72.26166	67.19056	0.00000	0.00000	0.00000	1
262	C	70.97963	71.90753	66.30515	0.00000	0.00000	0.00000	1
263	C	70.71413	70.40517	66.31212	0.00000	0.00000	0.00000	1
264	C	69.72437	72.65871	66.74136	0.00000	0.00000	0.00000	1
265	H	74.62283	72.66158	68.21925	0.00000	0.00000	0.00000	1
266	H	73.63012	71.02904	65.89435	0.00000	0.00000	0.00000	1
267	H	72.14064	71.64680	68.11560	0.00000	0.00000	0.00000	1
268	H	72.06261	73.31913	67.53443	0.00000	0.00000	0.00000	1
269	H	71.22628	72.21988	65.26307	0.00000	0.00000	0.00000	1
270	H	70.28661	70.06780	67.29052	0.00000	0.00000	0.00000	1
271	H	71.65359	69.81912	66.14295	0.00000	0.00000	0.00000	1

272	H	69.98990	70.10553	65.51448	0.00000	0.00000	0.00000	1
273	H	68.82775	72.35045	66.14519	0.00000	0.00000	0.00000	1
274	H	69.84236	73.76549	66.62011	0.00000	0.00000	0.00000	1
275	H	69.48894	72.46627	67.81918	0.00000	0.00000	0.00000	1
276		273						
277		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	1.0000 4000
		0.2500	300.00	0.00	0.00	0.00 -1291.2195	0.0000	0.0000
278	N	68.27731	77.50660	77.65939	0.00000	0.00000	0.00000	1
279	C	68.90988	77.48424	76.45340	0.00000	0.00000	0.00000	1
280	C	68.27803	76.15502	75.58847	0.00000	0.00000	0.00000	1
281	O	67.97016	75.10793	76.10378	0.00000	0.00000	0.00000	1
282	C	70.50894	77.10608	76.70272	0.00000	0.00000	0.00000	1
283	C	71.07440	78.03374	77.70971	0.00000	0.00000	0.00000	1
284	C	72.37699	77.46417	78.26978	0.00000	0.00000	0.00000	1
285	C	71.32672	79.42610	77.13880	0.00000	0.00000	0.00000	1
286	H	68.28477	76.63085	78.14957	0.00000	0.00000	0.00000	1
287	H	68.74768	78.49212	75.99129	0.00000	0.00000	0.00000	1
288	H	70.60308	76.04143	77.05660	0.00000	0.00000	0.00000	1
289	H	71.06735	77.15489	75.74251	0.00000	0.00000	0.00000	1
290	H	70.34980	78.11862	78.55395	0.00000	0.00000	0.00000	1
291	H	73.20505	77.49083	77.51773	0.00000	0.00000	0.00000	1
292	H	72.25655	76.39329	78.58912	0.00000	0.00000	0.00000	1
293	H	72.72187	78.03721	79.16714	0.00000	0.00000	0.00000	1
294	H	72.29197	79.85799	77.50698	0.00000	0.00000	0.00000	1
295	H	70.51561	80.14227	77.42580	0.00000	0.00000	0.00000	1
296	H	71.37043	79.41549	76.02079	0.00000	0.00000	0.00000	1
297	N	68.31801	76.47854	74.30824	0.00000	0.00000	0.00000	1
298	C	67.77921	75.60898	73.27992	0.00000	0.00000	0.00000	1
299	C	68.84944	75.44003	72.01252	0.00000	0.00000	0.00000	1
300	O	68.59744	74.65760	71.12697	0.00000	0.00000	0.00000	1
301	C	66.52221	76.20080	72.64862	0.00000	0.00000	0.00000	1
302	C	65.33145	76.10005	73.58179	0.00000	0.00000	0.00000	1
303	C	66.71327	77.63288	72.19152	0.00000	0.00000	0.00000	1
304	H	68.60108	77.44504	74.16730	0.00000	0.00000	0.00000	1
305	H	67.59228	74.65793	73.83726	0.00000	0.00000	0.00000	1
306	H	66.29343	75.58753	71.74711	0.00000	0.00000	0.00000	1
307	H	65.11816	75.03210	73.86811	0.00000	0.00000	0.00000	1
308	H	65.51112	76.66991	74.53624	0.00000	0.00000	0.00000	1
309	H	64.39654	76.51548	73.11149	0.00000	0.00000	0.00000	1
310	H	65.83154	78.00028	71.59517	0.00000	0.00000	0.00000	1
311	H	66.83756	78.33129	73.06553	0.00000	0.00000	0.00000	1
312	H	67.62762	77.74280	71.54298	0.00000	0.00000	0.00000	1
313	N	69.86975	76.27807	72.10057	0.00000	0.00000	0.00000	1
314	C	70.86090	76.24332	71.08516	0.00000	0.00000	0.00000	1
315	C	72.33863	75.89222	71.70396	0.00000	0.00000	0.00000	1
316	O	73.28453	75.85867	70.94925	0.00000	0.00000	0.00000	1
317	C	71.01354	77.71559	70.49947	0.00000	0.00000	0.00000	1
318	C	71.59412	77.56397	69.06408	0.00000	0.00000	0.00000	1
319	C	70.41972	76.90667	68.19671	0.00000	0.00000	0.00000	1
320	N	70.77240	77.18683	66.87159	0.00000	0.00000	0.00000	1
321	C	70.03614	76.94672	65.86335	0.00000	0.00000	0.00000	1
322	N	68.79118	76.35000	66.09124	0.00000	0.00000	0.00000	1
323	N	70.65992	77.35771	64.67698	0.00000	0.00000	0.00000	1
324	H	69.89448	76.88405	72.91660	0.00000	0.00000	0.00000	1
325	H	70.48534	75.49203	70.34986	0.00000	0.00000	0.00000	1
326	H	70.03814	78.25164	70.48700	0.00000	0.00000	0.00000	1
327	H	71.68850	78.32526	71.14240	0.00000	0.00000	0.00000	1
328	H	71.90484	78.54786	68.64716	0.00000	0.00000	0.00000	1
329	H	72.51040	76.92552	69.07660	0.00000	0.00000	0.00000	1
330	H	70.31237	75.79678	68.29689	0.00000	0.00000	0.00000	1
331	H	69.40633	77.35582	68.34221	0.00000	0.00000	0.00000	1
332	H	71.67507	77.60994	66.72295	0.00000	0.00000	0.00000	1

333	H	68.36219	76.05563	66.96783	0.00000	0.00000	0.00000	1
334	H	68.11590	76.11544	65.36294	0.00000	0.00000	0.00000	1
335	H	71.57639	77.77179	64.51347	0.00000	0.00000	0.00000	1
336	H	70.24036	77.24047	63.75398	0.00000	0.00000	0.00000	1
337	N	72.30826	75.75029	73.02263	0.00000	0.00000	0.00000	1
338	C	73.48089	75.34612	73.71401	0.00000	0.00000	0.00000	1
339	C	73.12592	73.95796	74.48384	0.00000	0.00000	0.00000	1
340	O	72.47277	73.09600	73.93764	0.00000	0.00000	0.00000	1
341	C	73.92902	76.52660	74.69808	0.00000	0.00000	0.00000	1
342	C	74.08704	77.85145	73.93169	0.00000	0.00000	0.00000	1
343	C	74.63391	77.87508	72.61307	0.00000	0.00000	0.00000	1
344	C	73.71322	79.07799	74.55837	0.00000	0.00000	0.00000	1
345	C	74.76605	79.09312	71.94281	0.00000	0.00000	0.00000	1
346	C	73.86944	80.27382	73.85558	0.00000	0.00000	0.00000	1
347	C	74.39267	80.33615	72.53137	0.00000	0.00000	0.00000	1
348	O	74.52411	81.57825	71.85696	0.00000	0.00000	0.00000	1
349	H	71.39906	75.79198	73.47982	0.00000	0.00000	0.00000	1
350	H	74.19926	75.19892	72.87452	0.00000	0.00000	0.00000	1
351	H	73.19477	76.65212	75.52555	0.00000	0.00000	0.00000	1
352	H	74.89511	76.26420	75.18717	0.00000	0.00000	0.00000	1
353	H	74.93171	76.93545	72.11144	0.00000	0.00000	0.00000	1
354	H	73.31570	79.08269	75.58827	0.00000	0.00000	0.00000	1
355	H	75.17572	79.08161	70.91744	0.00000	0.00000	0.00000	1
356	H	73.57866	81.21797	74.34791	0.00000	0.00000	0.00000	1
357	H	74.94804	81.27033	71.02104	0.00000	0.00000	0.00000	1
358	N	73.81371	73.85215	75.62553	0.00000	0.00000	0.00000	1
359	C	73.43064	72.80690	76.52738	0.00000	0.00000	0.00000	1
360	C	72.30829	73.36156	77.56651	0.00000	0.00000	0.00000	1
361	O	71.66267	74.36962	77.38576	0.00000	0.00000	0.00000	1
362	C	74.74679	72.26141	77.24021	0.00000	0.00000	0.00000	1
363	O	74.53148	71.09976	78.13283	0.00000	0.00000	0.00000	1
364	C	75.40877	73.50218	77.92208	0.00000	0.00000	0.00000	1
365	H	74.28037	74.69019	75.96248	0.00000	0.00000	0.00000	1
366	H	72.97726	72.06345	75.82834	0.00000	0.00000	0.00000	1
367	H	75.45806	71.88477	76.45967	0.00000	0.00000	0.00000	1
368	H	75.18119	70.48747	77.75743	0.00000	0.00000	0.00000	1
369	H	76.34844	73.21772	78.45330	0.00000	0.00000	0.00000	1
370	H	74.72928	73.97278	78.67422	0.00000	0.00000	0.00000	1
371	H	75.67660	74.29256	77.18326	0.00000	0.00000	0.00000	1
372	N	72.17113	72.45402	78.52642	0.00000	0.00000	0.00000	1
373	C	71.26906	72.72554	79.58790	0.00000	0.00000	0.00000	1
374	C	72.04331	73.41209	80.85920	0.00000	0.00000	0.00000	1
375	O	71.40079	73.88945	81.76686	0.00000	0.00000	0.00000	1
376	C	70.79225	71.33788	80.20247	0.00000	0.00000	0.00000	1
377	C	69.89795	70.53905	79.20356	0.00000	0.00000	0.00000	1
378	C	68.39385	70.99711	79.37321	0.00000	0.00000	0.00000	1
379	C	68.13902	72.29238	78.56753	0.00000	0.00000	0.00000	1
380	N	66.59288	72.53633	78.56624	0.00000	0.00000	0.00000	1
381	H	72.79686	71.63464	78.56128	0.00000	0.00000	0.00000	1
382	H	70.48125	73.38491	79.15874	0.00000	0.00000	0.00000	1
383	H	71.68930	70.73268	80.46440	0.00000	0.00000	0.00000	1
384	H	70.24908	71.50317	81.15947	0.00000	0.00000	0.00000	1
385	H	70.24902	70.67524	78.15569	0.00000	0.00000	0.00000	1
386	H	69.98160	69.44889	79.41477	0.00000	0.00000	0.00000	1
387	H	67.70834	70.19457	79.01675	0.00000	0.00000	0.00000	1
388	H	68.14555	71.14305	80.44977	0.00000	0.00000	0.00000	1
389	H	68.56439	73.21760	79.00422	0.00000	0.00000	0.00000	1
390	H	68.40462	72.22391	77.49341	0.00000	0.00000	0.00000	1
391	H	65.95918	71.69459	78.43554	0.00000	0.00000	0.00000	1
392	H	66.25208	73.18112	77.79646	0.00000	0.00000	0.00000	1
393	H	66.17381	72.99850	79.42486	0.00000	0.00000	0.00000	1
394	N	73.35775	73.18658	80.81095	0.00000	0.00000	0.00000	1

395	C	74.18184	73.98915	81.66541	0.00000	0.00000	0.00000	1
396	C	74.57752	75.35670	80.87847	0.00000	0.00000	0.00000	1
397	O	74.00700	75.75401	79.89144	0.00000	0.00000	0.00000	1
398	C	75.47028	73.13381	82.01709	0.00000	0.00000	0.00000	1
399	C	75.68115	73.15737	83.56556	0.00000	0.00000	0.00000	1
400	C	74.94495	71.91235	84.20480	0.00000	0.00000	0.00000	1
401	C	73.40978	72.06154	84.09675	0.00000	0.00000	0.00000	1
402	N	72.78491	70.78454	84.75445	0.00000	0.00000	0.00000	1
403	H	73.70973	72.76984	79.94980	0.00000	0.00000	0.00000	1
404	H	73.50583	74.18678	82.53033	0.00000	0.00000	0.00000	1
405	H	75.37000	72.08910	81.64743	0.00000	0.00000	0.00000	1
406	H	76.36132	73.55350	81.49755	0.00000	0.00000	0.00000	1
407	H	76.76749	73.11159	83.80331	0.00000	0.00000	0.00000	1
408	H	75.31380	74.10981	84.00970	0.00000	0.00000	0.00000	1
409	H	75.27665	70.97149	83.70890	0.00000	0.00000	0.00000	1
410	H	75.23641	71.80247	85.27468	0.00000	0.00000	0.00000	1
411	H	72.98603	72.90833	84.67280	0.00000	0.00000	0.00000	1
412	H	73.01004	72.06963	83.06205	0.00000	0.00000	0.00000	1
413	H	73.08272	70.55661	85.74766	0.00000	0.00000	0.00000	1
414	H	72.94605	69.85873	84.26085	0.00000	0.00000	0.00000	1
415	H	71.72879	70.78877	84.85042	0.00000	0.00000	0.00000	1
416	N	75.54447	75.97279	81.56467	0.00000	0.00000	0.00000	1
417	C	76.10463	77.25542	81.09890	0.00000	0.00000	0.00000	1
418	C	76.86481	76.97114	79.67070	0.00000	0.00000	0.00000	1
419	O	77.64220	76.04047	79.55384	0.00000	0.00000	0.00000	1
420	C	77.09232	77.72512	82.15123	0.00000	0.00000	0.00000	1
421	C	77.83987	78.97041	81.71107	0.00000	0.00000	0.00000	1
422	C	76.41736	77.97213	83.48837	0.00000	0.00000	0.00000	1
423	H	75.90800	75.46863	82.37078	0.00000	0.00000	0.00000	1
424	H	75.20933	77.90929	80.98684	0.00000	0.00000	0.00000	1
425	H	77.84475	76.91665	82.29322	0.00000	0.00000	0.00000	1
426	H	78.63588	79.25963	82.45323	0.00000	0.00000	0.00000	1
427	H	78.36546	78.81293	80.72514	0.00000	0.00000	0.00000	1
428	H	77.15263	79.85329	81.59343	0.00000	0.00000	0.00000	1
429	H	75.92569	77.04145	83.88418	0.00000	0.00000	0.00000	1
430	H	77.14997	78.32070	84.26703	0.00000	0.00000	0.00000	1
431	H	75.61701	78.75808	83.40833	0.00000	0.00000	0.00000	1
432	N	76.56314	77.91530	78.77689	0.00000	0.00000	0.00000	1
433	C	77.13070	77.87631	77.45907	0.00000	0.00000	0.00000	1
434	C	78.68827	78.38224	77.59251	0.00000	0.00000	0.00000	1
435	O	79.01682	79.50943	77.32484	0.00000	0.00000	0.00000	1
436	C	76.20984	78.86522	76.63647	0.00000	0.00000	0.00000	1
437	C	75.82716	79.92099	77.72229	0.00000	0.00000	0.00000	1
438	C	75.62201	79.00371	79.00283	0.00000	0.00000	0.00000	1
439	H	77.06999	76.80341	77.17223	0.00000	0.00000	0.00000	1
440	H	76.73006	79.31022	75.75768	0.00000	0.00000	0.00000	1
441	H	75.30868	78.34564	76.24236	0.00000	0.00000	0.00000	1
442	H	76.65899	80.64481	77.87566	0.00000	0.00000	0.00000	1
443	H	74.92563	80.52056	77.46242	0.00000	0.00000	0.00000	1
444	H	75.86153	79.49101	79.97619	0.00000	0.00000	0.00000	1
445	H	74.62051	78.51996	79.06950	0.00000	0.00000	0.00000	1
446	N	79.40930	77.36869	78.05805	0.00000	0.00000	0.00000	1
447	C	80.82701	77.52269	78.09013	0.00000	0.00000	0.00000	1
448	C	81.41631	76.98878	76.66416	0.00000	0.00000	0.00000	1
449	O	80.74590	76.94195	75.66130	0.00000	0.00000	0.00000	1
450	C	81.33226	76.66280	79.32441	0.00000	0.00000	0.00000	1
451	C	82.44019	77.44522	80.09245	0.00000	0.00000	0.00000	1
452	C	81.69543	78.37669	81.12764	0.00000	0.00000	0.00000	1
453	O	80.51017	78.30919	81.33832	0.00000	0.00000	0.00000	1
454	N	82.58249	79.18903	81.73800	0.00000	0.00000	0.00000	1
455	H	78.94446	76.48789	78.35908	0.00000	0.00000	0.00000	1
456	H	80.93382	78.62730	78.20355	0.00000	0.00000	0.00000	1

457	H	80.48397	76.44381	80.01665	0.00000	0.00000	0.00000	1
458	H	81.71227	75.67523	78.97674	0.00000	0.00000	0.00000	1
459	H	83.12501	76.74754	80.62302	0.00000	0.00000	0.00000	1
460	H	83.09804	78.02976	79.41219	0.00000	0.00000	0.00000	1
461	H	83.59830	79.23711	81.59388	0.00000	0.00000	0.00000	1
462	H	82.35576	79.85084	82.48772	0.00000	0.00000	0.00000	1
463	N	82.71008	76.67916	76.78893	0.00000	0.00000	0.00000	1
464	C	83.52222	76.28956	75.63451	0.00000	0.00000	0.00000	1
465	C	83.20354	74.72897	75.16467	0.00000	0.00000	0.00000	1
466	O	83.73638	74.29716	74.16934	0.00000	0.00000	0.00000	1
467	C	84.99951	76.29687	75.97271	0.00000	0.00000	0.00000	1
468	C	85.57497	77.69958	76.03268	0.00000	0.00000	0.00000	1
469	C	85.30600	75.55208	77.25882	0.00000	0.00000	0.00000	1
470	H	83.10541	76.81331	77.71670	0.00000	0.00000	0.00000	1
471	H	83.22552	77.01393	74.83889	0.00000	0.00000	0.00000	1
472	H	85.51660	75.76078	75.14188	0.00000	0.00000	0.00000	1
473	H	85.07287	78.31712	76.82783	0.00000	0.00000	0.00000	1
474	H	86.67637	77.68582	76.26394	0.00000	0.00000	0.00000	1
475	H	85.44491	78.24393	75.05637	0.00000	0.00000	0.00000	1
476	H	84.63925	74.65373	77.38201	0.00000	0.00000	0.00000	1
477	H	86.36969	75.18631	77.28498	0.00000	0.00000	0.00000	1
478	H	85.15696	76.20414	78.16317	0.00000	0.00000	0.00000	1
479	N	82.46426	74.06823	76.04838	0.00000	0.00000	0.00000	1
480	C	81.90407	72.83298	75.62938	0.00000	0.00000	0.00000	1
481	C	80.27772	73.00784	75.67814	0.00000	0.00000	0.00000	1
482	O	79.70207	73.28919	76.70124	0.00000	0.00000	0.00000	1
483	C	82.36017	71.78790	76.75583	0.00000	0.00000	0.00000	1
484	O	81.95463	70.41471	76.54696	0.00000	0.00000	0.00000	1
485	H	82.09000	74.62773	76.81243	0.00000	0.00000	0.00000	1
486	H	82.32346	72.62405	74.61687	0.00000	0.00000	0.00000	1
487	H	83.46740	71.90660	76.88485	0.00000	0.00000	0.00000	1
488	H	81.89315	72.14868	77.71293	0.00000	0.00000	0.00000	1
489	H	82.75971	70.06781	76.12032	0.00000	0.00000	0.00000	1
490	N	79.78292	72.79320	74.47130	0.00000	0.00000	0.00000	1
491	C	78.36597	72.83173	74.27798	0.00000	0.00000	0.00000	1
492	C	78.23641	72.00672	72.90243	0.00000	0.00000	0.00000	1
493	O	79.25571	71.74376	72.29490	0.00000	0.00000	0.00000	1
494	C	77.87091	74.36284	74.08751	0.00000	0.00000	0.00000	1
495	O	78.49977	75.12165	73.05079	0.00000	0.00000	0.00000	1
496	C	77.96870	74.93991	75.54523	0.00000	0.00000	0.00000	1
497	H	80.32453	72.54155	73.62470	0.00000	0.00000	0.00000	1
498	H	77.90806	72.36308	75.17884	0.00000	0.00000	0.00000	1
499	H	76.78233	74.32841	73.79837	0.00000	0.00000	0.00000	1
500	H	77.74442	75.28905	72.44848	0.00000	0.00000	0.00000	1
501	H	79.01619	75.25671	75.78344	0.00000	0.00000	0.00000	1
502	H	77.65774	74.19261	76.31596	0.00000	0.00000	0.00000	1
503	H	77.31874	75.83722	75.66635	0.00000	0.00000	0.00000	1
504	N	76.96894	71.69322	72.62065	0.00000	0.00000	0.00000	1
505	C	76.61134	71.09050	71.37015	0.00000	0.00000	0.00000	1
506	C	76.52308	72.25073	70.21419	0.00000	0.00000	0.00000	1
507	O	75.95199	73.29873	70.38969	0.00000	0.00000	0.00000	1
508	C	75.15417	70.53761	71.65854	0.00000	0.00000	0.00000	1
509	C	74.60853	71.59670	72.66693	0.00000	0.00000	0.00000	1
510	C	75.88531	71.79573	73.59053	0.00000	0.00000	0.00000	1
511	H	77.38659	70.32453	71.14137	0.00000	0.00000	0.00000	1
512	H	74.53752	70.45387	70.73509	0.00000	0.00000	0.00000	1
513	H	75.18588	69.52135	72.11104	0.00000	0.00000	0.00000	1
514	H	74.33591	72.54224	72.14455	0.00000	0.00000	0.00000	1
515	H	73.70106	71.27556	73.23120	0.00000	0.00000	0.00000	1
516	H	75.93984	72.77502	74.11916	0.00000	0.00000	0.00000	1
517	H	76.05983	70.97443	74.32576	0.00000	0.00000	0.00000	1
518	N	77.08202	71.77191	69.11043	0.00000	0.00000	0.00000	1

519	C	76.96527	72.49123	67.89777	0.00000	0.00000	0.00000	1	
520	C	75.82020	71.72908	66.99976	0.00000	0.00000	0.00000	1	
521	O	76.09114	70.99673	66.07869	0.00000	0.00000	0.00000	1	
522	C	78.40593	72.40527	67.18296	0.00000	0.00000	0.00000	1	
523	O	79.00067	71.10095	67.10827	0.00000	0.00000	0.00000	1	
524	C	79.19173	73.47361	68.02568	0.00000	0.00000	0.00000	1	
525	H	77.52302	70.85321	69.09368	0.00000	0.00000	0.00000	1	
526	H	76.64571	73.50889	68.22131	0.00000	0.00000	0.00000	1	
527	H	78.29141	72.77561	66.12820	0.00000	0.00000	0.00000	1	
528	H	78.90684	70.90224	66.15378	0.00000	0.00000	0.00000	1	
529	H	78.71337	74.47965	67.97664	0.00000	0.00000	0.00000	1	
530	H	80.24183	73.58432	67.66833	0.00000	0.00000	0.00000	1	
531	H	79.23746	73.17854	69.10128	0.00000	0.00000	0.00000	1	
532	N	74.61540	71.98717	67.50776	0.00000	0.00000	0.00000	1	
533	C	73.52317	72.08857	66.35665	0.00000	0.00000	0.00000	1	
534	C	73.72596	73.17795	65.42268	0.00000	0.00000	0.00000	1	
535	O	73.89449	74.06162	64.65475	0.00000	0.00000	0.00000	1	
536	C	72.12399	72.28436	67.19673	0.00000	0.00000	0.00000	1	
537	C	70.98369	71.93663	66.30376	0.00000	0.00000	0.00000	1	
538	C	70.72956	70.43207	66.31597	0.00000	0.00000	0.00000	1	
539	C	69.72550	72.68233	66.74140	0.00000	0.00000	0.00000	1	
540	H	74.63484	72.67839	68.25351	0.00000	0.00000	0.00000	1	
541	H	73.66148	71.07842	65.89877	0.00000	0.00000	0.00000	1	
542	H	72.13093	71.65507	68.11552	0.00000	0.00000	0.00000	1	
543	H	72.05195	73.33747	67.55226	0.00000	0.00000	0.00000	1	
544	H	71.22905	72.25212	65.26308	0.00000	0.00000	0.00000	1	
545	H	70.40404	70.07805	67.32732	0.00000	0.00000	0.00000	1	
546	H	71.65084	69.85537	66.04602	0.00000	0.00000	0.00000	1	
547	H	69.92945	70.13917	65.58957	0.00000	0.00000	0.00000	1	
548	H	68.84212	72.41404	66.10820	0.00000	0.00000	0.00000	1	
549	H	69.86014	73.79262	66.67015	0.00000	0.00000	0.00000	1	
550	H	69.45735	72.44896	67.80347	0.00000	0.00000	0.00000	1	
551		273							
552		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	1.5000	6000
		0.2500	300.00	0.00	0.00	0.00	-1291.2768	0.0000	
553	N	68.27887	77.50069	77.66078	0.00000	0.00000	0.00000	0.00000	1
554	C	68.90955	77.47922	76.45375	0.00000	0.00000	0.00000	0.00000	1
555	C	68.27733	76.15123	75.58855	0.00000	0.00000	0.00000	0.00000	1
556	O	67.97027	75.10308	76.10197	0.00000	0.00000	0.00000	0.00000	1
557	C	70.50988	77.10209	76.69603	0.00000	0.00000	0.00000	0.00000	1
558	C	71.07664	78.02678	77.70503	0.00000	0.00000	0.00000	0.00000	1
559	C	72.38087	77.45612	78.25992	0.00000	0.00000	0.00000	0.00000	1
560	C	71.32344	79.42103	77.13634	0.00000	0.00000	0.00000	0.00000	1
561	H	68.27894	76.62310	78.14761	0.00000	0.00000	0.00000	0.00000	1
562	H	68.74634	78.48771	75.99347	0.00000	0.00000	0.00000	0.00000	1
563	H	70.60809	76.03600	77.04519	0.00000	0.00000	0.00000	0.00000	1
564	H	71.06485	77.15654	75.73404	0.00000	0.00000	0.00000	0.00000	1
565	H	70.35435	78.10775	78.55163	0.00000	0.00000	0.00000	0.00000	1
566	H	73.20867	77.49061	77.50795	0.00000	0.00000	0.00000	0.00000	1
567	H	72.26293	76.38228	78.57103	0.00000	0.00000	0.00000	0.00000	1
568	H	72.72471	78.02287	79.16168	0.00000	0.00000	0.00000	0.00000	1
569	H	72.27777	79.86393	77.51952	0.00000	0.00000	0.00000	0.00000	1
570	H	70.49972	80.12850	77.40852	0.00000	0.00000	0.00000	0.00000	1
571	H	71.38535	79.40927	76.01922	0.00000	0.00000	0.00000	0.00000	1
572	N	68.31647	76.47740	74.30875	0.00000	0.00000	0.00000	0.00000	1
573	C	67.77767	75.60889	73.28021	0.00000	0.00000	0.00000	0.00000	1
574	C	68.84846	75.44543	72.01365	0.00000	0.00000	0.00000	0.00000	1
575	O	68.59450	74.67020	71.12207	0.00000	0.00000	0.00000	0.00000	1
576	C	66.51938	76.20049	72.65229	0.00000	0.00000	0.00000	0.00000	1
577	C	65.33039	76.10272	73.58805	0.00000	0.00000	0.00000	0.00000	1
578	C	66.71422	77.63179	72.19384	0.00000	0.00000	0.00000	0.00000	1
579	H	68.59916	77.44418	74.16641	0.00000	0.00000	0.00000	0.00000	1

580	H	67.59275	74.65631	73.83634	0.00000	0.00000	0.00000	1
581	H	66.28658	75.58715	71.75177	0.00000	0.00000	0.00000	1
582	H	65.11582	75.03534	73.87577	0.00000	0.00000	0.00000	1
583	H	65.51294	76.67302	74.54171	0.00000	0.00000	0.00000	1
584	H	64.39490	76.51918	73.11962	0.00000	0.00000	0.00000	1
585	H	65.83202	78.00361	71.60100	0.00000	0.00000	0.00000	1
586	H	66.84594	78.32956	73.06730	0.00000	0.00000	0.00000	1
587	H	67.62667	77.73680	71.54174	0.00000	0.00000	0.00000	1
588	N	69.87373	76.27687	72.10870	0.00000	0.00000	0.00000	1
589	C	70.86229	76.24312	71.09028	0.00000	0.00000	0.00000	1
590	C	72.34069	75.89017	71.70556	0.00000	0.00000	0.00000	1
591	O	73.28680	75.86361	70.95112	0.00000	0.00000	0.00000	1
592	C	71.01150	77.71483	70.50231	0.00000	0.00000	0.00000	1
593	C	71.59100	77.56546	69.06618	0.00000	0.00000	0.00000	1
594	C	70.42073	76.90405	68.19651	0.00000	0.00000	0.00000	1
595	N	70.77621	77.18214	66.87165	0.00000	0.00000	0.00000	1
596	C	70.04067	76.94157	65.86303	0.00000	0.00000	0.00000	1
597	N	68.79479	76.34715	66.09244	0.00000	0.00000	0.00000	1
598	N	70.66522	77.34909	64.67589	0.00000	0.00000	0.00000	1
599	H	69.90332	76.87834	72.92801	0.00000	0.00000	0.00000	1
600	H	70.48288	75.49196	70.35651	0.00000	0.00000	0.00000	1
601	H	70.03484	78.24860	70.49068	0.00000	0.00000	0.00000	1
602	H	71.68559	78.32661	71.14415	0.00000	0.00000	0.00000	1
603	H	71.89766	78.55077	68.64961	0.00000	0.00000	0.00000	1
604	H	72.50995	76.93094	69.07804	0.00000	0.00000	0.00000	1
605	H	70.31600	75.79405	68.29836	0.00000	0.00000	0.00000	1
606	H	69.40577	77.35085	68.33813	0.00000	0.00000	0.00000	1
607	H	71.67981	77.60334	66.72343	0.00000	0.00000	0.00000	1
608	H	68.36594	76.05560	66.97004	0.00000	0.00000	0.00000	1
609	H	68.11885	76.11152	65.36516	0.00000	0.00000	0.00000	1
610	H	71.58231	77.76145	64.51144	0.00000	0.00000	0.00000	1
611	H	70.24558	77.23080	63.75302	0.00000	0.00000	0.00000	1
612	N	72.31026	75.73453	73.02258	0.00000	0.00000	0.00000	1
613	C	73.48846	75.34017	73.71032	0.00000	0.00000	0.00000	1
614	C	73.14083	73.95169	74.48257	0.00000	0.00000	0.00000	1
615	O	72.49437	73.08588	73.93448	0.00000	0.00000	0.00000	1
616	C	73.93097	76.52115	74.69642	0.00000	0.00000	0.00000	1
617	C	74.08812	77.84747	73.93260	0.00000	0.00000	0.00000	1
618	C	74.63771	77.87389	72.61520	0.00000	0.00000	0.00000	1
619	C	73.71220	79.07231	74.56133	0.00000	0.00000	0.00000	1
620	C	74.76831	79.09339	71.94734	0.00000	0.00000	0.00000	1
621	C	73.86795	80.26963	73.86114	0.00000	0.00000	0.00000	1
622	C	74.39127	80.33473	72.53710	0.00000	0.00000	0.00000	1
623	O	74.51979	81.57815	71.86461	0.00000	0.00000	0.00000	1
624	H	71.40158	75.76793	73.48180	0.00000	0.00000	0.00000	1
625	H	74.20608	75.19797	72.86919	0.00000	0.00000	0.00000	1
626	H	73.19398	76.64352	75.52192	0.00000	0.00000	0.00000	1
627	H	74.89654	76.26034	75.18734	0.00000	0.00000	0.00000	1
628	H	74.93807	76.93548	72.11269	0.00000	0.00000	0.00000	1
629	H	73.31334	79.07454	75.59069	0.00000	0.00000	0.00000	1
630	H	75.17968	79.08431	70.92267	0.00000	0.00000	0.00000	1
631	H	73.57636	81.21261	74.35525	0.00000	0.00000	0.00000	1
632	H	74.93832	81.27166	71.02548	0.00000	0.00000	0.00000	1
633	N	73.81838	73.85475	75.63114	0.00000	0.00000	0.00000	1
634	C	73.43443	72.80934	76.53191	0.00000	0.00000	0.00000	1
635	C	72.31121	73.36286	77.57036	0.00000	0.00000	0.00000	1
636	O	71.66414	74.37003	77.38851	0.00000	0.00000	0.00000	1
637	C	74.75402	72.26804	77.24366	0.00000	0.00000	0.00000	1
638	O	74.54260	71.10828	78.13362	0.00000	0.00000	0.00000	1
639	C	75.40886	73.51359	77.92478	0.00000	0.00000	0.00000	1
640	H	74.27432	74.69741	75.97157	0.00000	0.00000	0.00000	1
641	H	72.98331	72.06440	75.83291	0.00000	0.00000	0.00000	1

642	H	75.46657	71.89991	76.46020	0.00000	0.00000	0.00000	1
643	H	75.17804	70.48890	77.74326	0.00000	0.00000	0.00000	1
644	H	76.34822	73.23522	78.45959	0.00000	0.00000	0.00000	1
645	H	74.72484	73.98271	78.67351	0.00000	0.00000	0.00000	1
646	H	75.67525	74.30346	77.18486	0.00000	0.00000	0.00000	1
647	N	72.17409	72.45575	78.53073	0.00000	0.00000	0.00000	1
648	C	71.27012	72.72802	79.59039	0.00000	0.00000	0.00000	1
649	C	72.04448	73.41000	80.86408	0.00000	0.00000	0.00000	1
650	O	71.40308	73.88284	81.77485	0.00000	0.00000	0.00000	1
651	C	70.78795	71.34144	80.20334	0.00000	0.00000	0.00000	1
652	C	69.89618	70.54152	79.20306	0.00000	0.00000	0.00000	1
653	C	68.39051	70.99740	79.36458	0.00000	0.00000	0.00000	1
654	C	68.13907	72.29451	78.56085	0.00000	0.00000	0.00000	1
655	N	66.59382	72.54391	78.56241	0.00000	0.00000	0.00000	1
656	H	72.80077	71.63755	78.56653	0.00000	0.00000	0.00000	1
657	H	70.48519	73.39045	79.16039	0.00000	0.00000	0.00000	1
658	H	71.68350	70.73544	80.46848	0.00000	0.00000	0.00000	1
659	H	70.24217	71.50827	81.15858	0.00000	0.00000	0.00000	1
660	H	70.25117	70.67573	78.15630	0.00000	0.00000	0.00000	1
661	H	69.97959	69.45185	79.41682	0.00000	0.00000	0.00000	1
662	H	67.70814	70.19514	79.00144	0.00000	0.00000	0.00000	1
663	H	68.13502	71.13995	80.43992	0.00000	0.00000	0.00000	1
664	H	68.56832	73.21750	78.99839	0.00000	0.00000	0.00000	1
665	H	68.40287	72.22673	77.48623	0.00000	0.00000	0.00000	1
666	H	65.95792	71.70760	78.40950	0.00000	0.00000	0.00000	1
667	H	66.25706	73.20821	77.80757	0.00000	0.00000	0.00000	1
668	H	66.17408	72.98617	79.43114	0.00000	0.00000	0.00000	1
669	N	73.35911	73.18630	80.81226	0.00000	0.00000	0.00000	1
670	C	74.18444	73.98908	81.66538	0.00000	0.00000	0.00000	1
671	C	74.57628	75.35830	80.87948	0.00000	0.00000	0.00000	1
672	O	74.00143	75.75859	79.89617	0.00000	0.00000	0.00000	1
673	C	75.47404	73.13358	82.01257	0.00000	0.00000	0.00000	1
674	C	75.68624	73.15538	83.56085	0.00000	0.00000	0.00000	1
675	C	74.94670	71.91323	84.20192	0.00000	0.00000	0.00000	1
676	C	73.41189	72.06410	84.09120	0.00000	0.00000	0.00000	1
677	N	72.78337	70.78898	84.74907	0.00000	0.00000	0.00000	1
678	H	73.71023	72.77255	79.94934	0.00000	0.00000	0.00000	1
679	H	73.51063	74.18526	82.53231	0.00000	0.00000	0.00000	1
680	H	75.37365	72.08946	81.64125	0.00000	0.00000	0.00000	1
681	H	76.36408	73.55464	81.49236	0.00000	0.00000	0.00000	1
682	H	76.77266	73.10606	83.79740	0.00000	0.00000	0.00000	1
683	H	75.32252	74.10909	84.00520	0.00000	0.00000	0.00000	1
684	H	75.27776	70.97057	83.70904	0.00000	0.00000	0.00000	1
685	H	75.23633	71.80578	85.27254	0.00000	0.00000	0.00000	1
686	H	72.98809	72.91220	84.66529	0.00000	0.00000	0.00000	1
687	H	73.01398	72.07116	83.05580	0.00000	0.00000	0.00000	1
688	H	73.07356	70.56518	85.74546	0.00000	0.00000	0.00000	1
689	H	72.94884	69.86136	84.26031	0.00000	0.00000	0.00000	1
690	H	71.72653	70.79292	84.83681	0.00000	0.00000	0.00000	1
691	N	75.54487	75.97340	81.56435	0.00000	0.00000	0.00000	1
692	C	76.10649	77.25440	81.09700	0.00000	0.00000	0.00000	1
693	C	76.86406	76.96822	79.66795	0.00000	0.00000	0.00000	1
694	O	77.63871	76.03514	79.55019	0.00000	0.00000	0.00000	1
695	C	77.09616	77.72162	82.14846	0.00000	0.00000	0.00000	1
696	C	77.84954	78.96199	81.70421	0.00000	0.00000	0.00000	1
697	C	76.42238	77.97295	83.48533	0.00000	0.00000	0.00000	1
698	H	75.91281	75.46682	82.36707	0.00000	0.00000	0.00000	1
699	H	75.21235	77.91023	80.98575	0.00000	0.00000	0.00000	1
700	H	77.84492	76.90995	82.29192	0.00000	0.00000	0.00000	1
701	H	78.65557	79.24350	82.43909	0.00000	0.00000	0.00000	1
702	H	78.36512	78.80182	80.71335	0.00000	0.00000	0.00000	1
703	H	77.16799	79.85029	81.59358	0.00000	0.00000	0.00000	1

704	H	75.92567	77.04489	83.88123	0.00000	0.00000	0.00000	1
705	H	77.15647	78.31775	84.26428	0.00000	0.00000	0.00000	1
706	H	75.62597	78.76292	83.40507	0.00000	0.00000	0.00000	1
707	N	76.56384	77.91310	78.77451	0.00000	0.00000	0.00000	1
708	C	77.13034	77.87486	77.45616	0.00000	0.00000	0.00000	1
709	C	78.68776	78.38149	77.58863	0.00000	0.00000	0.00000	1
710	O	79.01892	79.50695	77.31673	0.00000	0.00000	0.00000	1
711	C	76.20716	78.86257	76.63480	0.00000	0.00000	0.00000	1
712	C	75.82681	79.91891	77.72085	0.00000	0.00000	0.00000	1
713	C	75.62265	79.00135	79.00134	0.00000	0.00000	0.00000	1
714	H	77.07028	76.80191	77.16922	0.00000	0.00000	0.00000	1
715	H	76.72472	79.30699	75.75416	0.00000	0.00000	0.00000	1
716	H	75.30515	78.34216	76.24374	0.00000	0.00000	0.00000	1
717	H	76.65944	80.64204	77.87313	0.00000	0.00000	0.00000	1
718	H	74.92533	80.51911	77.46227	0.00000	0.00000	0.00000	1
719	H	75.86251	79.48851	79.97473	0.00000	0.00000	0.00000	1
720	H	74.62151	78.51686	79.06835	0.00000	0.00000	0.00000	1
721	N	79.40649	77.36915	78.06010	0.00000	0.00000	0.00000	1
722	C	80.82448	77.52040	78.09146	0.00000	0.00000	0.00000	1
723	C	81.41141	76.97815	76.66776	0.00000	0.00000	0.00000	1
724	O	80.73809	76.91862	75.66746	0.00000	0.00000	0.00000	1
725	C	81.32872	76.66206	79.32744	0.00000	0.00000	0.00000	1
726	C	82.43756	77.44417	80.09425	0.00000	0.00000	0.00000	1
727	C	81.69353	78.37840	81.12750	0.00000	0.00000	0.00000	1
728	O	80.50820	78.31127	81.34031	0.00000	0.00000	0.00000	1
729	N	82.58123	79.19320	81.73334	0.00000	0.00000	0.00000	1
730	H	78.94069	76.48879	78.36140	0.00000	0.00000	0.00000	1
731	H	80.93381	78.62528	78.20068	0.00000	0.00000	0.00000	1
732	H	80.48030	76.44522	80.02021	0.00000	0.00000	0.00000	1
733	H	81.70769	75.67353	78.98109	0.00000	0.00000	0.00000	1
734	H	83.12132	76.74634	80.62608	0.00000	0.00000	0.00000	1
735	H	83.09646	78.02652	79.41308	0.00000	0.00000	0.00000	1
736	H	83.59711	79.23994	81.58886	0.00000	0.00000	0.00000	1
737	H	82.35505	79.85829	82.48033	0.00000	0.00000	0.00000	1
738	N	82.70622	76.67352	76.79297	0.00000	0.00000	0.00000	1
739	C	83.52057	76.28933	75.63754	0.00000	0.00000	0.00000	1
740	C	83.20414	74.72855	75.16756	0.00000	0.00000	0.00000	1
741	O	83.73934	74.29628	74.17386	0.00000	0.00000	0.00000	1
742	C	84.99830	76.29981	75.97565	0.00000	0.00000	0.00000	1
743	C	85.57034	77.70377	76.03626	0.00000	0.00000	0.00000	1
744	C	85.30638	75.55423	77.26079	0.00000	0.00000	0.00000	1
745	H	83.10248	76.81642	77.71889	0.00000	0.00000	0.00000	1
746	H	83.22219	77.01448	74.84356	0.00000	0.00000	0.00000	1
747	H	85.51642	75.76575	75.14422	0.00000	0.00000	0.00000	1
748	H	85.06702	78.31991	76.83168	0.00000	0.00000	0.00000	1
749	H	86.67181	77.69241	76.26728	0.00000	0.00000	0.00000	1
750	H	85.43900	78.24819	75.06014	0.00000	0.00000	0.00000	1
751	H	84.65645	74.64209	77.37212	0.00000	0.00000	0.00000	1
752	H	86.37687	75.20973	77.29599	0.00000	0.00000	0.00000	1
753	H	85.13494	76.19803	78.16705	0.00000	0.00000	0.00000	1
754	N	82.46252	74.06867	76.05011	0.00000	0.00000	0.00000	1
755	C	81.90000	72.83512	75.62954	0.00000	0.00000	0.00000	1
756	C	80.27365	73.01112	75.68197	0.00000	0.00000	0.00000	1
757	O	79.70191	73.29406	76.70667	0.00000	0.00000	0.00000	1
758	C	82.35594	71.78816	76.75429	0.00000	0.00000	0.00000	1
759	O	81.94880	70.41566	76.54401	0.00000	0.00000	0.00000	1
760	H	82.08682	74.62828	76.81343	0.00000	0.00000	0.00000	1
761	H	82.31794	72.62725	74.61625	0.00000	0.00000	0.00000	1
762	H	83.46332	71.90565	76.88302	0.00000	0.00000	0.00000	1
763	H	81.88967	72.14864	77.71188	0.00000	0.00000	0.00000	1
764	H	82.75368	70.06814	76.11753	0.00000	0.00000	0.00000	1
765	N	79.77596	72.79595	74.47659	0.00000	0.00000	0.00000	1

766	C	78.35936	72.83463	74.28191	0.00000	0.00000	0.00000	1
767	C	78.23145	72.00615	72.90836	0.00000	0.00000	0.00000	1
768	O	79.25145	71.73747	72.30416	0.00000	0.00000	0.00000	1
769	C	77.86355	74.36480	74.08616	0.00000	0.00000	0.00000	1
770	O	78.48334	75.11563	73.03809	0.00000	0.00000	0.00000	1
771	C	77.97668	74.95218	75.53850	0.00000	0.00000	0.00000	1
772	H	80.31737	72.54119	73.63065	0.00000	0.00000	0.00000	1
773	H	77.89899	72.36848	75.18273	0.00000	0.00000	0.00000	1
774	H	76.77221	74.32884	73.80771	0.00000	0.00000	0.00000	1
775	H	77.72447	75.27118	72.43692	0.00000	0.00000	0.00000	1
776	H	79.02930	75.25983	75.76799	0.00000	0.00000	0.00000	1
777	H	77.66231	74.21401	76.31662	0.00000	0.00000	0.00000	1
778	H	77.33735	75.85749	75.65688	0.00000	0.00000	0.00000	1
779	N	76.96408	71.69513	72.62384	0.00000	0.00000	0.00000	1
780	C	76.60952	71.09007	71.37329	0.00000	0.00000	0.00000	1
781	C	76.52333	72.24771	70.21477	0.00000	0.00000	0.00000	1
782	O	75.94909	73.29429	70.38864	0.00000	0.00000	0.00000	1
783	C	75.15163	70.53826	71.65988	0.00000	0.00000	0.00000	1
784	C	74.60574	71.60175	72.66277	0.00000	0.00000	0.00000	1
785	C	75.87899	71.79850	73.59186	0.00000	0.00000	0.00000	1
786	H	77.38456	70.32294	71.14849	0.00000	0.00000	0.00000	1
787	H	74.53567	70.45083	70.73638	0.00000	0.00000	0.00000	1
788	H	75.18100	69.52487	72.11891	0.00000	0.00000	0.00000	1
789	H	74.33740	72.54785	72.13829	0.00000	0.00000	0.00000	1
790	H	73.69754	71.27714	73.22239	0.00000	0.00000	0.00000	1
791	H	75.93323	72.77681	74.12260	0.00000	0.00000	0.00000	1
792	H	76.04935	70.97550	74.32609	0.00000	0.00000	0.00000	1
793	N	77.08706	71.77088	69.11259	0.00000	0.00000	0.00000	1
794	C	76.96799	72.48937	67.89937	0.00000	0.00000	0.00000	1
795	C	75.82057	71.72716	67.00431	0.00000	0.00000	0.00000	1
796	O	76.08838	70.99278	66.08389	0.00000	0.00000	0.00000	1
797	C	78.40763	72.40470	67.18261	0.00000	0.00000	0.00000	1
798	O	79.00272	71.10061	67.10643	0.00000	0.00000	0.00000	1
799	C	79.19234	73.47305	68.02641	0.00000	0.00000	0.00000	1
800	H	77.53028	70.85317	69.09591	0.00000	0.00000	0.00000	1
801	H	76.64838	73.50718	68.22221	0.00000	0.00000	0.00000	1
802	H	78.29161	72.77614	66.12842	0.00000	0.00000	0.00000	1
803	H	78.89932	70.89851	66.15367	0.00000	0.00000	0.00000	1
804	H	78.70922	74.47712	67.98368	0.00000	0.00000	0.00000	1
805	H	80.24053	73.59014	67.66561	0.00000	0.00000	0.00000	1
806	H	79.24335	73.17360	69.10056	0.00000	0.00000	0.00000	1
807	N	74.61718	71.98859	67.51410	0.00000	0.00000	0.00000	1
808	C	73.52458	72.09576	66.36428	0.00000	0.00000	0.00000	1
809	C	73.72962	73.18526	65.43070	0.00000	0.00000	0.00000	1
810	O	73.89787	74.07365	64.66886	0.00000	0.00000	0.00000	1
811	C	72.12340	72.29037	67.20064	0.00000	0.00000	0.00000	1
812	C	70.98378	71.94250	66.30453	0.00000	0.00000	0.00000	1
813	C	70.72882	70.43857	66.31457	0.00000	0.00000	0.00000	1
814	C	69.72347	72.68415	66.74127	0.00000	0.00000	0.00000	1
815	H	74.64127	72.68076	68.25880	0.00000	0.00000	0.00000	1
816	H	73.66419	71.08566	65.90395	0.00000	0.00000	0.00000	1
817	H	72.12800	71.66107	68.11889	0.00000	0.00000	0.00000	1
818	H	72.05033	73.34340	67.55505	0.00000	0.00000	0.00000	1
819	H	71.23136	72.26025	65.26519	0.00000	0.00000	0.00000	1
820	H	70.40687	70.08269	67.32645	0.00000	0.00000	0.00000	1
821	H	71.64783	69.86080	66.03921	0.00000	0.00000	0.00000	1
822	H	69.92487	70.14873	65.59111	0.00000	0.00000	0.00000	1
823	H	68.84211	72.41346	66.10619	0.00000	0.00000	0.00000	1
824	H	69.85404	73.79504	66.67172	0.00000	0.00000	0.00000	1
825	H	69.45393	72.44830	67.80247	0.00000	0.00000	0.00000	1
826	273							
827		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000***** 2.0000	8000

		0.2500	300.00	0.00	0.00	0.00	-1291.3155	0.0000	0.0000	
828	N	68.28035	77.49520	77.66227		0.00000	0.00000	0.00000		1
829	C	68.90885	77.47547	76.45409		0.00000	0.00000	0.00000		1
830	C	68.27639	76.14795	75.58906		0.00000	0.00000	0.00000		1
831	O	67.96987	75.09921	76.10141		0.00000	0.00000	0.00000		1
832	C	70.51011	77.09870	76.69057		0.00000	0.00000	0.00000		1
833	C	71.07851	78.02076	77.70108		0.00000	0.00000	0.00000		1
834	C	72.38439	77.44898	78.25075		0.00000	0.00000	0.00000		1
835	C	71.32072	79.41675	77.13469		0.00000	0.00000	0.00000		1
836	H	68.27681	76.61583	78.14582		0.00000	0.00000	0.00000		1
837	H	68.74448	78.48448	75.99538		0.00000	0.00000	0.00000		1
838	H	70.61080	76.03157	77.03624		0.00000	0.00000	0.00000		1
839	H	71.06233	77.15701	75.72718		0.00000	0.00000	0.00000		1
840	H	70.35857	78.09836	78.55000		0.00000	0.00000	0.00000		1
841	H	73.21166	77.49082	77.49863		0.00000	0.00000	0.00000		1
842	H	72.26885	76.37242	78.55416		0.00000	0.00000	0.00000		1
843	H	72.72760	78.00983	79.15645		0.00000	0.00000	0.00000		1
844	H	72.26505	79.86902	77.53139		0.00000	0.00000	0.00000		1
845	H	70.48620	80.11648	77.39362		0.00000	0.00000	0.00000		1
846	H	71.39903	79.40443	76.01863		0.00000	0.00000	0.00000		1
847	N	68.31595	76.47634	74.31028		0.00000	0.00000	0.00000		1
848	C	67.77660	75.60731	73.28037		0.00000	0.00000	0.00000		1
849	C	68.84766	75.44894	72.01324		0.00000	0.00000	0.00000		1
850	O	68.59089	74.67991	71.11736		0.00000	0.00000	0.00000		1
851	C	66.51634	76.20106	72.65460		0.00000	0.00000	0.00000		1
852	C	65.33002	76.10534	73.59332		0.00000	0.00000	0.00000		1
853	C	66.71441	77.63133	72.19549		0.00000	0.00000	0.00000		1
854	H	68.59777	77.44269	74.16701		0.00000	0.00000	0.00000		1
855	H	67.59266	74.65435	73.83487		0.00000	0.00000	0.00000		1
856	H	66.28128	75.58722	71.75535		0.00000	0.00000	0.00000		1
857	H	65.11450	75.03847	73.88231		0.00000	0.00000	0.00000		1
858	H	65.51535	76.67604	74.54622		0.00000	0.00000	0.00000		1
859	H	64.39412	76.52274	73.12659		0.00000	0.00000	0.00000		1
860	H	65.83129	78.00593	71.60589		0.00000	0.00000	0.00000		1
861	H	66.85185	78.32874	73.06836		0.00000	0.00000	0.00000		1
862	H	67.62487	77.73311	71.54007		0.00000	0.00000	0.00000		1
863	N	69.87685	76.27458	72.11439		0.00000	0.00000	0.00000		1
864	C	70.86313	76.24256	71.09351		0.00000	0.00000	0.00000		1
865	C	72.34286	75.89036	71.70562		0.00000	0.00000	0.00000		1
866	O	73.28874	75.87014	70.95071		0.00000	0.00000	0.00000		1
867	C	71.00942	77.71424	70.50465		0.00000	0.00000	0.00000		1
868	C	71.58879	77.56675	69.06823		0.00000	0.00000	0.00000		1
869	C	70.42181	76.90177	68.19693		0.00000	0.00000	0.00000		1
870	N	70.77933	77.17785	66.87218		0.00000	0.00000	0.00000		1
871	C	70.04440	76.93683	65.86325		0.00000	0.00000	0.00000		1
872	N	68.79761	76.34444	66.09324		0.00000	0.00000	0.00000		1
873	N	70.66985	77.34138	64.67557		0.00000	0.00000	0.00000		1
874	H	69.91007	76.87182	72.93675		0.00000	0.00000	0.00000		1
875	H	70.48199	75.49155	70.36037		0.00000	0.00000	0.00000		1
876	H	70.03172	78.24607	70.49351		0.00000	0.00000	0.00000		1
877	H	71.68257	78.32747	71.14610		0.00000	0.00000	0.00000		1
878	H	71.89217	78.55320	68.65194		0.00000	0.00000	0.00000		1
879	H	72.50996	76.93542	69.08010		0.00000	0.00000	0.00000		1
880	H	70.31930	75.79171	68.30044		0.00000	0.00000	0.00000		1
881	H	69.40558	77.34659	68.33558		0.00000	0.00000	0.00000		1
882	H	71.68372	77.59742	66.72421		0.00000	0.00000	0.00000		1
883	H	68.36831	76.05497	66.97130		0.00000	0.00000	0.00000		1
884	H	68.12153	76.10830	65.36629		0.00000	0.00000	0.00000		1
885	H	71.58760	77.75208	64.51054		0.00000	0.00000	0.00000		1
886	H	70.25031	77.22206	63.75277		0.00000	0.00000	0.00000		1
887	N	72.31300	75.72602	73.02158		0.00000	0.00000	0.00000		1
888	C	73.49336	75.33651	73.70823		0.00000	0.00000	0.00000		1

889	C	73.14569	73.95039	74.48458	0.00000	0.00000	0.00000	1
890	O	72.49927	73.08337	73.93861	0.00000	0.00000	0.00000	1
891	C	73.93341	76.51704	74.69606	0.00000	0.00000	0.00000	1
892	C	74.08971	77.84426	73.93360	0.00000	0.00000	0.00000	1
893	C	74.64076	77.87327	72.61685	0.00000	0.00000	0.00000	1
894	C	73.71182	79.06763	74.56401	0.00000	0.00000	0.00000	1
895	C	74.76977	79.09395	71.95079	0.00000	0.00000	0.00000	1
896	C	73.86623	80.26620	73.86571	0.00000	0.00000	0.00000	1
897	C	74.38971	80.33374	72.54188	0.00000	0.00000	0.00000	1
898	O	74.51604	81.57823	71.87100	0.00000	0.00000	0.00000	1
899	H	71.40437	75.75112	73.48152	0.00000	0.00000	0.00000	1
900	H	74.21154	75.19533	72.86732	0.00000	0.00000	0.00000	1
901	H	73.19450	76.63776	75.52008	0.00000	0.00000	0.00000	1
902	H	74.89864	76.25733	75.18821	0.00000	0.00000	0.00000	1
903	H	74.94341	76.93608	72.11349	0.00000	0.00000	0.00000	1
904	H	73.31263	79.06769	75.59323	0.00000	0.00000	0.00000	1
905	H	75.18241	79.08707	70.92661	0.00000	0.00000	0.00000	1
906	H	73.57332	81.20808	74.36115	0.00000	0.00000	0.00000	1
907	H	74.93159	81.27300	71.02992	0.00000	0.00000	0.00000	1
908	N	73.82051	73.85816	75.63530	0.00000	0.00000	0.00000	1
909	C	73.43787	72.81208	76.53566	0.00000	0.00000	0.00000	1
910	C	72.31367	73.36378	77.57363	0.00000	0.00000	0.00000	1
911	O	71.66534	74.37028	77.39121	0.00000	0.00000	0.00000	1
912	C	74.75992	72.27417	77.24658	0.00000	0.00000	0.00000	1
913	O	74.55068	71.11490	78.13429	0.00000	0.00000	0.00000	1
914	C	75.40931	73.52294	77.92768	0.00000	0.00000	0.00000	1
915	H	74.27247	74.70345	75.97525	0.00000	0.00000	0.00000	1
916	H	72.98857	72.06563	75.83699	0.00000	0.00000	0.00000	1
917	H	75.47382	71.91161	76.46169	0.00000	0.00000	0.00000	1
918	H	75.17759	70.49167	77.73504	0.00000	0.00000	0.00000	1
919	H	76.34841	73.24895	78.46511	0.00000	0.00000	0.00000	1
920	H	74.72186	73.99091	78.67394	0.00000	0.00000	0.00000	1
921	H	75.67474	74.31258	77.18713	0.00000	0.00000	0.00000	1
922	N	72.17635	72.45686	78.53419	0.00000	0.00000	0.00000	1
923	C	71.27084	72.72970	79.59240	0.00000	0.00000	0.00000	1
924	C	72.04555	73.40806	80.86778	0.00000	0.00000	0.00000	1
925	O	71.40504	73.87710	81.78108	0.00000	0.00000	0.00000	1
926	C	70.78401	71.34415	80.20410	0.00000	0.00000	0.00000	1
927	C	69.89491	70.54345	79.20209	0.00000	0.00000	0.00000	1
928	C	68.38809	70.99792	79.35700	0.00000	0.00000	0.00000	1
929	C	68.13937	72.29669	78.55516	0.00000	0.00000	0.00000	1
930	N	66.59485	72.55058	78.55893	0.00000	0.00000	0.00000	1
931	H	72.80388	71.63964	78.57067	0.00000	0.00000	0.00000	1
932	H	70.48832	73.39462	79.16164	0.00000	0.00000	0.00000	1
933	H	71.67798	70.73740	80.47282	0.00000	0.00000	0.00000	1
934	H	70.23532	71.51257	81.15740	0.00000	0.00000	0.00000	1
935	H	70.25345	70.67634	78.15640	0.00000	0.00000	0.00000	1
936	H	69.97795	69.45410	79.41763	0.00000	0.00000	0.00000	1
937	H	67.70815	70.19601	78.98848	0.00000	0.00000	0.00000	1
938	H	68.12696	71.13767	80.43134	0.00000	0.00000	0.00000	1
939	H	68.57152	73.21779	78.99378	0.00000	0.00000	0.00000	1
940	H	68.40193	72.22989	77.48017	0.00000	0.00000	0.00000	1
941	H	65.95706	71.71937	78.38728	0.00000	0.00000	0.00000	1
942	H	66.26169	73.23111	77.81706	0.00000	0.00000	0.00000	1
943	H	66.17440	72.97590	79.43575	0.00000	0.00000	0.00000	1
944	N	73.36038	73.18607	80.81300	0.00000	0.00000	0.00000	1
945	C	74.18645	73.98881	81.66551	0.00000	0.00000	0.00000	1
946	C	74.57459	75.35975	80.88084	0.00000	0.00000	0.00000	1
947	O	73.99563	75.76261	79.90101	0.00000	0.00000	0.00000	1
948	C	75.47720	73.13349	82.00904	0.00000	0.00000	0.00000	1
949	C	75.69086	73.15373	83.55711	0.00000	0.00000	0.00000	1
950	C	74.94828	71.91397	84.19933	0.00000	0.00000	0.00000	1

951	C	73.41380	72.06640	84.08620	0.00000	0.00000	0.00000	1
952	N	72.78215	70.79296	84.74434	0.00000	0.00000	0.00000	1
953	H	73.71098	72.77524	79.94848	0.00000	0.00000	0.00000	1
954	H	73.51426	74.18324	82.53405	0.00000	0.00000	0.00000	1
955	H	75.37683	72.08979	81.63645	0.00000	0.00000	0.00000	1
956	H	76.36628	73.55573	81.48812	0.00000	0.00000	0.00000	1
957	H	76.77737	73.10109	83.79252	0.00000	0.00000	0.00000	1
958	H	75.33051	74.10850	84.00189	0.00000	0.00000	0.00000	1
959	H	75.27870	70.96991	83.70872	0.00000	0.00000	0.00000	1
960	H	75.23624	71.80815	85.27057	0.00000	0.00000	0.00000	1
961	H	72.98998	72.91576	84.65842	0.00000	0.00000	0.00000	1
962	H	73.01752	72.07240	83.05017	0.00000	0.00000	0.00000	1
963	H	73.06597	70.57269	85.74334	0.00000	0.00000	0.00000	1
964	H	72.95124	69.86383	84.25972	0.00000	0.00000	0.00000	1
965	H	71.72477	70.79664	84.82520	0.00000	0.00000	0.00000	1
966	N	75.54480	75.97390	81.56437	0.00000	0.00000	0.00000	1
967	C	76.10803	77.25344	81.09545	0.00000	0.00000	0.00000	1
968	C	76.86300	76.96554	79.66554	0.00000	0.00000	0.00000	1
969	O	77.63547	76.03055	79.54699	0.00000	0.00000	0.00000	1
970	C	77.10022	77.71840	82.14556	0.00000	0.00000	0.00000	1
971	C	77.85920	78.95405	81.69754	0.00000	0.00000	0.00000	1
972	C	76.42764	77.97410	83.48214	0.00000	0.00000	0.00000	1
973	H	75.91679	75.46469	82.36363	0.00000	0.00000	0.00000	1
974	H	75.21500	77.91108	80.98531	0.00000	0.00000	0.00000	1
975	H	77.84549	76.90370	82.29010	0.00000	0.00000	0.00000	1
976	H	78.67566	79.22714	82.42483	0.00000	0.00000	0.00000	1
977	H	78.36401	78.79234	80.70149	0.00000	0.00000	0.00000	1
978	H	77.18329	79.84778	81.59512	0.00000	0.00000	0.00000	1
979	H	75.92633	77.04860	83.87844	0.00000	0.00000	0.00000	1
980	H	77.16311	78.31579	84.26116	0.00000	0.00000	0.00000	1
981	H	75.63485	78.76767	83.40133	0.00000	0.00000	0.00000	1
982	N	76.56373	77.91094	78.77243	0.00000	0.00000	0.00000	1
983	C	77.12964	77.87323	77.45378	0.00000	0.00000	0.00000	1
984	C	78.68697	78.38020	77.58582	0.00000	0.00000	0.00000	1
985	O	79.01976	79.50432	77.31047	0.00000	0.00000	0.00000	1
986	C	76.20500	78.86031	76.63334	0.00000	0.00000	0.00000	1
987	C	75.82646	79.91714	77.71954	0.00000	0.00000	0.00000	1
988	C	75.62305	78.99952	79.00010	0.00000	0.00000	0.00000	1
989	H	77.06993	76.80027	77.16673	0.00000	0.00000	0.00000	1
990	H	76.72070	79.30422	75.75136	0.00000	0.00000	0.00000	1
991	H	75.30234	78.33940	76.24450	0.00000	0.00000	0.00000	1
992	H	76.65970	80.63976	77.87091	0.00000	0.00000	0.00000	1
993	H	74.92504	80.51782	77.46187	0.00000	0.00000	0.00000	1
994	H	75.86376	79.48652	79.97339	0.00000	0.00000	0.00000	1
995	H	74.62193	78.51505	79.06774	0.00000	0.00000	0.00000	1
996	N	79.40388	77.36880	78.06202	0.00000	0.00000	0.00000	1
997	C	80.82203	77.51802	78.09249	0.00000	0.00000	0.00000	1
998	C	81.40672	76.96815	76.67078	0.00000	0.00000	0.00000	1
999	O	80.73011	76.89571	75.67343	0.00000	0.00000	0.00000	1
1000	C	81.32516	76.66181	79.33049	0.00000	0.00000	0.00000	1
1001	C	82.43467	77.44388	80.09653	0.00000	0.00000	0.00000	1
1002	C	81.69079	78.38036	81.12796	0.00000	0.00000	0.00000	1
1003	O	80.50581	78.31403	81.34314	0.00000	0.00000	0.00000	1
1004	N	82.57953	79.19675	81.72967	0.00000	0.00000	0.00000	1
1005	H	78.93749	76.48858	78.36352	0.00000	0.00000	0.00000	1
1006	H	80.93387	78.62300	78.19798	0.00000	0.00000	0.00000	1
1007	H	80.47654	76.44745	80.02371	0.00000	0.00000	0.00000	1
1008	H	81.70319	75.67229	78.98597	0.00000	0.00000	0.00000	1
1009	H	83.11732	76.74584	80.62954	0.00000	0.00000	0.00000	1
1010	H	83.09460	78.02434	79.41475	0.00000	0.00000	0.00000	1
1011	H	83.59527	79.24290	81.58360	0.00000	0.00000	0.00000	1
1012	H	82.35445	79.86463	82.47449	0.00000	0.00000	0.00000	1

1013	N	82.70288	76.66919	76.79551	0.00000	0.00000	0.00000	1
1014	C	83.51906	76.28867	75.64010	0.00000	0.00000	0.00000	1
1015	C	83.20446	74.72789	75.16991	0.00000	0.00000	0.00000	1
1016	O	83.74150	74.29519	74.17744	0.00000	0.00000	0.00000	1
1017	C	84.99664	76.30232	75.97811	0.00000	0.00000	0.00000	1
1018	C	85.56588	77.70742	76.03964	0.00000	0.00000	0.00000	1
1019	C	85.30664	75.55621	77.26252	0.00000	0.00000	0.00000	1
1020	H	83.09984	76.82194	77.71960	0.00000	0.00000	0.00000	1
1021	H	83.21937	77.01414	74.84685	0.00000	0.00000	0.00000	1
1022	H	85.51622	75.77020	75.14631	0.00000	0.00000	0.00000	1
1023	H	85.06149	78.32213	76.83547	0.00000	0.00000	0.00000	1
1024	H	86.66740	77.69813	76.27050	0.00000	0.00000	0.00000	1
1025	H	85.43345	78.25213	75.06384	0.00000	0.00000	0.00000	1
1026	H	84.67135	74.63270	77.36418	0.00000	0.00000	0.00000	1
1027	H	86.38252	75.22984	77.30531	0.00000	0.00000	0.00000	1
1028	H	85.11659	76.19276	78.17018	0.00000	0.00000	0.00000	1
1029	N	82.46109	74.06847	76.05154	0.00000	0.00000	0.00000	1
1030	C	81.89608	72.83644	75.62994	0.00000	0.00000	0.00000	1
1031	C	80.26984	73.01401	75.68547	0.00000	0.00000	0.00000	1
1032	O	79.70021	73.29804	76.71090	0.00000	0.00000	0.00000	1
1033	C	82.35220	71.78795	76.75314	0.00000	0.00000	0.00000	1
1034	O	81.94386	70.41599	76.54175	0.00000	0.00000	0.00000	1
1035	H	82.08433	74.62843	76.81408	0.00000	0.00000	0.00000	1
1036	H	82.31246	72.62919	74.61594	0.00000	0.00000	0.00000	1
1037	H	83.45975	71.90462	76.88119	0.00000	0.00000	0.00000	1
1038	H	81.88682	72.14806	77.71128	0.00000	0.00000	0.00000	1
1039	H	82.74831	70.06814	76.11474	0.00000	0.00000	0.00000	1
1040	N	79.77063	72.79903	74.48078	0.00000	0.00000	0.00000	1
1041	C	78.35429	72.83711	74.28520	0.00000	0.00000	0.00000	1
1042	C	78.22787	72.00530	72.91354	0.00000	0.00000	0.00000	1
1043	O	79.24854	71.73312	72.31180	0.00000	0.00000	0.00000	1
1044	C	77.85784	74.36641	74.08498	0.00000	0.00000	0.00000	1
1045	O	78.46939	75.10969	73.02669	0.00000	0.00000	0.00000	1
1046	C	77.98459	74.96369	75.53208	0.00000	0.00000	0.00000	1
1047	H	80.31207	72.54192	73.63547	0.00000	0.00000	0.00000	1
1048	H	77.89337	72.37329	75.18702	0.00000	0.00000	0.00000	1
1049	H	76.76413	74.32944	73.81608	0.00000	0.00000	0.00000	1
1050	H	77.70688	75.25625	72.42773	0.00000	0.00000	0.00000	1
1051	H	79.04131	75.26523	75.75322	0.00000	0.00000	0.00000	1
1052	H	77.66878	74.23366	76.31736	0.00000	0.00000	0.00000	1
1053	H	77.35313	75.87489	75.64751	0.00000	0.00000	0.00000	1
1054	N	76.96082	71.69540	72.62652	0.00000	0.00000	0.00000	1
1055	C	76.60958	71.08927	71.37541	0.00000	0.00000	0.00000	1
1056	C	76.52364	72.24582	70.21584	0.00000	0.00000	0.00000	1
1057	O	75.94636	73.29100	70.38825	0.00000	0.00000	0.00000	1
1058	C	75.15152	70.53666	71.65916	0.00000	0.00000	0.00000	1
1059	C	74.60297	71.60055	72.66006	0.00000	0.00000	0.00000	1
1060	C	75.87375	71.79896	73.59221	0.00000	0.00000	0.00000	1
1061	H	77.38570	70.32260	71.15285	0.00000	0.00000	0.00000	1
1062	H	74.53737	70.44784	70.73458	0.00000	0.00000	0.00000	1
1063	H	75.18026	69.52406	72.11992	0.00000	0.00000	0.00000	1
1064	H	74.33469	72.54646	72.13500	0.00000	0.00000	0.00000	1
1065	H	73.69431	71.27358	73.21731	0.00000	0.00000	0.00000	1
1066	H	75.92638	72.77767	74.12247	0.00000	0.00000	0.00000	1
1067	H	76.04265	70.97654	74.32739	0.00000	0.00000	0.00000	1
1068	N	77.09103	71.77053	69.11487	0.00000	0.00000	0.00000	1
1069	C	76.96985	72.48811	67.90113	0.00000	0.00000	0.00000	1
1070	C	75.82027	71.72583	67.00884	0.00000	0.00000	0.00000	1
1071	O	76.08580	70.98966	66.08917	0.00000	0.00000	0.00000	1
1072	C	78.40856	72.40407	67.18262	0.00000	0.00000	0.00000	1
1073	O	79.00391	71.10017	67.10475	0.00000	0.00000	0.00000	1
1074	C	79.19305	73.47228	68.02684	0.00000	0.00000	0.00000	1

1075	H	77.53623	70.85377	69.09877	0.00000	0.00000	0.00000	1	
1076	H	76.65039	73.50598	68.22378	0.00000	0.00000	0.00000	1	
1077	H	78.29120	72.77623	66.12883	0.00000	0.00000	0.00000	1	
1078	H	78.89392	70.89620	66.15313	0.00000	0.00000	0.00000	1	
1079	H	78.70651	74.47491	67.98904	0.00000	0.00000	0.00000	1	
1080	H	80.23962	73.59402	67.66289	0.00000	0.00000	0.00000	1	
1081	H	79.24862	73.16968	69.09987	0.00000	0.00000	0.00000	1	
1082	N	74.61775	71.98981	67.51961	0.00000	0.00000	0.00000	1	
1083	C	73.52563	72.10129	66.36998	0.00000	0.00000	0.00000	1	
1084	C	73.73184	73.19305	65.43914	0.00000	0.00000	0.00000	1	
1085	O	73.90202	74.08334	64.68002	0.00000	0.00000	0.00000	1	
1086	C	72.12253	72.29515	67.20347	0.00000	0.00000	0.00000	1	
1087	C	70.98440	71.94772	66.30579	0.00000	0.00000	0.00000	1	
1088	C	70.72887	70.44381	66.31334	0.00000	0.00000	0.00000	1	
1089	C	69.72195	72.68649	66.74147	0.00000	0.00000	0.00000	1	
1090	H	74.64516	72.68279	68.26344	0.00000	0.00000	0.00000	1	
1091	H	73.66532	71.09211	65.90754	0.00000	0.00000	0.00000	1	
1092	H	72.12560	71.66578	68.12172	0.00000	0.00000	0.00000	1	
1093	H	72.04882	73.34814	67.55803	0.00000	0.00000	0.00000	1	
1094	H	71.23306	72.26717	65.26720	0.00000	0.00000	0.00000	1	
1095	H	70.41000	70.08598	67.32551	0.00000	0.00000	0.00000	1	
1096	H	71.64649	69.86603	66.03356	0.00000	0.00000	0.00000	1	
1097	H	69.92216	70.15612	65.59206	0.00000	0.00000	0.00000	1	
1098	H	68.84212	72.41441	66.10479	0.00000	0.00000	0.00000	1	
1099	H	69.85004	73.79772	66.67323	0.00000	0.00000	0.00000	1	
1100	H	69.45124	72.44879	67.80194	0.00000	0.00000	0.00000	1	
1101		273							
1102		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	2.5000	10000
		0.2500	300.00	0.00	0.00	-1291.3565	0.0000	0.0000	
1103	N	68.28180	77.48947	77.66397	0.00000	0.00000	0.00000	0.00000	1
1104	C	68.90782	77.47184	76.45449	0.00000	0.00000	0.00000	0.00000	1
1105	C	68.27514	76.14462	75.58940	0.00000	0.00000	0.00000	0.00000	1
1106	O	67.96891	75.09550	76.10103	0.00000	0.00000	0.00000	0.00000	1
1107	C	70.50994	77.09534	76.68538	0.00000	0.00000	0.00000	0.00000	1
1108	C	71.08041	78.01470	77.69724	0.00000	0.00000	0.00000	0.00000	1
1109	C	72.38807	77.44161	78.24112	0.00000	0.00000	0.00000	0.00000	1
1110	C	71.31810	79.41250	77.13345	0.00000	0.00000	0.00000	0.00000	1
1111	H	68.27638	76.60848	78.14454	0.00000	0.00000	0.00000	0.00000	1
1112	H	68.74209	78.48138	75.99742	0.00000	0.00000	0.00000	0.00000	1
1113	H	70.61262	76.02729	77.02787	0.00000	0.00000	0.00000	0.00000	1
1114	H	71.05952	77.15702	75.72063	0.00000	0.00000	0.00000	0.00000	1
1115	H	70.36309	78.08893	78.54869	0.00000	0.00000	0.00000	0.00000	1
1116	H	73.21461	77.49128	77.48872	0.00000	0.00000	0.00000	0.00000	1
1117	H	72.27521	76.36217	78.53636	0.00000	0.00000	0.00000	0.00000	1
1118	H	72.73081	77.99612	79.15089	0.00000	0.00000	0.00000	0.00000	1
1119	H	72.25197	79.87401	77.54396	0.00000	0.00000	0.00000	0.00000	1
1120	H	70.47295	80.10432	77.37883	0.00000	0.00000	0.00000	0.00000	1
1121	H	71.41322	79.40005	76.01872	0.00000	0.00000	0.00000	0.00000	1
1122	N	68.31516	76.47394	74.31065	0.00000	0.00000	0.00000	0.00000	1
1123	C	67.77542	75.60695	73.28010	0.00000	0.00000	0.00000	0.00000	1
1124	C	68.84607	75.45185	72.01281	0.00000	0.00000	0.00000	0.00000	1
1125	O	68.58670	74.68879	71.11239	0.00000	0.00000	0.00000	0.00000	1
1126	C	66.51471	76.20123	72.65728	0.00000	0.00000	0.00000	0.00000	1
1127	C	65.33002	76.10808	73.59851	0.00000	0.00000	0.00000	0.00000	1
1128	C	66.71426	77.63109	72.19695	0.00000	0.00000	0.00000	0.00000	1
1129	H	68.59682	77.44077	74.16804	0.00000	0.00000	0.00000	0.00000	1
1130	H	67.59233	74.65246	73.83294	0.00000	0.00000	0.00000	0.00000	1
1131	H	66.27628	75.58752	71.75871	0.00000	0.00000	0.00000	0.00000	1
1132	H	65.11356	75.04174	73.88879	0.00000	0.00000	0.00000	0.00000	1
1133	H	65.51821	76.67921	74.55061	0.00000	0.00000	0.00000	0.00000	1
1134	H	64.39363	76.52647	73.13357	0.00000	0.00000	0.00000	0.00000	1
1135	H	65.82996	78.00800	71.61060	0.00000	0.00000	0.00000	0.00000	1

1136	H	66.85698	78.32828	73.06916	0.00000	0.00000	0.00000	1
1137	H	67.62257	77.73023	71.53812	0.00000	0.00000	0.00000	1
1138	N	69.87960	76.27160	72.11907	0.00000	0.00000	0.00000	1
1139	C	70.86401	76.24182	71.09616	0.00000	0.00000	0.00000	1
1140	C	72.34528	75.89142	71.70543	0.00000	0.00000	0.00000	1
1141	O	73.29121	75.87756	70.95055	0.00000	0.00000	0.00000	1
1142	C	71.00711	77.71368	70.50696	0.00000	0.00000	0.00000	1
1143	C	71.58679	77.56802	69.07045	0.00000	0.00000	0.00000	1
1144	C	70.42297	76.89943	68.19775	0.00000	0.00000	0.00000	1
1145	N	70.78235	77.17340	66.87304	0.00000	0.00000	0.00000	1
1146	C	70.04807	76.93191	65.86383	0.00000	0.00000	0.00000	1
1147	N	68.80030	76.34157	66.09394	0.00000	0.00000	0.00000	1
1148	N	70.67456	77.33351	64.67570	0.00000	0.00000	0.00000	1
1149	H	69.91596	76.86454	72.94446	0.00000	0.00000	0.00000	1
1150	H	70.48189	75.49095	70.36327	0.00000	0.00000	0.00000	1
1151	H	70.02827	78.24341	70.49601	0.00000	0.00000	0.00000	1
1152	H	71.67900	78.32833	71.14836	0.00000	0.00000	0.00000	1
1153	H	71.88721	78.55546	68.65439	0.00000	0.00000	0.00000	1
1154	H	72.51010	76.93974	69.08245	0.00000	0.00000	0.00000	1
1155	H	70.32264	75.78933	68.30302	0.00000	0.00000	0.00000	1
1156	H	69.40556	77.34234	68.33362	0.00000	0.00000	0.00000	1
1157	H	71.68753	77.59133	66.72531	0.00000	0.00000	0.00000	1
1158	H	68.37014	76.05404	66.97224	0.00000	0.00000	0.00000	1
1159	H	68.12430	76.10511	65.36702	0.00000	0.00000	0.00000	1
1160	H	71.59303	77.74246	64.51023	0.00000	0.00000	0.00000	1
1161	H	70.25525	77.21311	63.75290	0.00000	0.00000	0.00000	1
1162	N	72.31575	75.71959	73.02037	0.00000	0.00000	0.00000	1
1163	C	73.49722	75.33308	73.70664	0.00000	0.00000	0.00000	1
1164	C	73.14869	73.94901	74.48626	0.00000	0.00000	0.00000	1
1165	O	72.50227	73.08008	73.94284	0.00000	0.00000	0.00000	1
1166	C	73.93589	76.51321	74.69580	0.00000	0.00000	0.00000	1
1167	C	74.09171	77.84124	73.93478	0.00000	0.00000	0.00000	1
1168	C	74.64392	77.87273	72.61863	0.00000	0.00000	0.00000	1
1169	C	73.71181	79.06307	74.56688	0.00000	0.00000	0.00000	1
1170	C	74.77103	79.09448	71.95427	0.00000	0.00000	0.00000	1
1171	C	73.86442	80.26277	73.87024	0.00000	0.00000	0.00000	1
1172	C	74.38802	80.33277	72.54658	0.00000	0.00000	0.00000	1
1173	O	74.51201	81.57829	71.87723	0.00000	0.00000	0.00000	1
1174	H	71.40703	75.73774	73.48044	0.00000	0.00000	0.00000	1
1175	H	74.21620	75.19207	72.86646	0.00000	0.00000	0.00000	1
1176	H	73.19592	76.63247	75.51909	0.00000	0.00000	0.00000	1
1177	H	74.90086	76.25373	75.18872	0.00000	0.00000	0.00000	1
1178	H	74.94850	76.93643	72.11423	0.00000	0.00000	0.00000	1
1179	H	73.31259	79.06099	75.59607	0.00000	0.00000	0.00000	1
1180	H	75.18455	79.08969	70.93044	0.00000	0.00000	0.00000	1
1181	H	73.56985	81.20346	74.36691	0.00000	0.00000	0.00000	1
1182	H	74.92589	81.27453	71.03479	0.00000	0.00000	0.00000	1
1183	N	73.82184	73.86170	75.63846	0.00000	0.00000	0.00000	1
1184	C	73.44120	72.81553	76.53944	0.00000	0.00000	0.00000	1
1185	C	72.31599	73.36512	77.57705	0.00000	0.00000	0.00000	1
1186	O	71.66636	74.37099	77.39458	0.00000	0.00000	0.00000	1
1187	C	74.76535	72.28076	77.24976	0.00000	0.00000	0.00000	1
1188	O	74.55817	71.12152	78.13565	0.00000	0.00000	0.00000	1
1189	C	75.40992	73.53220	77.93093	0.00000	0.00000	0.00000	1
1190	H	74.27111	74.70930	75.97648	0.00000	0.00000	0.00000	1
1191	H	72.99365	72.06768	75.84112	0.00000	0.00000	0.00000	1
1192	H	75.48037	71.92240	76.46390	0.00000	0.00000	0.00000	1
1193	H	75.17890	70.49580	77.72972	0.00000	0.00000	0.00000	1
1194	H	76.34874	73.26180	78.47064	0.00000	0.00000	0.00000	1
1195	H	74.71951	73.99914	78.67516	0.00000	0.00000	0.00000	1
1196	H	75.67455	74.32170	77.18992	0.00000	0.00000	0.00000	1
1197	N	72.17848	72.45780	78.53727	0.00000	0.00000	0.00000	1

1198	C	71.27157	72.73103	79.59423	0.00000	0.00000	0.00000	1
1199	C	72.04665	73.40594	80.87116	0.00000	0.00000	0.00000	1
1200	O	71.40696	73.87128	81.78689	0.00000	0.00000	0.00000	1
1201	C	70.77998	71.34660	80.20478	0.00000	0.00000	0.00000	1
1202	C	69.89380	70.54528	79.20070	0.00000	0.00000	0.00000	1
1203	C	68.38599	70.99862	79.34935	0.00000	0.00000	0.00000	1
1204	C	68.13992	72.29916	78.54962	0.00000	0.00000	0.00000	1
1205	N	66.59610	72.55733	78.55535	0.00000	0.00000	0.00000	1
1206	H	72.80700	71.64158	78.57424	0.00000	0.00000	0.00000	1
1207	H	70.49140	73.39838	79.16276	0.00000	0.00000	0.00000	1
1208	H	71.67220	70.73906	80.47750	0.00000	0.00000	0.00000	1
1209	H	70.22802	71.51672	81.15589	0.00000	0.00000	0.00000	1
1210	H	70.25592	70.67720	78.15614	0.00000	0.00000	0.00000	1
1211	H	69.97641	69.45619	79.41765	0.00000	0.00000	0.00000	1
1212	H	67.70825	70.19721	78.97569	0.00000	0.00000	0.00000	1
1213	H	68.11958	71.13561	80.42276	0.00000	0.00000	0.00000	1
1214	H	68.57468	73.21836	78.98959	0.00000	0.00000	0.00000	1
1215	H	68.40148	72.23363	77.47429	0.00000	0.00000	0.00000	1
1216	H	65.95655	71.73145	78.36557	0.00000	0.00000	0.00000	1
1217	H	66.26660	73.25330	77.82628	0.00000	0.00000	0.00000	1
1218	H	66.17476	72.96615	79.43957	0.00000	0.00000	0.00000	1
1219	N	73.36171	73.18579	80.81353	0.00000	0.00000	0.00000	1
1220	C	74.18832	73.98842	81.66569	0.00000	0.00000	0.00000	1
1221	C	74.57261	75.36116	80.88236	0.00000	0.00000	0.00000	1
1222	O	73.98949	75.76655	79.90607	0.00000	0.00000	0.00000	1
1223	C	75.48027	73.13346	82.00573	0.00000	0.00000	0.00000	1
1224	C	75.69557	73.15211	83.55358	0.00000	0.00000	0.00000	1
1225	C	74.94990	71.91464	84.19669	0.00000	0.00000	0.00000	1
1226	C	73.41577	72.06872	84.08109	0.00000	0.00000	0.00000	1
1227	N	72.78103	70.79702	84.73958	0.00000	0.00000	0.00000	1
1228	H	73.71184	72.77791	79.94744	0.00000	0.00000	0.00000	1
1229	H	73.51752	74.18088	82.53572	0.00000	0.00000	0.00000	1
1230	H	75.38001	72.09017	81.63195	0.00000	0.00000	0.00000	1
1231	H	76.36833	73.55692	81.48406	0.00000	0.00000	0.00000	1
1232	H	76.78217	73.09604	83.78777	0.00000	0.00000	0.00000	1
1233	H	75.33868	74.10790	83.99895	0.00000	0.00000	0.00000	1
1234	H	75.27966	70.96929	83.70812	0.00000	0.00000	0.00000	1
1235	H	75.23617	71.81019	85.26851	0.00000	0.00000	0.00000	1
1236	H	72.99198	72.91941	84.65136	0.00000	0.00000	0.00000	1
1237	H	73.02113	72.07358	83.04443	0.00000	0.00000	0.00000	1
1238	H	73.05869	70.58023	85.74106	0.00000	0.00000	0.00000	1
1239	H	72.95354	69.86639	84.25906	0.00000	0.00000	0.00000	1
1240	H	71.72315	70.80046	84.81380	0.00000	0.00000	0.00000	1
1241	N	75.54439	75.97433	81.56464	0.00000	0.00000	0.00000	1
1242	C	76.10943	77.25244	81.09387	0.00000	0.00000	0.00000	1
1243	C	76.86157	76.96263	79.66298	0.00000	0.00000	0.00000	1
1244	O	77.63183	76.02574	79.54364	0.00000	0.00000	0.00000	1
1245	C	77.10469	77.71482	82.14229	0.00000	0.00000	0.00000	1
1246	C	77.86920	78.94578	81.69058	0.00000	0.00000	0.00000	1
1247	C	76.43374	77.97559	83.47863	0.00000	0.00000	0.00000	1
1248	H	75.92060	75.46245	82.36023	0.00000	0.00000	0.00000	1
1249	H	75.21775	77.91216	80.98520	0.00000	0.00000	0.00000	1
1250	H	77.84621	76.89685	82.28781	0.00000	0.00000	0.00000	1
1251	H	78.69268	79.21163	82.41286	0.00000	0.00000	0.00000	1
1252	H	78.36385	78.78252	80.68936	0.00000	0.00000	0.00000	1
1253	H	77.19989	79.84523	81.59670	0.00000	0.00000	0.00000	1
1254	H	75.92771	77.05296	83.87569	0.00000	0.00000	0.00000	1
1255	H	77.17085	78.31433	84.25741	0.00000	0.00000	0.00000	1
1256	H	75.64482	78.77297	83.39701	0.00000	0.00000	0.00000	1
1257	N	76.56312	77.90857	78.77031	0.00000	0.00000	0.00000	1
1258	C	77.12856	77.87130	77.45143	0.00000	0.00000	0.00000	1
1259	C	78.68582	78.37844	77.58329	0.00000	0.00000	0.00000	1

1260	O	79.02075	79.50126	77.30493	0.00000	0.00000	0.00000	1
1261	C	76.20290	78.85807	76.63182	0.00000	0.00000	0.00000	1
1262	C	75.82609	79.91534	77.71818	0.00000	0.00000	0.00000	1
1263	C	75.62340	78.99783	78.99892	0.00000	0.00000	0.00000	1
1264	H	77.06906	76.79835	77.16428	0.00000	0.00000	0.00000	1
1265	H	76.71713	79.30147	75.74874	0.00000	0.00000	0.00000	1
1266	H	75.29963	78.33687	76.24486	0.00000	0.00000	0.00000	1
1267	H	76.65989	80.63750	77.86865	0.00000	0.00000	0.00000	1
1268	H	74.92474	80.51648	77.46135	0.00000	0.00000	0.00000	1
1269	H	75.86541	79.48465	79.97202	0.00000	0.00000	0.00000	1
1270	H	74.62208	78.51387	79.06751	0.00000	0.00000	0.00000	1
1271	N	79.40103	77.36811	78.06413	0.00000	0.00000	0.00000	1
1272	C	80.81937	77.51531	78.09343	0.00000	0.00000	0.00000	1
1273	C	81.40137	76.95683	76.67390	0.00000	0.00000	0.00000	1
1274	O	80.72063	76.86913	75.68039	0.00000	0.00000	0.00000	1
1275	C	81.32135	76.66161	79.33374	0.00000	0.00000	0.00000	1
1276	C	82.43139	77.44355	80.09874	0.00000	0.00000	0.00000	1
1277	C	81.68898	78.38271	81.12818	0.00000	0.00000	0.00000	1
1278	O	80.50403	78.31579	81.34433	0.00000	0.00000	0.00000	1
1279	N	82.57786	79.20123	81.72672	0.00000	0.00000	0.00000	1
1280	H	78.93421	76.48790	78.36555	0.00000	0.00000	0.00000	1
1281	H	80.93344	78.62069	78.19439	0.00000	0.00000	0.00000	1
1282	H	80.47194	76.44880	80.02656	0.00000	0.00000	0.00000	1
1283	H	81.69854	75.67104	78.99151	0.00000	0.00000	0.00000	1
1284	H	83.11280	76.74573	80.63362	0.00000	0.00000	0.00000	1
1285	H	83.09234	78.02255	79.41674	0.00000	0.00000	0.00000	1
1286	H	83.59320	79.24627	81.57823	0.00000	0.00000	0.00000	1
1287	H	82.35381	79.87164	82.46952	0.00000	0.00000	0.00000	1
1288	N	82.69914	76.66512	76.79764	0.00000	0.00000	0.00000	1
1289	C	83.51723	76.28780	75.64237	0.00000	0.00000	0.00000	1
1290	C	83.20455	74.72688	75.17218	0.00000	0.00000	0.00000	1
1291	O	83.74329	74.29382	74.18085	0.00000	0.00000	0.00000	1
1292	C	84.99468	76.30480	75.98054	0.00000	0.00000	0.00000	1
1293	C	85.56093	77.71108	76.04321	0.00000	0.00000	0.00000	1
1294	C	85.30668	75.55825	77.26422	0.00000	0.00000	0.00000	1
1295	H	83.09701	76.82988	77.71929	0.00000	0.00000	0.00000	1
1296	H	83.21645	77.01331	74.84962	0.00000	0.00000	0.00000	1
1297	H	85.51585	75.77474	75.14840	0.00000	0.00000	0.00000	1
1298	H	85.05545	78.32418	76.83954	0.00000	0.00000	0.00000	1
1299	H	86.66251	77.70390	76.27393	0.00000	0.00000	0.00000	1
1300	H	85.42741	78.25624	75.06782	0.00000	0.00000	0.00000	1
1301	H	84.68592	74.62398	77.35675	0.00000	0.00000	0.00000	1
1302	H	86.38745	75.24955	77.31433	0.00000	0.00000	0.00000	1
1303	H	85.09886	76.18748	78.17306	0.00000	0.00000	0.00000	1
1304	N	82.45993	74.06775	76.05320	0.00000	0.00000	0.00000	1
1305	C	81.89190	72.83753	75.63050	0.00000	0.00000	0.00000	1
1306	C	80.26603	73.01851	75.68877	0.00000	0.00000	0.00000	1
1307	O	79.69999	73.30661	76.71498	0.00000	0.00000	0.00000	1
1308	C	82.34828	71.78747	76.75211	0.00000	0.00000	0.00000	1
1309	O	81.93878	70.41602	76.53966	0.00000	0.00000	0.00000	1
1310	H	82.08201	74.62831	76.81476	0.00000	0.00000	0.00000	1
1311	H	82.30660	72.63062	74.61580	0.00000	0.00000	0.00000	1
1312	H	83.45603	71.90330	76.87924	0.00000	0.00000	0.00000	1
1313	H	81.88405	72.14711	77.71099	0.00000	0.00000	0.00000	1
1314	H	82.74270	70.06798	76.11176	0.00000	0.00000	0.00000	1
1315	N	79.76508	72.80273	74.48507	0.00000	0.00000	0.00000	1
1316	C	78.34905	72.83962	74.28758	0.00000	0.00000	0.00000	1
1317	C	78.22444	72.00425	72.91809	0.00000	0.00000	0.00000	1
1318	O	79.24606	71.72886	72.31924	0.00000	0.00000	0.00000	1
1319	C	77.85236	74.36832	74.08387	0.00000	0.00000	0.00000	1
1320	O	78.45576	75.10327	73.01501	0.00000	0.00000	0.00000	1
1321	C	77.99388	74.97518	75.52559	0.00000	0.00000	0.00000	1

1322	H	80.30683	72.54274	73.64070	0.00000	0.00000	0.00000	1	
1323	H	77.88802	72.37808	75.19046	0.00000	0.00000	0.00000	1	
1324	H	76.75621	74.33076	73.82521	0.00000	0.00000	0.00000	1	
1325	H	77.68938	75.24177	72.41902	0.00000	0.00000	0.00000	1	
1326	H	79.05524	75.26961	75.73858	0.00000	0.00000	0.00000	1	
1327	H	77.67654	74.25365	76.31816	0.00000	0.00000	0.00000	1	
1328	H	77.37050	75.89241	75.63799	0.00000	0.00000	0.00000	1	
1329	N	76.95771	71.69500	72.62891	0.00000	0.00000	0.00000	1	
1330	C	76.60965	71.08816	71.37723	0.00000	0.00000	0.00000	1	
1331	C	76.52369	72.24428	70.21719	0.00000	0.00000	0.00000	1	
1332	O	75.94350	73.28804	70.38853	0.00000	0.00000	0.00000	1	
1333	C	75.15157	70.53427	71.65824	0.00000	0.00000	0.00000	1	
1334	C	74.60007	71.59798	72.65763	0.00000	0.00000	0.00000	1	
1335	C	75.86861	71.79886	73.59224	0.00000	0.00000	0.00000	1	
1336	H	77.38719	70.32240	71.15648	0.00000	0.00000	0.00000	1	
1337	H	74.53938	70.44455	70.73243	0.00000	0.00000	0.00000	1	
1338	H	75.18027	69.52197	72.11963	0.00000	0.00000	0.00000	1	
1339	H	74.33131	72.54341	72.13183	0.00000	0.00000	0.00000	1	
1340	H	73.69104	71.26923	73.21308	0.00000	0.00000	0.00000	1	
1341	H	75.91927	72.77834	74.12134	0.00000	0.00000	0.00000	1	
1342	H	76.03659	70.97763	74.32893	0.00000	0.00000	0.00000	1	
1343	N	77.09469	71.77060	69.11739	0.00000	0.00000	0.00000	1	
1344	C	76.97135	72.48709	67.90312	0.00000	0.00000	0.00000	1	
1345	C	75.81960	71.72473	67.01366	0.00000	0.00000	0.00000	1	
1346	O	76.08305	70.98677	66.09475	0.00000	0.00000	0.00000	1	
1347	C	78.40904	72.40344	67.18275	0.00000	0.00000	0.00000	1	
1348	O	79.00451	71.09968	67.10316	0.00000	0.00000	0.00000	1	
1349	C	79.19387	73.47138	68.02707	0.00000	0.00000	0.00000	1	
1350	H	77.54184	70.85475	69.10191	0.00000	0.00000	0.00000	1	
1351	H	76.65212	73.50509	68.22550	0.00000	0.00000	0.00000	1	
1352	H	78.29026	72.77623	66.12933	0.00000	0.00000	0.00000	1	
1353	H	78.88928	70.89451	66.15242	0.00000	0.00000	0.00000	1	
1354	H	78.70452	74.47281	67.99381	0.00000	0.00000	0.00000	1	
1355	H	80.23885	73.59697	67.65992	0.00000	0.00000	0.00000	1	
1356	H	79.25384	73.16599	69.09907	0.00000	0.00000	0.00000	1	
1357	N	74.61786	71.99113	67.52520	0.00000	0.00000	0.00000	1	
1358	C	73.52577	72.10670	66.37516	0.00000	0.00000	0.00000	1	
1359	C	73.73538	73.20086	65.44806	0.00000	0.00000	0.00000	1	
1360	O	73.90598	74.09303	64.69093	0.00000	0.00000	0.00000	1	
1361	C	72.12157	72.29988	67.20644	0.00000	0.00000	0.00000	1	
1362	C	70.98474	71.95282	66.30714	0.00000	0.00000	0.00000	1	
1363	C	70.72940	70.44911	66.31210	0.00000	0.00000	0.00000	1	
1364	C	69.72083	72.68918	66.74180	0.00000	0.00000	0.00000	1	
1365	H	74.64815	72.68489	68.26815	0.00000	0.00000	0.00000	1	
1366	H	73.66609	71.09850	65.91081	0.00000	0.00000	0.00000	1	
1367	H	72.12334	71.67014	68.12446	0.00000	0.00000	0.00000	1	
1368	H	72.04725	73.35274	67.56136	0.00000	0.00000	0.00000	1	
1369	H	71.23460	72.27406	65.26925	0.00000	0.00000	0.00000	1	
1370	H	70.41347	70.08898	67.32445	0.00000	0.00000	0.00000	1	
1371	H	71.64598	69.87159	66.02822	0.00000	0.00000	0.00000	1	
1372	H	69.92034	70.16301	65.59273	0.00000	0.00000	0.00000	1	
1373	H	68.84223	72.41628	66.10368	0.00000	0.00000	0.00000	1	
1374	H	69.84686	73.80076	66.67493	0.00000	0.00000	0.00000	1	
1375	H	69.44883	72.44988	67.80164	0.00000	0.00000	0.00000	1	
1376		273							
1377		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	3.0000	12000
		0.2500	300.00	0.00	0.00	0.00	-1291.3801	0.0000	0.0000
1378	N	68.28269	77.48574	77.66511	0.00000	0.00000	0.00000	0.00000	1
1379	C	68.90706	77.46954	76.45478	0.00000	0.00000	0.00000	0.00000	1
1380	C	68.27424	76.14251	75.58955	0.00000	0.00000	0.00000	0.00000	1
1381	O	67.96802	75.09319	76.10074	0.00000	0.00000	0.00000	0.00000	1
1382	C	70.50970	77.09322	76.68221	0.00000	0.00000	0.00000	0.00000	1

1383	C	71.08169	78.01074	77.69490	0.00000	0.00000	0.00000	1
1384	C	72.39056	77.43680	78.23485	0.00000	0.00000	0.00000	1
1385	C	71.31649	79.40974	77.13289	0.00000	0.00000	0.00000	1
1386	H	68.27674	76.60384	78.14401	0.00000	0.00000	0.00000	1
1387	H	68.74036	78.47941	75.99878	0.00000	0.00000	0.00000	1
1388	H	70.61348	76.02459	77.02273	0.00000	0.00000	0.00000	1
1389	H	71.05760	77.15689	75.71661	0.00000	0.00000	0.00000	1
1390	H	70.36616	78.08283	78.54804	0.00000	0.00000	0.00000	1
1391	H	73.21651	77.49167	77.48222	0.00000	0.00000	0.00000	1
1392	H	72.27964	76.35547	78.52479	0.00000	0.00000	0.00000	1
1393	H	72.73308	77.98717	79.14722	0.00000	0.00000	0.00000	1
1394	H	72.24351	79.87706	77.55225	0.00000	0.00000	0.00000	1
1395	H	70.46471	80.09643	77.36958	0.00000	0.00000	0.00000	1
1396	H	71.42240	79.39744	76.01915	0.00000	0.00000	0.00000	1
1397	N	68.31489	76.47244	74.31097	0.00000	0.00000	0.00000	1
1398	C	67.77478	75.60649	73.27978	0.00000	0.00000	0.00000	1
1399	C	68.84519	75.45352	72.01212	0.00000	0.00000	0.00000	1
1400	O	68.58396	74.69414	71.10910	0.00000	0.00000	0.00000	1
1401	C	66.51354	76.20150	72.65877	0.00000	0.00000	0.00000	1
1402	C	65.33014	76.10986	73.60177	0.00000	0.00000	0.00000	1
1403	C	66.71403	77.63104	72.19779	0.00000	0.00000	0.00000	1
1404	H	68.59644	77.43940	74.16880	0.00000	0.00000	0.00000	1
1405	H	67.59210	74.65127	73.83153	0.00000	0.00000	0.00000	1
1406	H	66.27315	75.58779	71.76073	0.00000	0.00000	0.00000	1
1407	H	65.11312	75.04384	73.89288	0.00000	0.00000	0.00000	1
1408	H	65.52021	76.68125	74.55335	0.00000	0.00000	0.00000	1
1409	H	64.39343	76.52887	73.13802	0.00000	0.00000	0.00000	1
1410	H	65.82892	78.00923	71.61350	0.00000	0.00000	0.00000	1
1411	H	66.85995	78.32810	73.06958	0.00000	0.00000	0.00000	1
1412	H	67.62095	77.72868	71.53681	0.00000	0.00000	0.00000	1
1413	N	69.88135	76.26955	72.12151	0.00000	0.00000	0.00000	1
1414	C	70.86487	76.24120	71.09763	0.00000	0.00000	0.00000	1
1415	C	72.34684	75.89194	71.70566	0.00000	0.00000	0.00000	1
1416	O	73.29273	75.88108	70.95072	0.00000	0.00000	0.00000	1
1417	C	71.00577	77.71318	70.50826	0.00000	0.00000	0.00000	1
1418	C	71.58545	77.56909	69.07155	0.00000	0.00000	0.00000	1
1419	C	70.42348	76.89803	68.19835	0.00000	0.00000	0.00000	1
1420	N	70.78419	77.17055	66.87370	0.00000	0.00000	0.00000	1
1421	C	70.05032	76.92870	65.86423	0.00000	0.00000	0.00000	1
1422	N	68.80188	76.33967	66.09435	0.00000	0.00000	0.00000	1
1423	N	70.67764	77.32842	64.67588	0.00000	0.00000	0.00000	1
1424	H	69.91933	76.85973	72.94882	0.00000	0.00000	0.00000	1
1425	H	70.48233	75.49046	70.36486	0.00000	0.00000	0.00000	1
1426	H	70.02612	78.24141	70.49757	0.00000	0.00000	0.00000	1
1427	H	71.67670	78.32882	71.14971	0.00000	0.00000	0.00000	1
1428	H	71.88358	78.55734	68.65577	0.00000	0.00000	0.00000	1
1429	H	72.51020	76.94301	69.08291	0.00000	0.00000	0.00000	1
1430	H	70.32471	75.78790	68.30487	0.00000	0.00000	0.00000	1
1431	H	69.40528	77.33964	68.33255	0.00000	0.00000	0.00000	1
1432	H	71.68987	77.58741	66.72614	0.00000	0.00000	0.00000	1
1433	H	68.37113	76.05336	66.97272	0.00000	0.00000	0.00000	1
1434	H	68.12607	76.10306	65.36734	0.00000	0.00000	0.00000	1
1435	H	71.59656	77.73626	64.51026	0.00000	0.00000	0.00000	1
1436	H	70.25852	77.20735	63.75310	0.00000	0.00000	0.00000	1
1437	N	72.31715	75.71602	73.02011	0.00000	0.00000	0.00000	1
1438	C	73.49927	75.33098	73.70593	0.00000	0.00000	0.00000	1
1439	C	73.15043	73.94802	74.48731	0.00000	0.00000	0.00000	1
1440	O	72.50446	73.07780	73.94515	0.00000	0.00000	0.00000	1
1441	C	73.93742	76.51093	74.69557	0.00000	0.00000	0.00000	1
1442	C	74.09305	77.83947	73.93548	0.00000	0.00000	0.00000	1
1443	C	74.64598	77.87240	72.61968	0.00000	0.00000	0.00000	1
1444	C	73.71189	79.06034	74.56870	0.00000	0.00000	0.00000	1

1445	C	74.77184	79.09489	71.95643	0.00000	0.00000	0.00000	1
1446	C	73.86325	80.26074	73.87306	0.00000	0.00000	0.00000	1
1447	C	74.38692	80.33221	72.54951	0.00000	0.00000	0.00000	1
1448	O	74.50933	81.57837	71.88108	0.00000	0.00000	0.00000	1
1449	H	71.40825	75.73054	73.47997	0.00000	0.00000	0.00000	1
1450	H	74.21862	75.18995	72.86604	0.00000	0.00000	0.00000	1
1451	H	73.19697	76.62947	75.51855	0.00000	0.00000	0.00000	1
1452	H	74.90231	76.25150	75.18873	0.00000	0.00000	0.00000	1
1453	H	74.95229	76.93715	72.11513	0.00000	0.00000	0.00000	1
1454	H	73.31276	79.05692	75.59791	0.00000	0.00000	0.00000	1
1455	H	75.18580	79.09145	70.93279	0.00000	0.00000	0.00000	1
1456	H	73.56758	81.20071	74.37047	0.00000	0.00000	0.00000	1
1457	H	74.92265	81.27561	71.03800	0.00000	0.00000	0.00000	1
1458	N	73.82249	73.86356	75.64035	0.00000	0.00000	0.00000	1
1459	C	73.44310	72.81749	76.54184	0.00000	0.00000	0.00000	1
1460	C	72.31737	73.36602	77.57925	0.00000	0.00000	0.00000	1
1461	O	71.66706	74.37162	77.39697	0.00000	0.00000	0.00000	1
1462	C	74.76859	72.28499	77.25194	0.00000	0.00000	0.00000	1
1463	O	74.56275	71.12581	78.13692	0.00000	0.00000	0.00000	1
1464	C	75.41035	73.53801	77.93313	0.00000	0.00000	0.00000	1
1465	H	74.27095	74.71201	75.97750	0.00000	0.00000	0.00000	1
1466	H	72.99658	72.06869	75.84384	0.00000	0.00000	0.00000	1
1467	H	75.48430	71.92900	76.46561	0.00000	0.00000	0.00000	1
1468	H	75.18042	70.49893	77.72760	0.00000	0.00000	0.00000	1
1469	H	76.34899	73.26966	78.47413	0.00000	0.00000	0.00000	1
1470	H	74.71828	74.00434	78.67615	0.00000	0.00000	0.00000	1
1471	H	75.67458	74.32742	77.19186	0.00000	0.00000	0.00000	1
1472	N	72.17973	72.45836	78.53915	0.00000	0.00000	0.00000	1
1473	C	71.27196	72.73178	79.59535	0.00000	0.00000	0.00000	1
1474	C	72.04731	73.40452	80.87321	0.00000	0.00000	0.00000	1
1475	O	71.40815	73.86755	81.79046	0.00000	0.00000	0.00000	1
1476	C	70.77740	71.34803	80.20515	0.00000	0.00000	0.00000	1
1477	C	69.89315	70.54642	79.19962	0.00000	0.00000	0.00000	1
1478	C	68.38477	70.99915	79.34447	0.00000	0.00000	0.00000	1
1479	C	68.14039	72.30087	78.54618	0.00000	0.00000	0.00000	1
1480	N	66.59701	72.56164	78.55302	0.00000	0.00000	0.00000	1
1481	H	72.80882	71.64270	78.57628	0.00000	0.00000	0.00000	1
1482	H	70.49328	73.40066	79.16344	0.00000	0.00000	0.00000	1
1483	H	71.66846	70.73999	80.48050	0.00000	0.00000	0.00000	1
1484	H	70.22326	71.51924	81.15481	0.00000	0.00000	0.00000	1
1485	H	70.25754	70.67787	78.15580	0.00000	0.00000	0.00000	1
1486	H	69.97546	69.45745	79.41731	0.00000	0.00000	0.00000	1
1487	H	67.70835	70.19811	78.96761	0.00000	0.00000	0.00000	1
1488	H	68.11518	71.13436	80.41730	0.00000	0.00000	0.00000	1
1489	H	68.57670	73.21885	78.98715	0.00000	0.00000	0.00000	1
1490	H	68.40144	72.23628	77.47066	0.00000	0.00000	0.00000	1
1491	H	65.95640	71.73924	78.35209	0.00000	0.00000	0.00000	1
1492	H	66.26983	73.26697	77.83193	0.00000	0.00000	0.00000	1
1493	H	66.17501	72.96027	79.44158	0.00000	0.00000	0.00000	1
1494	N	73.36250	73.18545	80.81380	0.00000	0.00000	0.00000	1
1495	C	74.18937	73.98808	81.66579	0.00000	0.00000	0.00000	1
1496	C	74.57099	75.36195	80.88326	0.00000	0.00000	0.00000	1
1497	O	73.98510	75.76903	79.90927	0.00000	0.00000	0.00000	1
1498	C	75.48216	73.13347	82.00371	0.00000	0.00000	0.00000	1
1499	C	75.69857	73.15109	83.55140	0.00000	0.00000	0.00000	1
1500	C	74.95095	71.91502	84.19498	0.00000	0.00000	0.00000	1
1501	C	73.41705	72.07019	84.07781	0.00000	0.00000	0.00000	1
1502	N	72.78036	70.79961	84.73656	0.00000	0.00000	0.00000	1
1503	H	73.71239	72.77951	79.94672	0.00000	0.00000	0.00000	1
1504	H	73.51943	74.17925	82.53675	0.00000	0.00000	0.00000	1
1505	H	75.38204	72.09043	81.62920	0.00000	0.00000	0.00000	1
1506	H	76.36956	73.55775	81.48156	0.00000	0.00000	0.00000	1

1507	H	76.78522	73.09283	83.78480	0.00000	0.00000	0.00000	1
1508	H	75.34389	74.10750	83.99721	0.00000	0.00000	0.00000	1
1509	H	75.28028	70.96891	83.70762	0.00000	0.00000	0.00000	1
1510	H	75.23614	71.81135	85.26716	0.00000	0.00000	0.00000	1
1511	H	72.99329	72.92175	84.64680	0.00000	0.00000	0.00000	1
1512	H	73.02346	72.07429	83.04075	0.00000	0.00000	0.00000	1
1513	H	73.05422	70.58500	85.73955	0.00000	0.00000	0.00000	1
1514	H	72.95494	69.86804	84.25861	0.00000	0.00000	0.00000	1
1515	H	71.72220	70.80294	84.80670	0.00000	0.00000	0.00000	1
1516	N	75.54378	75.97448	81.56472	0.00000	0.00000	0.00000	1
1517	C	76.10985	77.25176	81.09275	0.00000	0.00000	0.00000	1
1518	C	76.86044	76.96070	79.66131	0.00000	0.00000	0.00000	1
1519	O	77.62921	76.02257	79.54146	0.00000	0.00000	0.00000	1
1520	C	77.10654	77.71276	82.14032	0.00000	0.00000	0.00000	1
1521	C	77.87233	78.94283	81.68813	0.00000	0.00000	0.00000	1
1522	C	76.43711	77.97629	83.47691	0.00000	0.00000	0.00000	1
1523	H	75.92275	75.46097	82.35798	0.00000	0.00000	0.00000	1
1524	H	75.21903	77.91273	80.98485	0.00000	0.00000	0.00000	1
1525	H	77.84654	76.89341	82.28588	0.00000	0.00000	0.00000	1
1526	H	78.69462	79.20831	82.41179	0.00000	0.00000	0.00000	1
1527	H	78.36582	78.77873	80.68655	0.00000	0.00000	0.00000	1
1528	H	77.20448	79.84318	81.59392	0.00000	0.00000	0.00000	1
1529	H	75.92827	77.05552	83.87467	0.00000	0.00000	0.00000	1
1530	H	77.17581	78.31323	84.25502	0.00000	0.00000	0.00000	1
1531	H	75.65093	78.77634	83.39488	0.00000	0.00000	0.00000	1
1532	N	76.56255	77.90697	78.76888	0.00000	0.00000	0.00000	1
1533	C	77.12785	77.87002	77.44992	0.00000	0.00000	0.00000	1
1534	C	78.68509	78.37716	77.58185	0.00000	0.00000	0.00000	1
1535	O	79.02107	79.49915	77.30152	0.00000	0.00000	0.00000	1
1536	C	76.20163	78.85666	76.63081	0.00000	0.00000	0.00000	1
1537	C	75.82585	79.91420	77.71727	0.00000	0.00000	0.00000	1
1538	C	75.62359	78.99680	78.99813	0.00000	0.00000	0.00000	1
1539	H	77.06832	76.79709	77.16270	0.00000	0.00000	0.00000	1
1540	H	76.71502	79.29976	75.74711	0.00000	0.00000	0.00000	1
1541	H	75.29796	78.33537	76.24490	0.00000	0.00000	0.00000	1
1542	H	76.65999	80.63609	77.86719	0.00000	0.00000	0.00000	1
1543	H	74.92453	80.51561	77.46095	0.00000	0.00000	0.00000	1
1544	H	75.86660	79.48351	79.97105	0.00000	0.00000	0.00000	1
1545	H	74.62207	78.51337	79.06749	0.00000	0.00000	0.00000	1
1546	N	79.39916	77.36743	78.06559	0.00000	0.00000	0.00000	1
1547	C	80.81759	77.51320	78.09399	0.00000	0.00000	0.00000	1
1548	C	81.39790	76.94898	76.67612	0.00000	0.00000	0.00000	1
1549	O	80.71500	76.85172	75.68459	0.00000	0.00000	0.00000	1
1550	C	81.31993	76.66043	79.33493	0.00000	0.00000	0.00000	1
1551	C	82.43098	77.44218	80.09878	0.00000	0.00000	0.00000	1
1552	C	81.69131	78.38367	81.12734	0.00000	0.00000	0.00000	1
1553	O	80.50637	78.31512	81.34441	0.00000	0.00000	0.00000	1
1554	N	82.57867	79.20486	81.72480	0.00000	0.00000	0.00000	1
1555	H	78.93200	76.48720	78.36678	0.00000	0.00000	0.00000	1
1556	H	80.93359	78.61860	78.19221	0.00000	0.00000	0.00000	1
1557	H	80.47019	76.44667	80.02675	0.00000	0.00000	0.00000	1
1558	H	81.69703	75.66974	78.99312	0.00000	0.00000	0.00000	1
1559	H	83.11133	76.74430	80.63465	0.00000	0.00000	0.00000	1
1560	H	83.09244	78.01969	79.41625	0.00000	0.00000	0.00000	1
1561	H	83.59372	79.25011	81.57587	0.00000	0.00000	0.00000	1
1562	H	82.35446	79.87636	82.46657	0.00000	0.00000	0.00000	1
1563	N	82.69675	76.66254	76.79881	0.00000	0.00000	0.00000	1
1564	C	83.51595	76.28717	75.64357	0.00000	0.00000	0.00000	1
1565	C	83.20463	74.72612	75.17349	0.00000	0.00000	0.00000	1
1566	O	83.74437	74.29289	74.18283	0.00000	0.00000	0.00000	1
1567	C	84.99327	76.30639	75.98205	0.00000	0.00000	0.00000	1
1568	C	85.55754	77.71344	76.04554	0.00000	0.00000	0.00000	1

1569	C	85.30654	75.55957	77.26528	0.00000	0.00000	0.00000	1
1570	H	83.09516	76.83611	77.71848	0.00000	0.00000	0.00000	1
1571	H	83.21450	77.01267	74.85108	0.00000	0.00000	0.00000	1
1572	H	85.51550	75.77768	75.14972	0.00000	0.00000	0.00000	1
1573	H	85.05134	78.32543	76.84224	0.00000	0.00000	0.00000	1
1574	H	86.65914	77.70761	76.27619	0.00000	0.00000	0.00000	1
1575	H	85.42330	78.25895	75.07045	0.00000	0.00000	0.00000	1
1576	H	84.69488	74.61880	77.35224	0.00000	0.00000	0.00000	1
1577	H	86.39015	75.26180	77.31988	0.00000	0.00000	0.00000	1
1578	H	85.08787	76.18414	78.17476	0.00000	0.00000	0.00000	1
1579	N	82.45958	74.06707	76.05438	0.00000	0.00000	0.00000	1
1580	C	81.88931	72.83816	75.63087	0.00000	0.00000	0.00000	1
1581	C	80.26377	73.02179	75.69068	0.00000	0.00000	0.00000	1
1582	O	79.69914	73.31225	76.71702	0.00000	0.00000	0.00000	1
1583	C	82.34572	71.78705	76.75146	0.00000	0.00000	0.00000	1
1584	O	81.93539	70.41595	76.53830	0.00000	0.00000	0.00000	1
1585	H	82.08079	74.62805	76.81520	0.00000	0.00000	0.00000	1
1586	H	82.30293	72.63134	74.61575	0.00000	0.00000	0.00000	1
1587	H	83.45361	71.90225	76.87800	0.00000	0.00000	0.00000	1
1588	H	81.88230	72.14641	77.71083	0.00000	0.00000	0.00000	1
1589	H	82.73892	70.06777	76.10980	0.00000	0.00000	0.00000	1
1590	N	79.76180	72.80503	74.48768	0.00000	0.00000	0.00000	1
1591	C	78.34593	72.84127	74.28951	0.00000	0.00000	0.00000	1
1592	C	78.22227	72.00372	72.92129	0.00000	0.00000	0.00000	1
1593	O	79.24446	71.72631	72.32422	0.00000	0.00000	0.00000	1
1594	C	77.84929	74.36957	74.08311	0.00000	0.00000	0.00000	1
1595	O	78.44709	75.09956	73.00765	0.00000	0.00000	0.00000	1
1596	C	78.00004	74.98246	75.52130	0.00000	0.00000	0.00000	1
1597	H	80.30366	72.54287	73.64400	0.00000	0.00000	0.00000	1
1598	H	77.88438	72.38125	75.19291	0.00000	0.00000	0.00000	1
1599	H	76.75161	74.33200	73.83116	0.00000	0.00000	0.00000	1
1600	H	77.67811	75.23282	72.41376	0.00000	0.00000	0.00000	1
1601	H	79.06356	75.27210	75.72860	0.00000	0.00000	0.00000	1
1602	H	77.68245	74.26641	76.31865	0.00000	0.00000	0.00000	1
1603	H	77.38226	75.90357	75.63186	0.00000	0.00000	0.00000	1
1604	N	76.95587	71.69470	72.63047	0.00000	0.00000	0.00000	1
1605	C	76.60969	71.08747	71.37842	0.00000	0.00000	0.00000	1
1606	C	76.52365	72.24334	70.21818	0.00000	0.00000	0.00000	1
1607	O	75.94169	73.28624	70.38878	0.00000	0.00000	0.00000	1
1608	C	75.15165	70.53256	71.65761	0.00000	0.00000	0.00000	1
1609	C	74.59822	71.59610	72.65611	0.00000	0.00000	0.00000	1
1610	C	75.86539	71.79869	73.59221	0.00000	0.00000	0.00000	1
1611	H	77.38806	70.32229	71.15852	0.00000	0.00000	0.00000	1
1612	H	74.54068	70.44228	70.73105	0.00000	0.00000	0.00000	1
1613	H	75.18043	69.52038	72.11924	0.00000	0.00000	0.00000	1
1614	H	74.32906	72.54112	72.12978	0.00000	0.00000	0.00000	1
1615	H	73.68879	71.26663	73.21069	0.00000	0.00000	0.00000	1
1616	H	75.91480	72.77874	74.12034	0.00000	0.00000	0.00000	1
1617	H	76.03292	70.97829	74.32992	0.00000	0.00000	0.00000	1
1618	N	77.09691	71.77068	69.11911	0.00000	0.00000	0.00000	1
1619	C	76.97209	72.48656	67.90449	0.00000	0.00000	0.00000	1
1620	C	75.81915	71.72410	67.01680	0.00000	0.00000	0.00000	1
1621	O	76.08120	70.98504	66.09841	0.00000	0.00000	0.00000	1
1622	C	78.40915	72.40309	67.18287	0.00000	0.00000	0.00000	1
1623	O	79.00462	71.09938	67.10220	0.00000	0.00000	0.00000	1
1624	C	79.19441	73.47077	68.02711	0.00000	0.00000	0.00000	1
1625	H	77.54525	70.85541	69.10392	0.00000	0.00000	0.00000	1
1626	H	76.65305	73.50459	68.22689	0.00000	0.00000	0.00000	1
1627	H	78.28943	72.77625	66.12968	0.00000	0.00000	0.00000	1
1628	H	78.88663	70.89371	66.15192	0.00000	0.00000	0.00000	1
1629	H	78.70357	74.47156	67.99657	0.00000	0.00000	0.00000	1
1630	H	80.23843	73.59846	67.65796	0.00000	0.00000	0.00000	1

1631	H	79.25707	73.16377	69.09851	0.00000	0.00000	0.00000	1
1632	N	74.61761	71.99202	67.52877	0.00000	0.00000	0.00000	1
1633	C	73.52601	72.11043	66.37887	0.00000	0.00000	0.00000	1
1634	C	73.73678	73.20549	65.45284	0.00000	0.00000	0.00000	1
1635	O	73.90888	74.09939	64.69841	0.00000	0.00000	0.00000	1
1636	C	72.12134	72.30286	67.20832	0.00000	0.00000	0.00000	1
1637	C	70.98521	71.95622	66.30781	0.00000	0.00000	0.00000	1
1638	C	70.72988	70.45214	66.31133	0.00000	0.00000	0.00000	1
1639	C	69.71998	72.69121	66.74219	0.00000	0.00000	0.00000	1
1640	H	74.64971	72.68624	68.27125	0.00000	0.00000	0.00000	1
1641	H	73.66651	71.10233	65.91278	0.00000	0.00000	0.00000	1
1642	H	72.12198	71.67286	68.12608	0.00000	0.00000	0.00000	1
1643	H	72.04630	73.35556	67.56352	0.00000	0.00000	0.00000	1
1644	H	71.23556	72.27846	65.27054	0.00000	0.00000	0.00000	1
1645	H	70.41576	70.09085	67.32373	0.00000	0.00000	0.00000	1
1646	H	71.64599	69.87526	66.02500	0.00000	0.00000	0.00000	1
1647	H	69.91955	70.16723	65.59302	0.00000	0.00000	0.00000	1
1648	H	68.84235	72.41779	66.10307	0.00000	0.00000	0.00000	1
1649	H	69.84516	73.80285	66.67610	0.00000	0.00000	0.00000	1
1650	H	69.44745	72.45078	67.80154	0.00000	0.00000	0.00000	1
1651		273						
1652		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	3.5000 14000
		0.2500	300.00	0.00	0.00	0.00	-1291.3972 0.0000	0.0000
1653	N	68.28347	77.48227	77.66618	0.00000	0.00000	0.00000	1
1654	C	68.90629	77.46742	76.45506	0.00000	0.00000	0.00000	1
1655	C	68.27337	76.14059	75.58966	0.00000	0.00000	0.00000	1
1656	O	67.96705	75.09112	76.10041	0.00000	0.00000	0.00000	1
1657	C	70.50940	77.09126	76.67938	0.00000	0.00000	0.00000	1
1658	C	71.08290	78.00705	77.69283	0.00000	0.00000	0.00000	1
1659	C	72.39292	77.43231	78.22903	0.00000	0.00000	0.00000	1
1660	C	71.31506	79.40717	77.13255	0.00000	0.00000	0.00000	1
1661	H	68.27741	76.59963	78.14370	0.00000	0.00000	0.00000	1
1662	H	68.73868	78.47760	76.00007	0.00000	0.00000	0.00000	1
1663	H	70.61411	76.02213	77.01810	0.00000	0.00000	0.00000	1
1664	H	71.05578	77.15671	75.71301	0.00000	0.00000	0.00000	1
1665	H	70.36908	78.07712	78.54757	0.00000	0.00000	0.00000	1
1666	H	73.21828	77.49208	77.47615	0.00000	0.00000	0.00000	1
1667	H	72.28390	76.34921	78.51404	0.00000	0.00000	0.00000	1
1668	H	72.73530	77.97880	79.14379	0.00000	0.00000	0.00000	1
1669	H	72.23568	79.87973	77.56000	0.00000	0.00000	0.00000	1
1670	H	70.45731	80.08912	77.36124	0.00000	0.00000	0.00000	1
1671	H	71.43087	79.39515	76.01980	0.00000	0.00000	0.00000	1
1672	N	68.31477	76.47108	74.31126	0.00000	0.00000	0.00000	1
1673	C	67.77422	75.60597	73.27941	0.00000	0.00000	0.00000	1
1674	C	68.84429	75.45487	72.01131	0.00000	0.00000	0.00000	1
1675	O	68.58142	74.69882	71.10599	0.00000	0.00000	0.00000	1
1676	C	66.51241	76.20183	72.66004	0.00000	0.00000	0.00000	1
1677	C	65.33032	76.11149	73.60473	0.00000	0.00000	0.00000	1
1678	C	66.71376	77.63105	72.19850	0.00000	0.00000	0.00000	1
1679	H	68.59625	77.43809	74.16951	0.00000	0.00000	0.00000	1
1680	H	67.59187	74.65018	73.83016	0.00000	0.00000	0.00000	1
1681	H	66.27031	75.58810	71.76251	0.00000	0.00000	0.00000	1
1682	H	65.11283	75.04578	73.89660	0.00000	0.00000	0.00000	1
1683	H	65.52214	76.68312	74.55582	0.00000	0.00000	0.00000	1
1684	H	64.39330	76.53108	73.14211	0.00000	0.00000	0.00000	1
1685	H	65.82789	78.01034	71.61610	0.00000	0.00000	0.00000	1
1686	H	66.86251	78.32799	73.06990	0.00000	0.00000	0.00000	1
1687	H	67.61939	77.72741	71.53557	0.00000	0.00000	0.00000	1
1688	N	69.88274	76.26762	72.12356	0.00000	0.00000	0.00000	1
1689	C	70.86543	76.24062	71.09880	0.00000	0.00000	0.00000	1
1690	C	72.34806	75.89245	71.70571	0.00000	0.00000	0.00000	1
1691	O	73.29432	75.88441	70.95112	0.00000	0.00000	0.00000	1

1692	C	71.00442	77.71278	70.50945	0.00000	0.00000	0.00000	1
1693	C	71.58426	77.57001	69.07264	0.00000	0.00000	0.00000	1
1694	C	70.42400	76.89668	68.19898	0.00000	0.00000	0.00000	1
1695	N	70.78581	77.16790	66.87436	0.00000	0.00000	0.00000	1
1696	C	70.05235	76.92574	65.86466	0.00000	0.00000	0.00000	1
1697	N	68.80331	76.33792	66.09470	0.00000	0.00000	0.00000	1
1698	N	70.68047	77.32373	64.67616	0.00000	0.00000	0.00000	1
1699	H	69.92220	76.85535	72.95257	0.00000	0.00000	0.00000	1
1700	H	70.48280	75.48991	70.36604	0.00000	0.00000	0.00000	1
1701	H	70.02404	78.23966	70.49891	0.00000	0.00000	0.00000	1
1702	H	71.67451	78.32925	71.15097	0.00000	0.00000	0.00000	1
1703	H	71.88043	78.55889	68.65704	0.00000	0.00000	0.00000	1
1704	H	72.51021	76.94606	69.08352	0.00000	0.00000	0.00000	1
1705	H	70.32656	75.78655	68.30665	0.00000	0.00000	0.00000	1
1706	H	69.40513	77.33717	68.33168	0.00000	0.00000	0.00000	1
1707	H	71.69196	77.58379	66.72697	0.00000	0.00000	0.00000	1
1708	H	68.37193	76.05270	66.97311	0.00000	0.00000	0.00000	1
1709	H	68.12769	76.10116	65.36757	0.00000	0.00000	0.00000	1
1710	H	71.59983	77.73053	64.51045	0.00000	0.00000	0.00000	1
1711	H	70.26160	77.20204	63.75334	0.00000	0.00000	0.00000	1
1712	N	72.31854	75.71307	73.01971	0.00000	0.00000	0.00000	1
1713	C	73.50105	75.32913	73.70529	0.00000	0.00000	0.00000	1
1714	C	73.15202	73.94710	74.48821	0.00000	0.00000	0.00000	1
1715	O	72.50615	73.07629	73.94735	0.00000	0.00000	0.00000	1
1716	C	73.93883	76.50888	74.69536	0.00000	0.00000	0.00000	1
1717	C	74.09424	77.83793	73.93616	0.00000	0.00000	0.00000	1
1718	C	74.64793	77.87230	72.62072	0.00000	0.00000	0.00000	1
1719	C	73.71200	79.05794	74.57035	0.00000	0.00000	0.00000	1
1720	C	74.77252	79.09537	71.95833	0.00000	0.00000	0.00000	1
1721	C	73.86220	80.25896	73.87559	0.00000	0.00000	0.00000	1
1722	C	74.38586	80.33180	72.55213	0.00000	0.00000	0.00000	1
1723	O	74.50686	81.57852	71.88452	0.00000	0.00000	0.00000	1
1724	H	71.40957	75.72453	73.47949	0.00000	0.00000	0.00000	1
1725	H	74.22066	75.18807	72.86563	0.00000	0.00000	0.00000	1
1726	H	73.19805	76.62686	75.51814	0.00000	0.00000	0.00000	1
1727	H	74.90369	76.24948	75.18866	0.00000	0.00000	0.00000	1
1728	H	74.95566	76.93758	72.11574	0.00000	0.00000	0.00000	1
1729	H	73.31304	79.05331	75.59960	0.00000	0.00000	0.00000	1
1730	H	75.18692	79.09310	70.93486	0.00000	0.00000	0.00000	1
1731	H	73.56552	81.19825	74.37366	0.00000	0.00000	0.00000	1
1732	H	74.91989	81.27665	71.04098	0.00000	0.00000	0.00000	1
1733	N	73.82305	73.86510	75.64202	0.00000	0.00000	0.00000	1
1734	C	73.44477	72.81921	76.54403	0.00000	0.00000	0.00000	1
1735	C	72.31863	73.36685	77.58127	0.00000	0.00000	0.00000	1
1736	O	71.66781	74.37232	77.39928	0.00000	0.00000	0.00000	1
1737	C	74.77142	72.28885	77.25407	0.00000	0.00000	0.00000	1
1738	O	74.56683	71.12975	78.13839	0.00000	0.00000	0.00000	1
1739	C	75.41074	73.54325	77.93520	0.00000	0.00000	0.00000	1
1740	H	74.27103	74.71415	75.97838	0.00000	0.00000	0.00000	1
1741	H	72.99914	72.06946	75.84644	0.00000	0.00000	0.00000	1
1742	H	75.48776	71.93487	76.46738	0.00000	0.00000	0.00000	1
1743	H	75.18225	70.50207	77.72647	0.00000	0.00000	0.00000	1
1744	H	76.34924	73.27669	78.47734	0.00000	0.00000	0.00000	1
1745	H	74.71725	74.00913	78.67723	0.00000	0.00000	0.00000	1
1746	H	75.67462	74.33258	77.19371	0.00000	0.00000	0.00000	1
1747	N	72.18078	72.45882	78.54080	0.00000	0.00000	0.00000	1
1748	C	71.27227	72.73240	79.59636	0.00000	0.00000	0.00000	1
1749	C	72.04789	73.40316	80.87505	0.00000	0.00000	0.00000	1
1750	O	71.40921	73.86410	81.79366	0.00000	0.00000	0.00000	1
1751	C	70.77502	71.34927	80.20545	0.00000	0.00000	0.00000	1
1752	C	69.89259	70.54744	79.19851	0.00000	0.00000	0.00000	1
1753	C	68.38373	70.99968	79.33999	0.00000	0.00000	0.00000	1

1754	C	68.14090	72.30253	78.54309	0.00000	0.00000	0.00000	1
1755	N	66.59791	72.56561	78.55085	0.00000	0.00000	0.00000	1
1756	H	72.81034	71.64363	78.57804	0.00000	0.00000	0.00000	1
1757	H	70.49493	73.40267	79.16407	0.00000	0.00000	0.00000	1
1758	H	71.66500	70.74077	80.48322	0.00000	0.00000	0.00000	1
1759	H	70.21885	71.52143	81.15375	0.00000	0.00000	0.00000	1
1760	H	70.25904	70.67858	78.15538	0.00000	0.00000	0.00000	1
1761	H	69.97461	69.45856	79.41676	0.00000	0.00000	0.00000	1
1762	H	67.70845	70.19903	78.96022	0.00000	0.00000	0.00000	1
1763	H	68.11131	71.13325	80.41231	0.00000	0.00000	0.00000	1
1764	H	68.57854	73.21937	78.98509	0.00000	0.00000	0.00000	1
1765	H	68.40157	72.23889	77.46741	0.00000	0.00000	0.00000	1
1766	H	65.95640	71.74641	78.34001	0.00000	0.00000	0.00000	1
1767	H	66.27286	73.27917	77.83694	0.00000	0.00000	0.00000	1
1768	H	66.17525	72.95513	79.44314	0.00000	0.00000	0.00000	1
1769	N	73.36320	73.18508	80.81406	0.00000	0.00000	0.00000	1
1770	C	74.19029	73.98774	81.66585	0.00000	0.00000	0.00000	1
1771	C	74.56937	75.36270	80.88402	0.00000	0.00000	0.00000	1
1772	O	73.98094	75.77116	79.91221	0.00000	0.00000	0.00000	1
1773	C	75.48383	73.13351	82.00188	0.00000	0.00000	0.00000	1
1774	C	75.70129	73.15017	83.54944	0.00000	0.00000	0.00000	1
1775	C	74.95192	71.91535	84.19341	0.00000	0.00000	0.00000	1
1776	C	73.41824	72.07151	84.07480	0.00000	0.00000	0.00000	1
1777	N	72.77976	70.80198	84.73381	0.00000	0.00000	0.00000	1
1778	H	73.71286	72.78089	79.94605	0.00000	0.00000	0.00000	1
1779	H	73.52107	74.17768	82.53764	0.00000	0.00000	0.00000	1
1780	H	75.38390	72.09068	81.62671	0.00000	0.00000	0.00000	1
1781	H	76.37061	73.55856	81.47930	0.00000	0.00000	0.00000	1
1782	H	76.78800	73.08990	83.78209	0.00000	0.00000	0.00000	1
1783	H	75.34864	74.10712	83.99567	0.00000	0.00000	0.00000	1
1784	H	75.28085	70.96855	83.70711	0.00000	0.00000	0.00000	1
1785	H	75.23613	71.81233	85.26591	0.00000	0.00000	0.00000	1
1786	H	72.99452	72.92389	84.64261	0.00000	0.00000	0.00000	1
1787	H	73.02559	72.07491	83.03738	0.00000	0.00000	0.00000	1
1788	H	73.05023	70.58935	85.73813	0.00000	0.00000	0.00000	1
1789	H	72.95616	69.86956	84.25819	0.00000	0.00000	0.00000	1
1790	H	71.72137	70.80523	84.80031	0.00000	0.00000	0.00000	1
1791	N	75.54307	75.97470	81.56474	0.00000	0.00000	0.00000	1
1792	C	76.11003	77.25125	81.09182	0.00000	0.00000	0.00000	1
1793	C	76.85926	76.95899	79.65991	0.00000	0.00000	0.00000	1
1794	O	77.62663	76.01968	79.53963	0.00000	0.00000	0.00000	1
1795	C	77.10786	77.71131	82.13866	0.00000	0.00000	0.00000	1
1796	C	77.87439	78.94079	81.68607	0.00000	0.00000	0.00000	1
1797	C	76.43984	77.97678	83.47559	0.00000	0.00000	0.00000	1
1798	H	75.92454	75.45964	82.35581	0.00000	0.00000	0.00000	1
1799	H	75.21986	77.91316	80.98442	0.00000	0.00000	0.00000	1
1800	H	77.84690	76.89105	82.28408	0.00000	0.00000	0.00000	1
1801	H	78.69534	79.20684	82.41099	0.00000	0.00000	0.00000	1
1802	H	78.36886	78.77577	80.68499	0.00000	0.00000	0.00000	1
1803	H	77.20702	79.84134	81.59074	0.00000	0.00000	0.00000	1
1804	H	75.92861	77.05756	83.87382	0.00000	0.00000	0.00000	1
1805	H	77.17997	78.31191	84.25315	0.00000	0.00000	0.00000	1
1806	H	75.65599	78.77914	83.39364	0.00000	0.00000	0.00000	1
1807	N	76.56195	77.90553	78.76763	0.00000	0.00000	0.00000	1
1808	C	77.12719	77.86880	77.44863	0.00000	0.00000	0.00000	1
1809	C	78.68451	78.37564	77.58058	0.00000	0.00000	0.00000	1
1810	O	79.02117	79.49704	77.29869	0.00000	0.00000	0.00000	1
1811	C	76.20056	78.85537	76.62990	0.00000	0.00000	0.00000	1
1812	C	75.82564	79.91318	77.71640	0.00000	0.00000	0.00000	1
1813	C	75.62373	78.99591	78.99739	0.00000	0.00000	0.00000	1
1814	H	77.06756	76.79589	77.16131	0.00000	0.00000	0.00000	1
1815	H	76.71327	79.29820	75.74566	0.00000	0.00000	0.00000	1

1816	H	75.29656	78.33404	76.24487	0.00000	0.00000	0.00000	1
1817	H	76.66006	80.63483	77.86583	0.00000	0.00000	0.00000	1
1818	H	74.92435	80.51482	77.46049	0.00000	0.00000	0.00000	1
1819	H	75.86768	79.48251	79.97012	0.00000	0.00000	0.00000	1
1820	H	74.62198	78.51303	79.06746	0.00000	0.00000	0.00000	1
1821	N	79.39785	77.36630	78.06624	0.00000	0.00000	0.00000	1
1822	C	80.81639	77.51132	78.09438	0.00000	0.00000	0.00000	1
1823	C	81.39764	76.94630	76.67737	0.00000	0.00000	0.00000	1
1824	O	80.71738	76.84991	75.68415	0.00000	0.00000	0.00000	1
1825	C	81.31913	76.65937	79.33579	0.00000	0.00000	0.00000	1
1826	C	82.43108	77.44089	80.09882	0.00000	0.00000	0.00000	1
1827	C	81.69312	78.38413	81.12678	0.00000	0.00000	0.00000	1
1828	O	80.50883	78.31398	81.34437	0.00000	0.00000	0.00000	1
1829	N	82.57971	79.20754	81.72232	0.00000	0.00000	0.00000	1
1830	H	78.93015	76.48641	78.36790	0.00000	0.00000	0.00000	1
1831	H	80.93324	78.61669	78.19121	0.00000	0.00000	0.00000	1
1832	H	80.46950	76.44572	80.02794	0.00000	0.00000	0.00000	1
1833	H	81.69593	75.66849	78.99425	0.00000	0.00000	0.00000	1
1834	H	83.11066	76.74258	80.63517	0.00000	0.00000	0.00000	1
1835	H	83.09313	78.01694	79.41558	0.00000	0.00000	0.00000	1
1836	H	83.59483	79.25389	81.57336	0.00000	0.00000	0.00000	1
1837	H	82.35509	79.87998	82.46331	0.00000	0.00000	0.00000	1
1838	N	82.69674	76.66057	76.80105	0.00000	0.00000	0.00000	1
1839	C	83.51547	76.28644	75.64474	0.00000	0.00000	0.00000	1
1840	C	83.20484	74.72531	75.17474	0.00000	0.00000	0.00000	1
1841	O	83.74519	74.29188	74.18454	0.00000	0.00000	0.00000	1
1842	C	84.99266	76.30772	75.98327	0.00000	0.00000	0.00000	1
1843	C	85.55457	77.71567	76.04769	0.00000	0.00000	0.00000	1
1844	C	85.30661	75.56071	77.26623	0.00000	0.00000	0.00000	1
1845	H	83.09485	76.84024	77.71960	0.00000	0.00000	0.00000	1
1846	H	83.21282	77.01192	74.85267	0.00000	0.00000	0.00000	1
1847	H	85.51577	75.78029	75.15073	0.00000	0.00000	0.00000	1
1848	H	85.04744	78.32643	76.84476	0.00000	0.00000	0.00000	1
1849	H	86.65615	77.71130	76.27832	0.00000	0.00000	0.00000	1
1850	H	85.41947	78.26154	75.07291	0.00000	0.00000	0.00000	1
1851	H	84.70293	74.61434	77.34820	0.00000	0.00000	0.00000	1
1852	H	86.39258	75.27260	77.32506	0.00000	0.00000	0.00000	1
1853	H	85.07813	76.18111	78.17617	0.00000	0.00000	0.00000	1
1854	N	82.45912	74.06650	76.05532	0.00000	0.00000	0.00000	1
1855	C	81.88720	72.83859	75.63121	0.00000	0.00000	0.00000	1
1856	C	80.26177	73.02335	75.69269	0.00000	0.00000	0.00000	1
1857	O	79.69878	73.31355	76.71988	0.00000	0.00000	0.00000	1
1858	C	82.34345	71.78652	76.75091	0.00000	0.00000	0.00000	1
1859	O	81.93223	70.41580	76.53709	0.00000	0.00000	0.00000	1
1860	H	82.07999	74.62778	76.81576	0.00000	0.00000	0.00000	1
1861	H	82.29977	72.63196	74.61565	0.00000	0.00000	0.00000	1
1862	H	83.45145	71.90111	76.87694	0.00000	0.00000	0.00000	1
1863	H	81.88067	72.14565	77.71069	0.00000	0.00000	0.00000	1
1864	H	82.73535	70.06743	76.10796	0.00000	0.00000	0.00000	1
1865	N	79.75877	72.80720	74.49002	0.00000	0.00000	0.00000	1
1866	C	78.34302	72.84251	74.29132	0.00000	0.00000	0.00000	1
1867	C	78.22032	72.00304	72.92423	0.00000	0.00000	0.00000	1
1868	O	79.24298	71.72397	72.32863	0.00000	0.00000	0.00000	1
1869	C	77.84475	74.36990	74.08172	0.00000	0.00000	0.00000	1
1870	O	78.43878	75.09594	73.00140	0.00000	0.00000	0.00000	1
1871	C	78.00170	74.98710	75.51728	0.00000	0.00000	0.00000	1
1872	H	80.30076	72.54350	73.64683	0.00000	0.00000	0.00000	1
1873	H	77.88137	72.38391	75.19536	0.00000	0.00000	0.00000	1
1874	H	76.74601	74.33227	73.83514	0.00000	0.00000	0.00000	1
1875	H	77.66810	75.22507	72.40875	0.00000	0.00000	0.00000	1
1876	H	79.06703	75.26916	75.72017	0.00000	0.00000	0.00000	1
1877	H	77.68311	74.27632	76.31879	0.00000	0.00000	0.00000	1

1878	H	77.39122	75.91335	75.62615	0.00000	0.00000	0.00000	1	
1879	N	76.95417	71.69435	72.63196	0.00000	0.00000	0.00000	1	
1880	C	76.60975	71.08680	71.37956	0.00000	0.00000	0.00000	1	
1881	C	76.52356	72.24254	70.21920	0.00000	0.00000	0.00000	1	
1882	O	75.93997	73.28463	70.38926	0.00000	0.00000	0.00000	1	
1883	C	75.15177	70.53093	71.65710	0.00000	0.00000	0.00000	1	
1884	C	74.59651	71.59429	72.65481	0.00000	0.00000	0.00000	1	
1885	C	75.86243	71.79850	73.59223	0.00000	0.00000	0.00000	1	
1886	H	77.38893	70.32223	71.16042	0.00000	0.00000	0.00000	1	
1887	H	74.54194	70.44016	70.72982	0.00000	0.00000	0.00000	1	
1888	H	75.18065	69.51884	72.11891	0.00000	0.00000	0.00000	1	
1889	H	74.32703	72.53893	72.12792	0.00000	0.00000	0.00000	1	
1890	H	73.68713	71.26365	73.20831	0.00000	0.00000	0.00000	1	
1891	H	75.91067	72.77911	74.11948	0.00000	0.00000	0.00000	1	
1892	H	76.02958	70.97892	74.33093	0.00000	0.00000	0.00000	1	
1893	N	77.09880	71.77088	69.12071	0.00000	0.00000	0.00000	1	
1894	C	76.97271	72.48613	67.90580	0.00000	0.00000	0.00000	1	
1895	C	75.81853	71.72357	67.01977	0.00000	0.00000	0.00000	1	
1896	O	76.07950	70.98352	66.10180	0.00000	0.00000	0.00000	1	
1897	C	78.40913	72.40276	67.18300	0.00000	0.00000	0.00000	1	
1898	O	79.00456	71.09908	67.10137	0.00000	0.00000	0.00000	1	
1899	C	79.19491	73.47019	68.02710	0.00000	0.00000	0.00000	1	
1900	H	77.54823	70.85613	69.10579	0.00000	0.00000	0.00000	1	
1901	H	76.65382	73.50424	68.22809	0.00000	0.00000	0.00000	1	
1902	H	78.28853	72.77626	66.13003	0.00000	0.00000	0.00000	1	
1903	H	78.88436	70.89310	66.15143	0.00000	0.00000	0.00000	1	
1904	H	78.70288	74.47046	67.99891	0.00000	0.00000	0.00000	1	
1905	H	80.23807	73.59960	67.65612	0.00000	0.00000	0.00000	1	
1906	H	79.25996	73.16183	69.09796	0.00000	0.00000	0.00000	1	
1907	N	74.61739	71.99274	67.53210	0.00000	0.00000	0.00000	1	
1908	C	73.52652	72.11383	66.38243	0.00000	0.00000	0.00000	1	
1909	C	73.73885	73.20940	65.45700	0.00000	0.00000	0.00000	1	
1910	O	73.91117	74.10540	64.70503	0.00000	0.00000	0.00000	1	
1911	C	72.12075	72.30559	67.21029	0.00000	0.00000	0.00000	1	
1912	C	70.98539	71.95920	66.30850	0.00000	0.00000	0.00000	1	
1913	C	70.73042	70.45509	66.31058	0.00000	0.00000	0.00000	1	
1914	C	69.71943	72.69306	66.74250	0.00000	0.00000	0.00000	1	
1915	H	74.65099	72.68744	68.27407	0.00000	0.00000	0.00000	1	
1916	H	73.66685	71.10625	65.91441	0.00000	0.00000	0.00000	1	
1917	H	72.12074	71.67520	68.12773	0.00000	0.00000	0.00000	1	
1918	H	72.04546	73.35820	67.56560	0.00000	0.00000	0.00000	1	
1919	H	71.23640	72.28247	65.27171	0.00000	0.00000	0.00000	1	
1920	H	70.41787	70.09253	67.32304	0.00000	0.00000	0.00000	1	
1921	H	71.64617	69.87868	66.02216	0.00000	0.00000	0.00000	1	
1922	H	69.91901	70.17096	65.59319	0.00000	0.00000	0.00000	1	
1923	H	68.84245	72.41939	66.10258	0.00000	0.00000	0.00000	1	
1924	H	69.84380	73.80484	66.67722	0.00000	0.00000	0.00000	1	
1925	H	69.44629	72.45170	67.80151	0.00000	0.00000	0.00000	1	
1926		273							
1927		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	4.0000	16000
		0.2500	300.00	0.00	0.00	-1291.4020	0.0000	0.0000	
1928	N	68.28411	77.47941	77.66707	0.00000	0.00000	0.00000	0.00000	1
1929	C	68.90564	77.46568	76.45529	0.00000	0.00000	0.00000	0.00000	1
1930	C	68.27263	76.13903	75.58970	0.00000	0.00000	0.00000	0.00000	1
1931	O	67.96616	75.08945	76.10011	0.00000	0.00000	0.00000	0.00000	1
1932	C	70.50913	77.08965	76.67711	0.00000	0.00000	0.00000	0.00000	1
1933	C	71.08391	78.00397	77.69118	0.00000	0.00000	0.00000	0.00000	1
1934	C	72.39490	77.42858	78.22423	0.00000	0.00000	0.00000	0.00000	1
1935	C	71.31392	79.40503	77.13237	0.00000	0.00000	0.00000	0.00000	1
1936	H	68.27814	76.59620	78.14355	0.00000	0.00000	0.00000	0.00000	1
1937	H	68.73725	78.47611	76.00115	0.00000	0.00000	0.00000	0.00000	1
1938	H	70.61455	76.02011	77.01436	0.00000	0.00000	0.00000	0.00000	1

1939	H	71.05427	77.15654	75.71012	0.00000	0.00000	0.00000	1
1940	H	70.37153	78.07237	78.54726	0.00000	0.00000	0.00000	1
1941	H	73.21973	77.49242	77.47114	0.00000	0.00000	0.00000	1
1942	H	72.28749	76.34401	78.50516	0.00000	0.00000	0.00000	1
1943	H	72.73719	77.97184	79.14093	0.00000	0.00000	0.00000	1
1944	H	72.22924	79.88183	77.56644	0.00000	0.00000	0.00000	1
1945	H	70.45137	80.08308	77.35455	0.00000	0.00000	0.00000	1
1946	H	71.43781	79.39335	76.02052	0.00000	0.00000	0.00000	1
1947	N	68.31474	76.46993	74.31145	0.00000	0.00000	0.00000	1
1948	C	67.77377	75.60556	73.27904	0.00000	0.00000	0.00000	1
1949	C	68.84358	75.45593	72.01056	0.00000	0.00000	0.00000	1
1950	O	68.57935	74.70253	71.10343	0.00000	0.00000	0.00000	1
1951	C	66.51152	76.20212	72.66103	0.00000	0.00000	0.00000	1
1952	C	65.33050	76.11283	73.60713	0.00000	0.00000	0.00000	1
1953	C	66.71350	77.63109	72.19905	0.00000	0.00000	0.00000	1
1954	H	68.59619	77.43698	74.17010	0.00000	0.00000	0.00000	1
1955	H	67.59167	74.64931	73.82899	0.00000	0.00000	0.00000	1
1956	H	66.26801	75.58838	71.76392	0.00000	0.00000	0.00000	1
1957	H	65.11264	75.04736	73.89961	0.00000	0.00000	0.00000	1
1958	H	65.52377	76.68465	74.55782	0.00000	0.00000	0.00000	1
1959	H	64.39323	76.53288	73.14545	0.00000	0.00000	0.00000	1
1960	H	65.82700	78.01123	71.61818	0.00000	0.00000	0.00000	1
1961	H	66.86451	78.32794	73.07014	0.00000	0.00000	0.00000	1
1962	H	67.61808	77.72647	71.53454	0.00000	0.00000	0.00000	1
1963	N	69.88386	76.26600	72.12506	0.00000	0.00000	0.00000	1
1964	C	70.86608	76.24009	71.09975	0.00000	0.00000	0.00000	1
1965	C	72.34925	75.89289	71.70583	0.00000	0.00000	0.00000	1
1966	O	73.29512	75.88707	70.95128	0.00000	0.00000	0.00000	1
1967	C	71.00335	77.71241	70.51040	0.00000	0.00000	0.00000	1
1968	C	71.58324	77.57083	69.07347	0.00000	0.00000	0.00000	1
1969	C	70.42434	76.89559	68.19949	0.00000	0.00000	0.00000	1
1970	N	70.78705	77.16570	66.87486	0.00000	0.00000	0.00000	1
1971	C	70.05401	76.92330	65.86506	0.00000	0.00000	0.00000	1
1972	N	68.80454	76.33650	66.09494	0.00000	0.00000	0.00000	1
1973	N	70.68275	77.31985	64.67651	0.00000	0.00000	0.00000	1
1974	H	69.92442	76.85177	72.95542	0.00000	0.00000	0.00000	1
1975	H	70.48332	75.48943	70.36694	0.00000	0.00000	0.00000	1
1976	H	70.02235	78.23814	70.50000	0.00000	0.00000	0.00000	1
1977	H	71.67271	78.32959	71.15199	0.00000	0.00000	0.00000	1
1978	H	71.87775	78.56025	68.65803	0.00000	0.00000	0.00000	1
1979	H	72.51041	76.94840	69.08417	0.00000	0.00000	0.00000	1
1980	H	70.32805	75.78545	68.30816	0.00000	0.00000	0.00000	1
1981	H	69.40494	77.33515	68.33101	0.00000	0.00000	0.00000	1
1982	H	71.69361	77.58081	66.72767	0.00000	0.00000	0.00000	1
1983	H	68.37252	76.05215	66.97339	0.00000	0.00000	0.00000	1
1984	H	68.12900	76.09959	65.36772	0.00000	0.00000	0.00000	1
1985	H	71.60253	77.72582	64.51068	0.00000	0.00000	0.00000	1
1986	H	70.26417	77.19768	63.75356	0.00000	0.00000	0.00000	1
1987	N	72.31956	75.71082	73.01944	0.00000	0.00000	0.00000	1
1988	C	73.50242	75.32758	73.70487	0.00000	0.00000	0.00000	1
1989	C	73.15332	73.94615	74.48888	0.00000	0.00000	0.00000	1
1990	O	72.50842	73.07417	73.94871	0.00000	0.00000	0.00000	1
1991	C	73.93999	76.50726	74.69520	0.00000	0.00000	0.00000	1
1992	C	74.09523	77.83670	73.93669	0.00000	0.00000	0.00000	1
1993	C	74.64944	77.87218	72.62150	0.00000	0.00000	0.00000	1
1994	C	73.71213	79.05602	74.57167	0.00000	0.00000	0.00000	1
1995	C	74.77307	79.09577	71.95986	0.00000	0.00000	0.00000	1
1996	C	73.86135	80.25754	73.87763	0.00000	0.00000	0.00000	1
1997	C	74.38502	80.33148	72.55423	0.00000	0.00000	0.00000	1
1998	O	74.50484	81.57865	71.88728	0.00000	0.00000	0.00000	1
1999	H	71.41054	75.71997	73.47915	0.00000	0.00000	0.00000	1
2000	H	74.22217	75.18656	72.86534	0.00000	0.00000	0.00000	1

2001	H	73.19899	76.62481	75.51784	0.00000	0.00000	0.00000	1
2002	H	74.90484	76.24785	75.18854	0.00000	0.00000	0.00000	1
2003	H	74.95842	76.93812	72.11633	0.00000	0.00000	0.00000	1
2004	H	73.31333	79.05042	75.60097	0.00000	0.00000	0.00000	1
2005	H	75.18780	79.09446	70.93653	0.00000	0.00000	0.00000	1
2006	H	73.56384	81.19630	74.37622	0.00000	0.00000	0.00000	1
2007	H	74.91776	81.27755	71.04341	0.00000	0.00000	0.00000	1
2008	N	73.82345	73.86630	75.64327	0.00000	0.00000	0.00000	1
2009	C	73.44610	72.82059	76.54579	0.00000	0.00000	0.00000	1
2010	C	72.31967	73.36755	77.58294	0.00000	0.00000	0.00000	1
2011	O	71.66852	74.37298	77.40124	0.00000	0.00000	0.00000	1
2012	C	74.77365	72.29199	77.25588	0.00000	0.00000	0.00000	1
2013	O	74.57008	71.13296	78.13976	0.00000	0.00000	0.00000	1
2014	C	75.41103	73.54749	77.93695	0.00000	0.00000	0.00000	1
2015	H	74.27117	74.71573	75.97900	0.00000	0.00000	0.00000	1
2016	H	73.00119	72.07002	75.84862	0.00000	0.00000	0.00000	1
2017	H	75.49052	71.93953	76.46897	0.00000	0.00000	0.00000	1
2018	H	75.18401	70.50480	77.72605	0.00000	0.00000	0.00000	1
2019	H	76.34943	73.28234	78.47994	0.00000	0.00000	0.00000	1
2020	H	74.71645	74.01302	78.67823	0.00000	0.00000	0.00000	1
2021	H	75.67460	74.33675	77.19528	0.00000	0.00000	0.00000	1
2022	N	72.18158	72.45917	78.54210	0.00000	0.00000	0.00000	1
2023	C	71.27250	72.73287	79.59717	0.00000	0.00000	0.00000	1
2024	C	72.04836	73.40202	80.87653	0.00000	0.00000	0.00000	1
2025	O	71.41006	73.86126	81.79624	0.00000	0.00000	0.00000	1
2026	C	70.77307	71.35023	80.20566	0.00000	0.00000	0.00000	1
2027	C	69.89215	70.54827	79.19752	0.00000	0.00000	0.00000	1
2028	C	68.38292	71.00013	79.33633	0.00000	0.00000	0.00000	1
2029	C	68.14137	72.30394	78.54061	0.00000	0.00000	0.00000	1
2030	N	66.59870	72.56885	78.54906	0.00000	0.00000	0.00000	1
2031	H	72.81147	71.64432	78.57940	0.00000	0.00000	0.00000	1
2032	H	70.49624	73.40428	79.16461	0.00000	0.00000	0.00000	1
2033	H	71.66217	70.74136	80.48542	0.00000	0.00000	0.00000	1
2034	H	70.21523	71.52315	81.15284	0.00000	0.00000	0.00000	1
2035	H	70.26028	70.67921	78.15497	0.00000	0.00000	0.00000	1
2036	H	69.97393	69.45945	79.41616	0.00000	0.00000	0.00000	1
2037	H	67.70854	70.19985	78.95420	0.00000	0.00000	0.00000	1
2038	H	68.10824	71.13235	80.40824	0.00000	0.00000	0.00000	1
2039	H	68.58004	73.21984	78.98351	0.00000	0.00000	0.00000	1
2040	H	68.40179	72.24114	77.46482	0.00000	0.00000	0.00000	1
2041	H	65.95647	71.75229	78.33032	0.00000	0.00000	0.00000	1
2042	H	66.27538	73.28891	77.84091	0.00000	0.00000	0.00000	1
2043	H	66.17546	72.95111	79.44422	0.00000	0.00000	0.00000	1
2044	N	73.36377	73.18476	80.81426	0.00000	0.00000	0.00000	1
2045	C	74.19101	73.98746	81.66588	0.00000	0.00000	0.00000	1
2046	C	74.56801	75.36333	80.88467	0.00000	0.00000	0.00000	1
2047	O	73.97746	75.77290	79.91458	0.00000	0.00000	0.00000	1
2048	C	75.48517	73.13358	82.00040	0.00000	0.00000	0.00000	1
2049	C	75.70350	73.14943	83.54784	0.00000	0.00000	0.00000	1
2050	C	74.95273	71.91561	84.19210	0.00000	0.00000	0.00000	1
2051	C	73.41921	72.07258	84.07233	0.00000	0.00000	0.00000	1
2052	N	72.77930	70.80391	84.73157	0.00000	0.00000	0.00000	1
2053	H	73.71323	72.78197	79.94551	0.00000	0.00000	0.00000	1
2054	H	73.52237	74.17638	82.53834	0.00000	0.00000	0.00000	1
2055	H	75.38541	72.09092	81.62470	0.00000	0.00000	0.00000	1
2056	H	76.37145	73.55927	81.47748	0.00000	0.00000	0.00000	1
2057	H	76.79024	73.08753	83.77988	0.00000	0.00000	0.00000	1
2058	H	75.35249	74.10681	83.99445	0.00000	0.00000	0.00000	1
2059	H	75.28133	70.96827	83.70665	0.00000	0.00000	0.00000	1
2060	H	75.23614	71.81309	85.26486	0.00000	0.00000	0.00000	1
2061	H	72.99554	72.92562	84.63918	0.00000	0.00000	0.00000	1
2062	H	73.02733	72.07540	83.03462	0.00000	0.00000	0.00000	1

2063	H	73.04705	70.59287	85.73696	0.00000	0.00000	0.00000	1
2064	H	72.95711	69.87080	84.25783	0.00000	0.00000	0.00000	1
2065	H	71.72073	70.80712	84.79516	0.00000	0.00000	0.00000	1
2066	N	75.54242	75.97496	81.56476	0.00000	0.00000	0.00000	1
2067	C	76.11012	77.25089	81.09113	0.00000	0.00000	0.00000	1
2068	C	76.85830	76.95766	79.65881	0.00000	0.00000	0.00000	1
2069	O	77.62459	76.01746	79.53825	0.00000	0.00000	0.00000	1
2070	C	77.10883	77.71036	82.13735	0.00000	0.00000	0.00000	1
2071	C	77.87591	78.93935	81.68435	0.00000	0.00000	0.00000	1
2072	C	76.44191	77.97712	83.47458	0.00000	0.00000	0.00000	1
2073	H	75.92591	75.45859	82.35402	0.00000	0.00000	0.00000	1
2074	H	75.22040	77.91348	80.98404	0.00000	0.00000	0.00000	1
2075	H	77.84721	76.88947	82.28261	0.00000	0.00000	0.00000	1
2076	H	78.69634	79.20574	82.40977	0.00000	0.00000	0.00000	1
2077	H	78.37157	78.77344	80.68380	0.00000	0.00000	0.00000	1
2078	H	77.20879	79.83994	81.58802	0.00000	0.00000	0.00000	1
2079	H	75.92885	77.05902	83.87304	0.00000	0.00000	0.00000	1
2080	H	77.18316	78.31070	84.25177	0.00000	0.00000	0.00000	1
2081	H	75.65985	78.78126	83.39291	0.00000	0.00000	0.00000	1
2082	N	76.56147	77.90438	78.76660	0.00000	0.00000	0.00000	1
2083	C	77.12665	77.86775	77.44770	0.00000	0.00000	0.00000	1
2084	C	78.68407	78.37424	77.57951	0.00000	0.00000	0.00000	1
2085	O	79.02090	79.49532	77.29648	0.00000	0.00000	0.00000	1
2086	C	76.19980	78.85426	76.62920	0.00000	0.00000	0.00000	1
2087	C	75.82550	79.91234	77.71565	0.00000	0.00000	0.00000	1
2088	C	75.62385	78.99518	78.99677	0.00000	0.00000	0.00000	1
2089	H	77.06686	76.79483	77.16030	0.00000	0.00000	0.00000	1
2090	H	76.71199	79.29688	75.74455	0.00000	0.00000	0.00000	1
2091	H	75.29550	78.33295	76.24481	0.00000	0.00000	0.00000	1
2092	H	76.66013	80.63382	77.86471	0.00000	0.00000	0.00000	1
2093	H	74.92424	80.51415	77.46003	0.00000	0.00000	0.00000	1
2094	H	75.86854	79.48175	79.96934	0.00000	0.00000	0.00000	1
2095	H	74.62189	78.51282	79.06742	0.00000	0.00000	0.00000	1
2096	N	79.39709	77.36524	78.06635	0.00000	0.00000	0.00000	1
2097	C	80.81574	77.51021	78.09468	0.00000	0.00000	0.00000	1
2098	C	81.39763	76.94561	76.67794	0.00000	0.00000	0.00000	1
2099	O	80.71820	76.84936	75.68393	0.00000	0.00000	0.00000	1
2100	C	81.31868	76.65858	79.33630	0.00000	0.00000	0.00000	1
2101	C	82.43131	77.43980	80.09877	0.00000	0.00000	0.00000	1
2102	C	81.69465	78.38433	81.12631	0.00000	0.00000	0.00000	1
2103	O	80.50976	78.31349	81.34499	0.00000	0.00000	0.00000	1
2104	N	82.58082	79.20952	81.72006	0.00000	0.00000	0.00000	1
2105	H	78.92912	76.48567	78.36854	0.00000	0.00000	0.00000	1
2106	H	80.93266	78.61546	78.19134	0.00000	0.00000	0.00000	1
2107	H	80.46922	76.44515	80.02871	0.00000	0.00000	0.00000	1
2108	H	81.69509	75.66750	78.99498	0.00000	0.00000	0.00000	1
2109	H	83.11024	76.74115	80.63547	0.00000	0.00000	0.00000	1
2110	H	83.09381	78.01480	79.41515	0.00000	0.00000	0.00000	1
2111	H	83.59583	79.25689	81.57093	0.00000	0.00000	0.00000	1
2112	H	82.35565	79.88256	82.46037	0.00000	0.00000	0.00000	1
2113	N	82.69669	76.65981	76.80240	0.00000	0.00000	0.00000	1
2114	C	83.51531	76.28585	75.64583	0.00000	0.00000	0.00000	1
2115	C	83.20502	74.72468	75.17592	0.00000	0.00000	0.00000	1
2116	O	83.74577	74.29108	74.18602	0.00000	0.00000	0.00000	1
2117	C	84.99241	76.30874	75.98428	0.00000	0.00000	0.00000	1
2118	C	85.55231	77.71747	76.04946	0.00000	0.00000	0.00000	1
2119	C	85.30693	75.56158	77.26702	0.00000	0.00000	0.00000	1
2120	H	83.09468	76.84179	77.72057	0.00000	0.00000	0.00000	1
2121	H	83.21177	77.01125	74.85401	0.00000	0.00000	0.00000	1
2122	H	85.51637	75.78242	75.15160	0.00000	0.00000	0.00000	1
2123	H	85.04429	78.32710	76.84683	0.00000	0.00000	0.00000	1
2124	H	86.65390	77.71454	76.28010	0.00000	0.00000	0.00000	1

2125	H	85.41641	78.26366	75.07497	0.00000	0.00000	0.00000	1
2126	H	84.70958	74.61084	77.34498	0.00000	0.00000	0.00000	1
2127	H	86.39467	75.28108	77.32938	0.00000	0.00000	0.00000	1
2128	H	85.07060	76.17862	78.17724	0.00000	0.00000	0.00000	1
2129	N	82.45849	74.06608	76.05602	0.00000	0.00000	0.00000	1
2130	C	81.88544	72.83888	75.63152	0.00000	0.00000	0.00000	1
2131	C	80.26007	73.02427	75.69429	0.00000	0.00000	0.00000	1
2132	O	79.69806	73.31466	76.72193	0.00000	0.00000	0.00000	1
2133	C	82.34164	71.78605	76.75045	0.00000	0.00000	0.00000	1
2134	O	81.92969	70.41561	76.53615	0.00000	0.00000	0.00000	1
2135	H	82.07942	74.62758	76.81633	0.00000	0.00000	0.00000	1
2136	H	82.29730	72.63246	74.61563	0.00000	0.00000	0.00000	1
2137	H	83.44974	71.90009	76.87612	0.00000	0.00000	0.00000	1
2138	H	81.87938	72.14495	77.71057	0.00000	0.00000	0.00000	1
2139	H	82.73241	70.06707	76.10642	0.00000	0.00000	0.00000	1
2140	N	79.75624	72.80904	74.49181	0.00000	0.00000	0.00000	1
2141	C	78.34059	72.84339	74.29283	0.00000	0.00000	0.00000	1
2142	C	78.21872	72.00240	72.92664	0.00000	0.00000	0.00000	1
2143	O	79.24175	71.72206	72.33218	0.00000	0.00000	0.00000	1
2144	C	77.84091	74.36998	74.08067	0.00000	0.00000	0.00000	1
2145	O	78.43183	75.09301	72.99659	0.00000	0.00000	0.00000	1
2146	C	78.00327	74.99068	75.51404	0.00000	0.00000	0.00000	1
2147	H	80.29835	72.54448	73.64894	0.00000	0.00000	0.00000	1
2148	H	77.87901	72.38578	75.19743	0.00000	0.00000	0.00000	1
2149	H	76.74132	74.33189	73.83788	0.00000	0.00000	0.00000	1
2150	H	77.65990	75.21877	72.40482	0.00000	0.00000	0.00000	1
2151	H	79.07046	75.26725	75.71432	0.00000	0.00000	0.00000	1
2152	H	77.68224	74.28400	76.31820	0.00000	0.00000	0.00000	1
2153	H	77.39806	75.92067	75.62115	0.00000	0.00000	0.00000	1
2154	N	76.95277	71.69399	72.63319	0.00000	0.00000	0.00000	1
2155	C	76.60974	71.08624	71.38049	0.00000	0.00000	0.00000	1
2156	C	76.52347	72.24190	70.22005	0.00000	0.00000	0.00000	1
2157	O	75.93861	73.28336	70.38964	0.00000	0.00000	0.00000	1
2158	C	75.15181	70.52961	71.65679	0.00000	0.00000	0.00000	1
2159	C	74.59501	71.59281	72.65384	0.00000	0.00000	0.00000	1
2160	C	75.85997	71.79831	73.59225	0.00000	0.00000	0.00000	1
2161	H	77.38964	70.32221	71.16195	0.00000	0.00000	0.00000	1
2162	H	74.54298	70.43837	70.72886	0.00000	0.00000	0.00000	1
2163	H	75.18088	69.51753	72.11865	0.00000	0.00000	0.00000	1
2164	H	74.32541	72.53708	72.12639	0.00000	0.00000	0.00000	1
2165	H	73.68518	71.26232	73.20678	0.00000	0.00000	0.00000	1
2166	H	75.90730	72.77939	74.11875	0.00000	0.00000	0.00000	1
2167	H	76.02685	70.97944	74.33180	0.00000	0.00000	0.00000	1
2168	N	77.10031	71.77103	69.12206	0.00000	0.00000	0.00000	1
2169	C	76.97314	72.48578	67.90695	0.00000	0.00000	0.00000	1
2170	C	75.81794	71.72320	67.02226	0.00000	0.00000	0.00000	1
2171	O	76.07807	70.98234	66.10459	0.00000	0.00000	0.00000	1
2172	C	78.40902	72.40252	67.18315	0.00000	0.00000	0.00000	1
2173	O	79.00442	71.09886	67.10072	0.00000	0.00000	0.00000	1
2174	C	79.19532	73.46972	68.02707	0.00000	0.00000	0.00000	1
2175	H	77.55061	70.85668	69.10734	0.00000	0.00000	0.00000	1
2176	H	76.65437	73.50393	68.22925	0.00000	0.00000	0.00000	1
2177	H	78.28770	72.77628	66.13034	0.00000	0.00000	0.00000	1
2178	H	78.88259	70.89269	66.15103	0.00000	0.00000	0.00000	1
2179	H	78.70242	74.46962	68.00070	0.00000	0.00000	0.00000	1
2180	H	80.23779	73.60038	67.65461	0.00000	0.00000	0.00000	1
2181	H	79.26227	73.16031	69.09750	0.00000	0.00000	0.00000	1
2182	N	74.61733	71.99340	67.53486	0.00000	0.00000	0.00000	1
2183	C	73.52642	72.11785	66.38601	0.00000	0.00000	0.00000	1
2184	C	73.74092	73.21021	65.45772	0.00000	0.00000	0.00000	1
2185	O	73.91281	74.11137	64.71216	0.00000	0.00000	0.00000	1
2186	C	72.12023	72.30781	67.21174	0.00000	0.00000	0.00000	1

2187	C	70.98581	71.96174	66.30915	0.00000	0.00000	0.00000	1	
2188	C	70.73093	70.45742	66.30999	0.00000	0.00000	0.00000	1	
2189	C	69.71897	72.69467	66.74283	0.00000	0.00000	0.00000	1	
2190	H	74.65196	72.68841	68.27643	0.00000	0.00000	0.00000	1	
2191	H	73.66712	71.10949	65.91588	0.00000	0.00000	0.00000	1	
2192	H	72.11975	71.67711	68.12899	0.00000	0.00000	0.00000	1	
2193	H	72.04475	73.36027	67.56737	0.00000	0.00000	0.00000	1	
2194	H	71.23711	72.28575	65.27270	0.00000	0.00000	0.00000	1	
2195	H	70.41960	70.09389	67.32245	0.00000	0.00000	0.00000	1	
2196	H	71.64642	69.88150	66.01992	0.00000	0.00000	0.00000	1	
2197	H	69.91871	70.17399	65.59327	0.00000	0.00000	0.00000	1	
2198	H	68.84259	72.42078	66.10221	0.00000	0.00000	0.00000	1	
2199	H	69.84280	73.80651	66.67818	0.00000	0.00000	0.00000	1	
2200	H	69.44539	72.45252	67.80151	0.00000	0.00000	0.00000	1	
2201		273							
2202		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	4.5000	18000
		0.2500	300.00	0.00	0.00	0.00	-1291.4365	0.0000	0.0000
2203	N	68.28519	77.47436	77.66864	0.00000	0.00000	0.00000	0.00000	1
2204	C	68.90446	77.46261	76.45571	0.00000	0.00000	0.00000	0.00000	1
2205	C	68.27129	76.13633	75.58969	0.00000	0.00000	0.00000	0.00000	1
2206	O	67.96442	75.08658	76.09948	0.00000	0.00000	0.00000	0.00000	1
2207	C	70.50859	77.08682	76.67322	0.00000	0.00000	0.00000	0.00000	1
2208	C	71.08577	77.99842	77.68842	0.00000	0.00000	0.00000	0.00000	1
2209	C	72.39848	77.42188	78.21577	0.00000	0.00000	0.00000	0.00000	1
2210	C	71.31196	79.40119	77.13233	0.00000	0.00000	0.00000	0.00000	1
2211	H	68.27976	76.59025	78.14346	0.00000	0.00000	0.00000	0.00000	1
2212	H	68.73467	78.47348	76.00307	0.00000	0.00000	0.00000	0.00000	1
2213	H	70.61514	76.01656	77.00785	0.00000	0.00000	0.00000	0.00000	1
2214	H	71.05158	77.15620	75.70517	0.00000	0.00000	0.00000	0.00000	1
2215	H	70.37597	78.06385	78.54688	0.00000	0.00000	0.00000	0.00000	1
2216	H	73.22231	77.49299	77.46227	0.00000	0.00000	0.00000	0.00000	1
2217	H	72.29392	76.33477	78.48940	0.00000	0.00000	0.00000	0.00000	1
2218	H	72.74070	77.95943	79.13586	0.00000	0.00000	0.00000	0.00000	1
2219	H	72.21789	79.88525	77.57787	0.00000	0.00000	0.00000	0.00000	1
2220	H	70.44122	80.07237	77.34315	0.00000	0.00000	0.00000	0.00000	1
2221	H	71.44991	79.39035	76.02215	0.00000	0.00000	0.00000	0.00000	1
2222	N	68.31474	76.46787	74.31167	0.00000	0.00000	0.00000	0.00000	1
2223	C	67.77303	75.60487	73.27829	0.00000	0.00000	0.00000	0.00000	1
2224	C	68.84229	75.45768	72.00912	0.00000	0.00000	0.00000	0.00000	1
2225	O	68.57575	74.70881	71.09893	0.00000	0.00000	0.00000	0.00000	1
2226	C	66.51001	76.20266	72.66271	0.00000	0.00000	0.00000	0.00000	1
2227	C	65.33090	76.11517	73.61130	0.00000	0.00000	0.00000	0.00000	1
2228	C	66.71300	77.63122	72.19997	0.00000	0.00000	0.00000	0.00000	1
2229	H	68.59627	77.43498	74.17112	0.00000	0.00000	0.00000	0.00000	1
2230	H	67.59131	74.64782	73.82684	0.00000	0.00000	0.00000	0.00000	1
2231	H	66.26401	75.58893	71.76630	0.00000	0.00000	0.00000	0.00000	1
2232	H	65.11243	75.05012	73.90484	0.00000	0.00000	0.00000	0.00000	1
2233	H	65.52673	76.68730	74.56127	0.00000	0.00000	0.00000	0.00000	1
2234	H	64.39316	76.53602	73.15130	0.00000	0.00000	0.00000	0.00000	1
2235	H	65.82539	78.01277	71.62175	0.00000	0.00000	0.00000	0.00000	1
2236	H	66.86786	78.32792	73.07049	0.00000	0.00000	0.00000	0.00000	1
2237	H	67.61573	77.72496	71.53271	0.00000	0.00000	0.00000	0.00000	1
2238	N	69.88570	76.26318	72.12745	0.00000	0.00000	0.00000	0.00000	1
2239	C	70.86704	76.23913	71.10124	0.00000	0.00000	0.00000	0.00000	1
2240	C	72.35100	75.89364	71.70611	0.00000	0.00000	0.00000	0.00000	1
2241	O	73.29735	75.89203	70.95175	0.00000	0.00000	0.00000	0.00000	1
2242	C	71.00145	77.71175	70.51199	0.00000	0.00000	0.00000	0.00000	1
2243	C	71.58159	77.57213	69.07496	0.00000	0.00000	0.00000	0.00000	1
2244	C	70.42495	76.89367	68.20052	0.00000	0.00000	0.00000	0.00000	1
2245	N	70.78927	77.16186	66.87596	0.00000	0.00000	0.00000	0.00000	1
2246	C	70.05680	76.91896	65.86572	0.00000	0.00000	0.00000	0.00000	1
2247	N	68.80637	76.33386	66.09539	0.00000	0.00000	0.00000	0.00000	1

2248	N	70.68691	77.31310	64.67697	0.00000	0.00000	0.00000	1
2249	H	69.92804	76.84558	72.96011	0.00000	0.00000	0.00000	1
2250	H	70.48437	75.48853	70.36836	0.00000	0.00000	0.00000	1
2251	H	70.01937	78.23545	70.50186	0.00000	0.00000	0.00000	1
2252	H	71.66954	78.33015	71.15374	0.00000	0.00000	0.00000	1
2253	H	71.87301	78.56260	68.65971	0.00000	0.00000	0.00000	1
2254	H	72.51064	76.95257	69.08549	0.00000	0.00000	0.00000	1
2255	H	70.33058	75.78354	68.31089	0.00000	0.00000	0.00000	1
2256	H	69.40457	77.33161	68.32993	0.00000	0.00000	0.00000	1
2257	H	71.69649	77.57559	66.72900	0.00000	0.00000	0.00000	1
2258	H	68.37344	76.05114	66.97383	0.00000	0.00000	0.00000	1
2259	H	68.13127	76.09680	65.36791	0.00000	0.00000	0.00000	1
2260	H	71.60730	77.71754	64.51125	0.00000	0.00000	0.00000	1
2261	H	70.26877	77.19002	63.75400	0.00000	0.00000	0.00000	1
2262	N	72.32137	75.70713	73.01914	0.00000	0.00000	0.00000	1
2263	C	73.50478	75.32518	73.70411	0.00000	0.00000	0.00000	1
2264	C	73.15561	73.94493	74.49017	0.00000	0.00000	0.00000	1
2265	O	72.51066	73.07207	73.95152	0.00000	0.00000	0.00000	1
2266	C	73.94207	76.50453	74.69495	0.00000	0.00000	0.00000	1
2267	C	74.09701	77.83463	73.93759	0.00000	0.00000	0.00000	1
2268	C	74.65208	77.87201	72.62283	0.00000	0.00000	0.00000	1
2269	C	73.71243	79.05277	74.57394	0.00000	0.00000	0.00000	1
2270	C	74.77401	79.09649	71.96250	0.00000	0.00000	0.00000	1
2271	C	73.85990	80.25517	73.88112	0.00000	0.00000	0.00000	1
2272	C	74.38356	80.33099	72.55783	0.00000	0.00000	0.00000	1
2273	O	74.50133	81.57895	71.89201	0.00000	0.00000	0.00000	1
2274	H	71.41223	75.71254	73.47870	0.00000	0.00000	0.00000	1
2275	H	74.22469	75.18405	72.86475	0.00000	0.00000	0.00000	1
2276	H	73.20076	76.62132	75.51743	0.00000	0.00000	0.00000	1
2277	H	74.90693	76.24502	75.18830	0.00000	0.00000	0.00000	1
2278	H	74.96252	76.93872	72.11688	0.00000	0.00000	0.00000	1
2279	H	73.31394	79.04552	75.60333	0.00000	0.00000	0.00000	1
2280	H	75.18927	79.09687	70.93939	0.00000	0.00000	0.00000	1
2281	H	73.56096	81.19298	74.38062	0.00000	0.00000	0.00000	1
2282	H	74.91425	81.27920	71.04766	0.00000	0.00000	0.00000	1
2283	N	73.82435	73.86815	75.64556	0.00000	0.00000	0.00000	1
2284	C	73.44840	72.82287	76.54895	0.00000	0.00000	0.00000	1
2285	C	72.32152	73.36883	77.58590	0.00000	0.00000	0.00000	1
2286	O	71.67007	74.37438	77.40489	0.00000	0.00000	0.00000	1
2287	C	74.77743	72.29742	77.25923	0.00000	0.00000	0.00000	1
2288	O	74.57558	71.13860	78.14251	0.00000	0.00000	0.00000	1
2289	C	75.41148	73.55483	77.94013	0.00000	0.00000	0.00000	1
2290	H	74.27162	74.71838	75.98009	0.00000	0.00000	0.00000	1
2291	H	73.00470	72.07087	75.85253	0.00000	0.00000	0.00000	1
2292	H	75.49522	71.94742	76.47202	0.00000	0.00000	0.00000	1
2293	H	75.18756	70.50983	77.72632	0.00000	0.00000	0.00000	1
2294	H	76.34976	73.29210	78.48449	0.00000	0.00000	0.00000	1
2295	H	74.71510	74.01971	78.68012	0.00000	0.00000	0.00000	1
2296	H	75.67446	74.34398	77.19812	0.00000	0.00000	0.00000	1
2297	N	72.18288	72.45973	78.54430	0.00000	0.00000	0.00000	1
2298	C	71.27287	72.73363	79.59858	0.00000	0.00000	0.00000	1
2299	C	72.04916	73.39998	80.87905	0.00000	0.00000	0.00000	1
2300	O	71.41153	73.85629	81.80066	0.00000	0.00000	0.00000	1
2301	C	70.76967	71.35182	80.20595	0.00000	0.00000	0.00000	1
2302	C	69.89140	70.54970	79.19564	0.00000	0.00000	0.00000	1
2303	C	68.38157	71.00099	79.32991	0.00000	0.00000	0.00000	1
2304	C	68.14228	72.30652	78.53639	0.00000	0.00000	0.00000	1
2305	N	66.60015	72.57455	78.54588	0.00000	0.00000	0.00000	1
2306	H	72.81323	71.64537	78.58162	0.00000	0.00000	0.00000	1
2307	H	70.49847	73.40701	79.16558	0.00000	0.00000	0.00000	1
2308	H	71.65721	70.74227	80.48916	0.00000	0.00000	0.00000	1
2309	H	70.20889	71.52600	81.15116	0.00000	0.00000	0.00000	1

2310	H	70.26243	70.68042	78.15410	0.00000	0.00000	0.00000	1
2311	H	69.97276	69.46096	79.41482	0.00000	0.00000	0.00000	1
2312	H	67.70872	70.20138	78.94368	0.00000	0.00000	0.00000	1
2313	H	68.10305	71.13078	80.40113	0.00000	0.00000	0.00000	1
2314	H	68.58266	73.22076	78.98100	0.00000	0.00000	0.00000	1
2315	H	68.40240	72.24533	77.46042	0.00000	0.00000	0.00000	1
2316	H	65.95677	71.76261	78.31378	0.00000	0.00000	0.00000	1
2317	H	66.27984	73.30547	77.84755	0.00000	0.00000	0.00000	1
2318	H	66.17583	72.94447	79.44570	0.00000	0.00000	0.00000	1
2319	N	73.36475	73.18418	80.81457	0.00000	0.00000	0.00000	1
2320	C	74.19223	73.98704	81.66591	0.00000	0.00000	0.00000	1
2321	C	74.56556	75.36454	80.88579	0.00000	0.00000	0.00000	1
2322	O	73.97133	75.77601	79.91880	0.00000	0.00000	0.00000	1
2323	C	75.48748	73.13376	81.99782	0.00000	0.00000	0.00000	1
2324	C	75.70732	73.14816	83.54505	0.00000	0.00000	0.00000	1
2325	C	74.95414	71.91603	84.18979	0.00000	0.00000	0.00000	1
2326	C	73.42093	72.07442	84.06802	0.00000	0.00000	0.00000	1
2327	N	72.77851	70.80726	84.72770	0.00000	0.00000	0.00000	1
2328	H	73.71385	72.78376	79.94459	0.00000	0.00000	0.00000	1
2329	H	73.52455	74.17412	82.53946	0.00000	0.00000	0.00000	1
2330	H	75.38801	72.09141	81.62117	0.00000	0.00000	0.00000	1
2331	H	76.37287	73.56058	81.47432	0.00000	0.00000	0.00000	1
2332	H	76.79413	73.08343	83.77602	0.00000	0.00000	0.00000	1
2333	H	75.35916	74.10625	83.99237	0.00000	0.00000	0.00000	1
2334	H	75.28217	70.96778	83.70575	0.00000	0.00000	0.00000	1
2335	H	75.23619	71.81435	85.26299	0.00000	0.00000	0.00000	1
2336	H	72.99735	72.92863	84.63319	0.00000	0.00000	0.00000	1
2337	H	73.03035	72.07620	83.02982	0.00000	0.00000	0.00000	1
2338	H	73.04164	70.59896	85.73487	0.00000	0.00000	0.00000	1
2339	H	72.95870	69.87296	84.25721	0.00000	0.00000	0.00000	1
2340	H	71.71966	70.81044	84.78635	0.00000	0.00000	0.00000	1
2341	N	75.54117	75.97556	81.56479	0.00000	0.00000	0.00000	1
2342	C	76.11018	77.25039	81.08997	0.00000	0.00000	0.00000	1
2343	C	76.85671	76.95537	79.65713	0.00000	0.00000	0.00000	1
2344	O	77.62129	76.01388	79.53606	0.00000	0.00000	0.00000	1
2345	C	77.11048	77.70894	82.13508	0.00000	0.00000	0.00000	1
2346	C	77.87868	78.93690	81.68109	0.00000	0.00000	0.00000	1
2347	C	76.44538	77.97763	83.47285	0.00000	0.00000	0.00000	1
2348	H	75.92816	75.45683	82.35080	0.00000	0.00000	0.00000	1
2349	H	75.22124	77.91409	80.98337	0.00000	0.00000	0.00000	1
2350	H	77.84779	76.88705	82.28008	0.00000	0.00000	0.00000	1
2351	H	78.69861	79.20374	82.40697	0.00000	0.00000	0.00000	1
2352	H	78.37429	78.76971	80.68092	0.00000	0.00000	0.00000	1
2353	H	77.21208	79.83771	81.58321	0.00000	0.00000	0.00000	1
2354	H	75.92931	77.06128	83.87146	0.00000	0.00000	0.00000	1
2355	H	77.18842	78.30840	84.24955	0.00000	0.00000	0.00000	1
2356	H	75.66624	78.78466	83.39187	0.00000	0.00000	0.00000	1
2357	N	76.56058	77.90243	78.76504	0.00000	0.00000	0.00000	1
2358	C	77.12569	77.86568	77.44601	0.00000	0.00000	0.00000	1
2359	C	78.68326	78.37167	77.57773	0.00000	0.00000	0.00000	1
2360	O	79.02065	79.49221	77.29323	0.00000	0.00000	0.00000	1
2361	C	76.19853	78.85233	76.62794	0.00000	0.00000	0.00000	1
2362	C	75.82530	79.91087	77.71429	0.00000	0.00000	0.00000	1
2363	C	75.62398	78.99407	78.99569	0.00000	0.00000	0.00000	1
2364	H	77.06554	76.79280	77.15881	0.00000	0.00000	0.00000	1
2365	H	76.71005	79.29449	75.74269	0.00000	0.00000	0.00000	1
2366	H	75.29383	78.33105	76.24457	0.00000	0.00000	0.00000	1
2367	H	76.66029	80.63208	77.86272	0.00000	0.00000	0.00000	1
2368	H	74.92410	80.51295	77.45908	0.00000	0.00000	0.00000	1
2369	H	75.86996	79.48055	79.96796	0.00000	0.00000	0.00000	1
2370	H	74.62169	78.51255	79.06732	0.00000	0.00000	0.00000	1
2371	N	79.39603	77.36333	78.06639	0.00000	0.00000	0.00000	1

2372	C	80.81465	77.50863	78.09538	0.00000	0.00000	0.00000	1
2373	C	81.39765	76.94531	76.67868	0.00000	0.00000	0.00000	1
2374	O	80.72002	76.85069	75.68346	0.00000	0.00000	0.00000	1
2375	C	81.31797	76.65742	79.33708	0.00000	0.00000	0.00000	1
2376	C	82.43169	77.43806	80.09880	0.00000	0.00000	0.00000	1
2377	C	81.69663	78.38459	81.12560	0.00000	0.00000	0.00000	1
2378	O	80.51312	78.31257	81.34693	0.00000	0.00000	0.00000	1
2379	N	82.58261	79.21250	81.71581	0.00000	0.00000	0.00000	1
2380	H	78.92774	76.48413	78.36924	0.00000	0.00000	0.00000	1
2381	H	80.93081	78.61404	78.19206	0.00000	0.00000	0.00000	1
2382	H	80.46886	76.44454	80.03004	0.00000	0.00000	0.00000	1
2383	H	81.69364	75.66599	78.99594	0.00000	0.00000	0.00000	1
2384	H	83.10953	76.73878	80.63603	0.00000	0.00000	0.00000	1
2385	H	83.09504	78.01139	79.41464	0.00000	0.00000	0.00000	1
2386	H	83.59749	79.26174	81.56592	0.00000	0.00000	0.00000	1
2387	H	82.35677	79.88671	82.45489	0.00000	0.00000	0.00000	1
2388	N	82.69672	76.65914	76.80415	0.00000	0.00000	0.00000	1
2389	C	83.51519	76.28490	75.64769	0.00000	0.00000	0.00000	1
2390	C	83.20518	74.72358	75.17814	0.00000	0.00000	0.00000	1
2391	O	83.74665	74.28963	74.18879	0.00000	0.00000	0.00000	1
2392	C	84.99208	76.31051	75.98610	0.00000	0.00000	0.00000	1
2393	C	85.54852	77.72059	76.05267	0.00000	0.00000	0.00000	1
2394	C	85.30772	75.56302	77.26842	0.00000	0.00000	0.00000	1
2395	H	83.09417	76.84250	77.72232	0.00000	0.00000	0.00000	1
2396	H	83.21044	77.00991	74.85587	0.00000	0.00000	0.00000	1
2397	H	85.51768	75.78615	75.15324	0.00000	0.00000	0.00000	1
2398	H	85.03888	78.32819	76.85057	0.00000	0.00000	0.00000	1
2399	H	86.65010	77.72030	76.28331	0.00000	0.00000	0.00000	1
2400	H	85.41120	78.26734	75.07867	0.00000	0.00000	0.00000	1
2401	H	84.72125	74.60500	77.33961	0.00000	0.00000	0.00000	1
2402	H	86.39834	75.29542	77.33674	0.00000	0.00000	0.00000	1
2403	H	85.05827	76.17421	78.17909	0.00000	0.00000	0.00000	1
2404	N	82.45709	74.06551	76.05730	0.00000	0.00000	0.00000	1
2405	C	81.88207	72.83946	75.63223	0.00000	0.00000	0.00000	1
2406	C	80.25678	73.02592	75.69705	0.00000	0.00000	0.00000	1
2407	O	79.69566	73.31649	76.72504	0.00000	0.00000	0.00000	1
2408	C	82.33846	71.78521	76.74968	0.00000	0.00000	0.00000	1
2409	O	81.92522	70.41524	76.53450	0.00000	0.00000	0.00000	1
2410	H	82.07831	74.62737	76.81746	0.00000	0.00000	0.00000	1
2411	H	82.29284	72.63346	74.61583	0.00000	0.00000	0.00000	1
2412	H	83.44675	71.89824	76.87461	0.00000	0.00000	0.00000	1
2413	H	81.87718	72.14360	77.71045	0.00000	0.00000	0.00000	1
2414	H	82.72723	70.06645	76.10369	0.00000	0.00000	0.00000	1
2415	N	79.75208	72.81232	74.49469	0.00000	0.00000	0.00000	1
2416	C	78.33645	72.84467	74.29544	0.00000	0.00000	0.00000	1
2417	C	78.21595	72.00111	72.93075	0.00000	0.00000	0.00000	1
2418	O	79.23958	71.71873	72.33817	0.00000	0.00000	0.00000	1
2419	C	77.83434	74.36989	74.07876	0.00000	0.00000	0.00000	1
2420	O	78.41975	75.08791	72.98833	0.00000	0.00000	0.00000	1
2421	C	78.00531	74.99653	75.50840	0.00000	0.00000	0.00000	1
2422	H	80.29433	72.54662	73.65224	0.00000	0.00000	0.00000	1
2423	H	77.87516	72.38873	75.20101	0.00000	0.00000	0.00000	1
2424	H	76.73342	74.33067	73.84238	0.00000	0.00000	0.00000	1
2425	H	77.64558	75.20779	72.39820	0.00000	0.00000	0.00000	1
2426	H	79.07538	75.26410	75.70452	0.00000	0.00000	0.00000	1
2427	H	77.68126	74.29661	76.31714	0.00000	0.00000	0.00000	1
2428	H	77.40921	75.93270	75.61214	0.00000	0.00000	0.00000	1
2429	N	76.95031	71.69318	72.63539	0.00000	0.00000	0.00000	1
2430	C	76.60974	71.08521	71.38210	0.00000	0.00000	0.00000	1
2431	C	76.52324	72.24084	70.22164	0.00000	0.00000	0.00000	1
2432	O	75.93621	73.28120	70.39053	0.00000	0.00000	0.00000	1
2433	C	75.15197	70.52708	71.65612	0.00000	0.00000	0.00000	1

2434	C	74.59272	71.59010	72.65196	0.00000	0.00000	0.00000	1	
2435	C	75.85580	71.79795	73.59238	0.00000	0.00000	0.00000	1	
2436	H	77.39080	70.32208	71.16456	0.00000	0.00000	0.00000	1	
2437	H	74.54469	70.43513	70.72728	0.00000	0.00000	0.00000	1	
2438	H	75.18123	69.51520	72.11834	0.00000	0.00000	0.00000	1	
2439	H	74.32252	72.53384	72.12378	0.00000	0.00000	0.00000	1	
2440	H	73.68279	71.25782	73.20350	0.00000	0.00000	0.00000	1	
2441	H	75.90149	72.77989	74.11746	0.00000	0.00000	0.00000	1	
2442	H	76.02203	70.98032	74.33341	0.00000	0.00000	0.00000	1	
2443	N	77.10283	71.77135	69.12450	0.00000	0.00000	0.00000	1	
2444	C	76.97381	72.48534	67.90898	0.00000	0.00000	0.00000	1	
2445	C	75.81704	71.72258	67.02653	0.00000	0.00000	0.00000	1	
2446	O	76.07550	70.98036	66.10950	0.00000	0.00000	0.00000	1	
2447	C	78.40874	72.40211	67.18340	0.00000	0.00000	0.00000	1	
2448	O	79.00402	71.09847	67.09961	0.00000	0.00000	0.00000	1	
2449	C	79.19604	73.46890	68.02694	0.00000	0.00000	0.00000	1	
2450	H	77.55458	70.85773	69.11008	0.00000	0.00000	0.00000	1	
2451	H	76.65528	73.50351	68.23128	0.00000	0.00000	0.00000	1	
2452	H	78.28611	72.77631	66.13091	0.00000	0.00000	0.00000	1	
2453	H	78.87965	70.89211	66.15030	0.00000	0.00000	0.00000	1	
2454	H	78.70182	74.46821	68.00361	0.00000	0.00000	0.00000	1	
2455	H	80.23736	73.60151	67.65196	0.00000	0.00000	0.00000	1	
2456	H	79.26618	73.15780	69.09668	0.00000	0.00000	0.00000	1	
2457	N	74.61695	71.99460	67.53971	0.00000	0.00000	0.00000	1	
2458	C	73.52720	72.12062	66.38822	0.00000	0.00000	0.00000	1	
2459	C	73.74259	73.22026	65.46886	0.00000	0.00000	0.00000	1	
2460	O	73.91686	74.11743	64.71883	0.00000	0.00000	0.00000	1	
2461	C	72.11978	72.31179	67.21461	0.00000	0.00000	0.00000	1	
2462	C	70.98586	71.96593	66.31007	0.00000	0.00000	0.00000	1	
2463	C	70.73193	70.46175	66.30898	0.00000	0.00000	0.00000	1	
2464	C	69.71842	72.69744	66.74339	0.00000	0.00000	0.00000	1	
2465	H	74.65349	72.69020	68.28066	0.00000	0.00000	0.00000	1	
2466	H	73.66760	71.11507	65.91834	0.00000	0.00000	0.00000	1	
2467	H	72.11809	71.68037	68.13118	0.00000	0.00000	0.00000	1	
2468	H	72.04349	73.36395	67.57055	0.00000	0.00000	0.00000	1	
2469	H	71.23836	72.29151	65.27444	0.00000	0.00000	0.00000	1	
2470	H	70.42259	70.09627	67.32136	0.00000	0.00000	0.00000	1	
2471	H	71.64702	69.88652	66.01617	0.00000	0.00000	0.00000	1	
2472	H	69.91844	70.17921	65.59331	0.00000	0.00000	0.00000	1	
2473	H	68.84287	72.42343	66.10166	0.00000	0.00000	0.00000	1	
2474	H	69.84121	73.80950	66.67993	0.00000	0.00000	0.00000	1	
2475	H	69.44391	72.45406	67.80155	0.00000	0.00000	0.00000	1	
2476	273								
2477		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	5.0000	20000
		0.2500	300.00	0.00	0.00	0.00	-1291.4519	0.0000	0.0000
2478	N	68.28601	77.47051	77.66983	0.00000	0.00000	0.00000	0.00000	1
2479	C	68.90355	77.46028	76.45603	0.00000	0.00000	0.00000	0.00000	1
2480	C	68.27023	76.13429	75.58959	0.00000	0.00000	0.00000	0.00000	1
2481	O	67.96299	75.08445	76.09894	0.00000	0.00000	0.00000	0.00000	1
2482	C	70.50813	77.08467	76.67031	0.00000	0.00000	0.00000	0.00000	1
2483	C	71.08717	77.99415	77.68640	0.00000	0.00000	0.00000	0.00000	1
2484	C	72.40121	77.41668	78.20927	0.00000	0.00000	0.00000	0.00000	1
2485	C	71.31052	79.39824	77.13250	0.00000	0.00000	0.00000	0.00000	1
2486	H	68.28121	76.58578	78.14351	0.00000	0.00000	0.00000	0.00000	1
2487	H	68.73269	78.47150	76.00455	0.00000	0.00000	0.00000	0.00000	1
2488	H	70.61547	76.01386	77.00292	0.00000	0.00000	0.00000	0.00000	1
2489	H	71.04953	77.15593	75.70148	0.00000	0.00000	0.00000	0.00000	1
2490	H	70.37941	78.05722	78.54671	0.00000	0.00000	0.00000	0.00000	1
2491	H	73.22426	77.49335	77.45550	0.00000	0.00000	0.00000	0.00000	1
2492	H	72.29856	76.32763	78.47707	0.00000	0.00000	0.00000	0.00000	1
2493	H	72.74348	77.94972	79.13198	0.00000	0.00000	0.00000	0.00000	1
2494	H	72.20928	79.88760	77.58664	0.00000	0.00000	0.00000	0.00000	1

2495	H	70.43377	80.06418	77.33484	0.00000	0.00000	0.00000	1
2496	H	71.45899	79.38822	76.02370	0.00000	0.00000	0.00000	1
2497	N	68.31462	76.46599	74.31141	0.00000	0.00000	0.00000	1
2498	C	67.77242	75.60481	73.27763	0.00000	0.00000	0.00000	1
2499	C	68.84112	75.45893	72.00815	0.00000	0.00000	0.00000	1
2500	O	68.57304	74.71340	71.09555	0.00000	0.00000	0.00000	1
2501	C	66.50928	76.20290	72.66411	0.00000	0.00000	0.00000	1
2502	C	65.33127	76.11693	73.61441	0.00000	0.00000	0.00000	1
2503	C	66.71259	77.63134	72.20063	0.00000	0.00000	0.00000	1
2504	H	68.59646	77.43343	74.17186	0.00000	0.00000	0.00000	1
2505	H	67.59103	74.64676	73.82514	0.00000	0.00000	0.00000	1
2506	H	66.26103	75.58939	71.76806	0.00000	0.00000	0.00000	1
2507	H	65.11235	75.05218	73.90875	0.00000	0.00000	0.00000	1
2508	H	65.52904	76.68928	74.56386	0.00000	0.00000	0.00000	1
2509	H	64.39313	76.53838	73.15572	0.00000	0.00000	0.00000	1
2510	H	65.82413	78.01393	71.62438	0.00000	0.00000	0.00000	1
2511	H	66.87027	78.32794	73.07073	0.00000	0.00000	0.00000	1
2512	H	67.61392	77.72393	71.53132	0.00000	0.00000	0.00000	1
2513	N	69.88700	76.26103	72.12908	0.00000	0.00000	0.00000	1
2514	C	70.86789	76.23836	71.10233	0.00000	0.00000	0.00000	1
2515	C	72.35237	75.89426	71.70650	0.00000	0.00000	0.00000	1
2516	O	73.29975	75.89557	70.95328	0.00000	0.00000	0.00000	1
2517	C	71.00001	77.71122	70.51321	0.00000	0.00000	0.00000	1
2518	C	71.58020	77.57321	69.07599	0.00000	0.00000	0.00000	1
2519	C	70.42533	76.89219	68.20117	0.00000	0.00000	0.00000	1
2520	N	70.79053	77.15881	66.87635	0.00000	0.00000	0.00000	1
2521	C	70.05906	76.91572	65.86643	0.00000	0.00000	0.00000	1
2522	N	68.80841	76.33216	66.09558	0.00000	0.00000	0.00000	1
2523	N	70.68973	77.30776	64.67802	0.00000	0.00000	0.00000	1
2524	H	69.93060	76.84097	72.96340	0.00000	0.00000	0.00000	1
2525	H	70.48527	75.48782	70.36934	0.00000	0.00000	0.00000	1
2526	H	70.01709	78.23340	70.50324	0.00000	0.00000	0.00000	1
2527	H	71.66712	78.33056	71.15507	0.00000	0.00000	0.00000	1
2528	H	71.86942	78.56436	68.66095	0.00000	0.00000	0.00000	1
2529	H	72.51064	76.95602	69.08572	0.00000	0.00000	0.00000	1
2530	H	70.33245	75.78206	68.31302	0.00000	0.00000	0.00000	1
2531	H	69.40427	77.32892	68.32917	0.00000	0.00000	0.00000	1
2532	H	71.69847	77.57156	66.72997	0.00000	0.00000	0.00000	1
2533	H	68.37406	76.05035	66.97412	0.00000	0.00000	0.00000	1
2534	H	68.13299	76.09468	65.36800	0.00000	0.00000	0.00000	1
2535	H	71.61095	77.71126	64.51181	0.00000	0.00000	0.00000	1
2536	H	70.27233	77.18420	63.75440	0.00000	0.00000	0.00000	1
2537	N	72.32257	75.70474	73.01909	0.00000	0.00000	0.00000	1
2538	C	73.50642	75.32353	73.70390	0.00000	0.00000	0.00000	1
2539	C	73.15711	73.94400	74.49126	0.00000	0.00000	0.00000	1
2540	O	72.51259	73.07024	73.95356	0.00000	0.00000	0.00000	1
2541	C	73.94398	76.50256	74.69467	0.00000	0.00000	0.00000	1
2542	C	74.09849	77.83332	73.93822	0.00000	0.00000	0.00000	1
2543	C	74.65402	77.87187	72.62367	0.00000	0.00000	0.00000	1
2544	C	73.71271	79.05049	74.57565	0.00000	0.00000	0.00000	1
2545	C	74.77469	79.09710	71.96439	0.00000	0.00000	0.00000	1
2546	C	73.85885	80.25352	73.88368	0.00000	0.00000	0.00000	1
2547	C	74.38249	80.33070	72.56049	0.00000	0.00000	0.00000	1
2548	O	74.49873	81.57924	71.89550	0.00000	0.00000	0.00000	1
2549	H	71.41340	75.70736	73.47838	0.00000	0.00000	0.00000	1
2550	H	74.22634	75.18226	72.86453	0.00000	0.00000	0.00000	1
2551	H	73.20195	76.61792	75.51638	0.00000	0.00000	0.00000	1
2552	H	74.90878	76.24303	75.18823	0.00000	0.00000	0.00000	1
2553	H	74.96491	76.93897	72.11691	0.00000	0.00000	0.00000	1
2554	H	73.31450	79.04195	75.60512	0.00000	0.00000	0.00000	1
2555	H	75.19032	79.09873	70.94141	0.00000	0.00000	0.00000	1
2556	H	73.55885	81.19062	74.38384	0.00000	0.00000	0.00000	1

2557	H	74.91177	81.28049	71.05085	0.00000	0.00000	0.00000	1
2558	N	73.82499	73.86946	75.64722	0.00000	0.00000	0.00000	1
2559	C	73.45014	72.82456	76.55136	0.00000	0.00000	0.00000	1
2560	C	72.32301	73.36987	77.58819	0.00000	0.00000	0.00000	1
2561	O	71.67158	74.37570	77.40789	0.00000	0.00000	0.00000	1
2562	C	74.78022	72.30145	77.26188	0.00000	0.00000	0.00000	1
2563	O	74.57961	71.14287	78.14488	0.00000	0.00000	0.00000	1
2564	C	75.41184	73.56029	77.94257	0.00000	0.00000	0.00000	1
2565	H	74.27209	74.72018	75.98081	0.00000	0.00000	0.00000	1
2566	H	73.00731	72.07144	75.85557	0.00000	0.00000	0.00000	1
2567	H	75.49870	71.95317	76.47454	0.00000	0.00000	0.00000	1
2568	H	75.19058	70.51380	77.72731	0.00000	0.00000	0.00000	1
2569	H	76.35004	73.29938	78.48795	0.00000	0.00000	0.00000	1
2570	H	74.71409	74.02463	78.68159	0.00000	0.00000	0.00000	1
2571	H	75.67432	74.34936	77.20030	0.00000	0.00000	0.00000	1
2572	N	72.18378	72.46014	78.54589	0.00000	0.00000	0.00000	1
2573	C	71.27312	72.73415	79.59964	0.00000	0.00000	0.00000	1
2574	C	72.04976	73.39843	80.88092	0.00000	0.00000	0.00000	1
2575	O	71.41262	73.85254	81.80393	0.00000	0.00000	0.00000	1
2576	C	70.76712	71.35294	80.20611	0.00000	0.00000	0.00000	1
2577	C	69.89086	70.55078	79.19410	0.00000	0.00000	0.00000	1
2578	C	68.38061	71.00167	79.32506	0.00000	0.00000	0.00000	1
2579	C	68.14305	72.30857	78.53329	0.00000	0.00000	0.00000	1
2580	N	66.60132	72.57886	78.54343	0.00000	0.00000	0.00000	1
2581	H	72.81434	71.64603	78.58315	0.00000	0.00000	0.00000	1
2582	H	70.50010	73.40901	79.16636	0.00000	0.00000	0.00000	1
2583	H	71.65348	70.74288	80.49189	0.00000	0.00000	0.00000	1
2584	H	70.20412	71.52803	81.14984	0.00000	0.00000	0.00000	1
2585	H	70.26404	70.68144	78.15333	0.00000	0.00000	0.00000	1
2586	H	69.97189	69.46207	79.41357	0.00000	0.00000	0.00000	1
2587	H	67.70887	70.20263	78.93573	0.00000	0.00000	0.00000	1
2588	H	68.09927	71.12959	80.39576	0.00000	0.00000	0.00000	1
2589	H	68.58462	73.22153	78.97931	0.00000	0.00000	0.00000	1
2590	H	68.40305	72.24868	77.45721	0.00000	0.00000	0.00000	1
2591	H	65.95713	71.77041	78.30164	0.00000	0.00000	0.00000	1
2592	H	66.28326	73.31757	77.85230	0.00000	0.00000	0.00000	1
2593	H	66.17612	72.93981	79.44649	0.00000	0.00000	0.00000	1
2594	N	73.36548	73.18377	80.81476	0.00000	0.00000	0.00000	1
2595	C	74.19311	73.98674	81.66590	0.00000	0.00000	0.00000	1
2596	C	74.56374	75.36550	80.88674	0.00000	0.00000	0.00000	1
2597	O	73.96678	75.77851	79.92210	0.00000	0.00000	0.00000	1
2598	C	75.48918	73.13395	81.99588	0.00000	0.00000	0.00000	1
2599	C	75.71016	73.14723	83.54296	0.00000	0.00000	0.00000	1
2600	C	74.95521	71.91634	84.18801	0.00000	0.00000	0.00000	1
2601	C	73.42222	72.07578	84.06477	0.00000	0.00000	0.00000	1
2602	N	72.77795	70.80977	84.72480	0.00000	0.00000	0.00000	1
2603	H	73.71431	72.78506	79.94388	0.00000	0.00000	0.00000	1
2604	H	73.52612	74.17244	82.54027	0.00000	0.00000	0.00000	1
2605	H	75.38996	72.09184	81.61849	0.00000	0.00000	0.00000	1
2606	H	76.37390	73.56166	81.47196	0.00000	0.00000	0.00000	1
2607	H	76.79701	73.08040	83.77310	0.00000	0.00000	0.00000	1
2608	H	75.36412	74.10582	83.99082	0.00000	0.00000	0.00000	1
2609	H	75.28282	70.96742	83.70499	0.00000	0.00000	0.00000	1
2610	H	75.23625	71.81525	85.26153	0.00000	0.00000	0.00000	1
2611	H	72.99873	72.93088	84.62866	0.00000	0.00000	0.00000	1
2612	H	73.03262	72.07676	83.02621	0.00000	0.00000	0.00000	1
2613	H	73.03768	70.60350	85.73327	0.00000	0.00000	0.00000	1
2614	H	72.95982	69.87459	84.25672	0.00000	0.00000	0.00000	1
2615	H	71.71890	70.81295	84.77985	0.00000	0.00000	0.00000	1
2616	N	75.54024	75.97609	81.56492	0.00000	0.00000	0.00000	1
2617	C	76.11019	77.25010	81.08914	0.00000	0.00000	0.00000	1
2618	C	76.85557	76.95376	79.65592	0.00000	0.00000	0.00000	1

2619	O	77.61903	76.01141	79.53459	0.00000	0.00000	0.00000	1
2620	C	77.11171	77.70800	82.13338	0.00000	0.00000	0.00000	1
2621	C	77.88080	78.93509	81.67852	0.00000	0.00000	0.00000	1
2622	C	76.44792	77.97796	83.47155	0.00000	0.00000	0.00000	1
2623	H	75.92981	75.45554	82.34844	0.00000	0.00000	0.00000	1
2624	H	75.22183	77.91462	80.98285	0.00000	0.00000	0.00000	1
2625	H	77.84823	76.88537	82.27818	0.00000	0.00000	0.00000	1
2626	H	78.70054	79.20218	82.40458	0.00000	0.00000	0.00000	1
2627	H	78.37673	78.76674	80.67873	0.00000	0.00000	0.00000	1
2628	H	77.21468	79.83617	81.57956	0.00000	0.00000	0.00000	1
2629	H	75.92968	77.06282	83.87014	0.00000	0.00000	0.00000	1
2630	H	77.19221	78.30662	84.24795	0.00000	0.00000	0.00000	1
2631	H	75.67084	78.78705	83.39117	0.00000	0.00000	0.00000	1
2632	N	76.55988	77.90098	78.76386	0.00000	0.00000	0.00000	1
2633	C	77.12496	77.86409	77.44486	0.00000	0.00000	0.00000	1
2634	C	78.68262	78.36978	77.57650	0.00000	0.00000	0.00000	1
2635	O	79.02015	79.49000	77.29102	0.00000	0.00000	0.00000	1
2636	C	76.19768	78.85079	76.62699	0.00000	0.00000	0.00000	1
2637	C	75.82518	79.90973	77.71321	0.00000	0.00000	0.00000	1
2638	C	75.62407	78.99325	78.99485	0.00000	0.00000	0.00000	1
2639	H	77.06447	76.79119	77.15785	0.00000	0.00000	0.00000	1
2640	H	76.70879	79.29259	75.74133	0.00000	0.00000	0.00000	1
2641	H	75.29265	78.32959	76.24429	0.00000	0.00000	0.00000	1
2642	H	76.66043	80.63073	77.86115	0.00000	0.00000	0.00000	1
2643	H	74.92405	80.51201	77.45823	0.00000	0.00000	0.00000	1
2644	H	75.87099	79.47974	79.96688	0.00000	0.00000	0.00000	1
2645	H	74.62149	78.51242	79.06721	0.00000	0.00000	0.00000	1
2646	N	79.39526	77.36193	78.06639	0.00000	0.00000	0.00000	1
2647	C	80.81389	77.50770	78.09594	0.00000	0.00000	0.00000	1
2648	C	81.39763	76.94548	76.67914	0.00000	0.00000	0.00000	1
2649	O	80.72093	76.85211	75.68315	0.00000	0.00000	0.00000	1
2650	C	81.31757	76.65677	79.33762	0.00000	0.00000	0.00000	1
2651	C	82.43183	77.43673	80.09876	0.00000	0.00000	0.00000	1
2652	C	81.69793	78.38469	81.12500	0.00000	0.00000	0.00000	1
2653	O	80.51485	78.31188	81.34820	0.00000	0.00000	0.00000	1
2654	N	82.58391	79.21463	81.71251	0.00000	0.00000	0.00000	1
2655	H	78.92693	76.48288	78.36958	0.00000	0.00000	0.00000	1
2656	H	80.92934	78.61316	78.19286	0.00000	0.00000	0.00000	1
2657	H	80.46858	76.44431	80.03104	0.00000	0.00000	0.00000	1
2658	H	81.69247	75.66495	78.99654	0.00000	0.00000	0.00000	1
2659	H	83.10900	76.73703	80.63648	0.00000	0.00000	0.00000	1
2660	H	83.09599	78.00896	79.41432	0.00000	0.00000	0.00000	1
2661	H	83.59858	79.26507	81.56167	0.00000	0.00000	0.00000	1
2662	H	82.35776	79.88973	82.45065	0.00000	0.00000	0.00000	1
2663	N	82.69650	76.65895	76.80531	0.00000	0.00000	0.00000	1
2664	C	83.51507	76.28423	75.64889	0.00000	0.00000	0.00000	1
2665	C	83.20510	74.72261	75.17997	0.00000	0.00000	0.00000	1
2666	O	83.74711	74.28832	74.19112	0.00000	0.00000	0.00000	1
2667	C	84.99204	76.31182	75.98756	0.00000	0.00000	0.00000	1
2668	C	85.54572	77.72291	76.05516	0.00000	0.00000	0.00000	1
2669	C	85.30844	75.56406	77.26948	0.00000	0.00000	0.00000	1
2670	H	83.09358	76.84198	77.72362	0.00000	0.00000	0.00000	1
2671	H	83.20965	77.00873	74.85697	0.00000	0.00000	0.00000	1
2672	H	85.51874	75.78897	75.15453	0.00000	0.00000	0.00000	1
2673	H	85.03486	78.32896	76.85347	0.00000	0.00000	0.00000	1
2674	H	86.64729	77.72459	76.28582	0.00000	0.00000	0.00000	1
2675	H	85.40735	78.27010	75.08156	0.00000	0.00000	0.00000	1
2676	H	84.72999	74.60082	77.33580	0.00000	0.00000	0.00000	1
2677	H	86.40104	75.30585	77.34205	0.00000	0.00000	0.00000	1
2678	H	85.04959	76.17086	78.18046	0.00000	0.00000	0.00000	1
2679	N	82.45567	74.06524	76.05845	0.00000	0.00000	0.00000	1
2680	C	81.87908	72.84005	75.63303	0.00000	0.00000	0.00000	1

2681	C	80.25391	73.02750	75.69899	0.00000	0.00000	0.00000	1
2682	O	79.69294	73.31827	76.72698	0.00000	0.00000	0.00000	1
2683	C	82.33582	71.78464	76.74917	0.00000	0.00000	0.00000	1
2684	O	81.92175	70.41502	76.53325	0.00000	0.00000	0.00000	1
2685	H	82.07722	74.62747	76.81846	0.00000	0.00000	0.00000	1
2686	H	82.28904	72.63440	74.61624	0.00000	0.00000	0.00000	1
2687	H	83.44429	71.89691	76.87332	0.00000	0.00000	0.00000	1
2688	H	81.87552	72.14253	77.71059	0.00000	0.00000	0.00000	1
2689	H	82.72327	70.06611	76.10164	0.00000	0.00000	0.00000	1
2690	N	79.74908	72.81481	74.49653	0.00000	0.00000	0.00000	1
2691	C	78.33344	72.84545	74.29719	0.00000	0.00000	0.00000	1
2692	C	78.21392	71.99996	72.93363	0.00000	0.00000	0.00000	1
2693	O	79.23798	71.71614	72.34240	0.00000	0.00000	0.00000	1
2694	C	77.82967	74.36969	74.07739	0.00000	0.00000	0.00000	1
2695	O	78.41070	75.08410	72.98224	0.00000	0.00000	0.00000	1
2696	C	78.00744	75.00070	75.50421	0.00000	0.00000	0.00000	1
2697	H	80.29154	72.54827	73.65448	0.00000	0.00000	0.00000	1
2698	H	77.87250	72.39068	75.20355	0.00000	0.00000	0.00000	1
2699	H	76.72775	74.32952	73.84583	0.00000	0.00000	0.00000	1
2700	H	77.63477	75.19947	72.39345	0.00000	0.00000	0.00000	1
2701	H	79.07930	75.26353	75.69644	0.00000	0.00000	0.00000	1
2702	H	77.68235	74.30528	76.31647	0.00000	0.00000	0.00000	1
2703	H	77.41668	75.94047	75.60589	0.00000	0.00000	0.00000	1
2704	N	76.94848	71.69238	72.63697	0.00000	0.00000	0.00000	1
2705	C	76.60969	71.08430	71.38325	0.00000	0.00000	0.00000	1
2706	C	76.52305	72.24003	70.22288	0.00000	0.00000	0.00000	1
2707	O	75.93453	73.27969	70.39099	0.00000	0.00000	0.00000	1
2708	C	75.15205	70.52510	71.65567	0.00000	0.00000	0.00000	1
2709	C	74.59090	71.58793	72.65067	0.00000	0.00000	0.00000	1
2710	C	75.85268	71.79758	73.59242	0.00000	0.00000	0.00000	1
2711	H	77.39166	70.32192	71.16640	0.00000	0.00000	0.00000	1
2712	H	74.54596	70.43255	70.72611	0.00000	0.00000	0.00000	1
2713	H	75.18156	69.51332	72.11810	0.00000	0.00000	0.00000	1
2714	H	74.32031	72.53122	72.12188	0.00000	0.00000	0.00000	1
2715	H	73.68070	71.25495	73.20134	0.00000	0.00000	0.00000	1
2716	H	75.89718	72.78022	74.11636	0.00000	0.00000	0.00000	1
2717	H	76.01844	70.98097	74.33467	0.00000	0.00000	0.00000	1
2718	N	77.10467	71.77164	69.12631	0.00000	0.00000	0.00000	1
2719	C	76.97429	72.48501	67.91062	0.00000	0.00000	0.00000	1
2720	C	75.81610	71.72219	67.02981	0.00000	0.00000	0.00000	1
2721	O	76.07351	70.97900	66.11325	0.00000	0.00000	0.00000	1
2722	C	78.40841	72.40184	67.18364	0.00000	0.00000	0.00000	1
2723	O	79.00360	71.09818	67.09882	0.00000	0.00000	0.00000	1
2724	C	79.19658	73.46829	68.02680	0.00000	0.00000	0.00000	1
2725	H	77.55745	70.85851	69.11216	0.00000	0.00000	0.00000	1
2726	H	76.65580	73.50321	68.23323	0.00000	0.00000	0.00000	1
2727	H	78.28479	72.77636	66.13135	0.00000	0.00000	0.00000	1
2728	H	78.87751	70.89178	66.14975	0.00000	0.00000	0.00000	1
2729	H	78.70151	74.46723	68.00561	0.00000	0.00000	0.00000	1
2730	H	80.23706	73.60219	67.64996	0.00000	0.00000	0.00000	1
2731	H	79.26903	73.15602	69.09604	0.00000	0.00000	0.00000	1
2732	N	74.61661	71.99554	67.54308	0.00000	0.00000	0.00000	1
2733	C	73.52815	72.12386	66.39144	0.00000	0.00000	0.00000	1
2734	C	73.74366	73.22594	65.47471	0.00000	0.00000	0.00000	1
2735	O	73.92001	74.12315	64.72513	0.00000	0.00000	0.00000	1
2736	C	72.11898	72.31460	67.21649	0.00000	0.00000	0.00000	1
2737	C	70.98633	71.96925	66.31097	0.00000	0.00000	0.00000	1
2738	C	70.73274	70.46490	66.30817	0.00000	0.00000	0.00000	1
2739	C	69.71797	72.69968	66.74385	0.00000	0.00000	0.00000	1
2740	H	74.65455	72.69147	68.28379	0.00000	0.00000	0.00000	1
2741	H	73.66795	71.11905	65.92021	0.00000	0.00000	0.00000	1
2742	H	72.11689	71.68276	68.13294	0.00000	0.00000	0.00000	1

2743	H	72.04264	73.36674	67.57301	0.00000	0.00000	0.00000	1
2744	H	71.23931	72.29589	65.27571	0.00000	0.00000	0.00000	1
2745	H	70.42480	70.09809	67.32054	0.00000	0.00000	0.00000	1
2746	H	71.64764	69.89035	66.01348	0.00000	0.00000	0.00000	1
2747	H	69.91839	70.18309	65.59322	0.00000	0.00000	0.00000	1
2748	H	68.84310	72.42555	66.10128	0.00000	0.00000	0.00000	1
2749	H	69.84015	73.81184	66.68131	0.00000	0.00000	0.00000	1
2750	H	69.44287	72.45527	67.80166	0.00000	0.00000	0.00000	1
2751		273						
2752		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	5.5000 22000
		0.2500	300.00	0.00	0.00	0.00	-1291.4690 0.0000	0.0000
2753	N	68.28662	77.46732	77.67074	0.00000	0.00000	0.00000	1
2754	C	68.90275	77.45836	76.45624	0.00000	0.00000	0.00000	1
2755	C	68.26935	76.13264	75.58951	0.00000	0.00000	0.00000	1
2756	O	67.96172	75.08267	76.09833	0.00000	0.00000	0.00000	1
2757	C	70.50771	77.08292	76.66790	0.00000	0.00000	0.00000	1
2758	C	71.08826	77.99067	77.68473	0.00000	0.00000	0.00000	1
2759	C	72.40335	77.41229	78.20383	0.00000	0.00000	0.00000	1
2760	C	71.30933	79.39585	77.13272	0.00000	0.00000	0.00000	1
2761	H	68.28251	76.58213	78.14355	0.00000	0.00000	0.00000	1
2762	H	68.73100	78.46984	76.00569	0.00000	0.00000	0.00000	1
2763	H	70.61564	76.01167	76.99885	0.00000	0.00000	0.00000	1
2764	H	71.04783	77.15570	75.69847	0.00000	0.00000	0.00000	1
2765	H	70.38218	78.05176	78.54657	0.00000	0.00000	0.00000	1
2766	H	73.22578	77.49358	77.44990	0.00000	0.00000	0.00000	1
2767	H	72.30201	76.32160	78.46654	0.00000	0.00000	0.00000	1
2768	H	72.74571	77.94141	79.12878	0.00000	0.00000	0.00000	1
2769	H	72.20223	79.88940	77.59383	0.00000	0.00000	0.00000	1
2770	H	70.42783	80.05755	77.32822	0.00000	0.00000	0.00000	1
2771	H	71.46632	79.38664	76.02511	0.00000	0.00000	0.00000	1
2772	N	68.31485	76.46489	74.31160	0.00000	0.00000	0.00000	1
2773	C	67.77197	75.60424	73.27714	0.00000	0.00000	0.00000	1
2774	C	68.84035	75.45993	72.00717	0.00000	0.00000	0.00000	1
2775	O	68.57081	74.71708	71.09290	0.00000	0.00000	0.00000	1
2776	C	66.50824	76.20334	72.66501	0.00000	0.00000	0.00000	1
2777	C	65.33158	76.11835	73.61694	0.00000	0.00000	0.00000	1
2778	C	66.71222	77.63147	72.20114	0.00000	0.00000	0.00000	1
2779	H	68.59670	77.43224	74.17246	0.00000	0.00000	0.00000	1
2780	H	67.59074	74.64592	73.82387	0.00000	0.00000	0.00000	1
2781	H	66.25863	75.58977	71.76946	0.00000	0.00000	0.00000	1
2782	H	65.11235	75.05385	73.91194	0.00000	0.00000	0.00000	1
2783	H	65.53097	76.69086	74.56595	0.00000	0.00000	0.00000	1
2784	H	64.39315	76.54029	73.15933	0.00000	0.00000	0.00000	1
2785	H	65.82307	78.01484	71.62650	0.00000	0.00000	0.00000	1
2786	H	66.87218	78.32798	73.07090	0.00000	0.00000	0.00000	1
2787	H	67.61241	77.72317	71.53018	0.00000	0.00000	0.00000	1
2788	N	69.88797	76.25933	72.13039	0.00000	0.00000	0.00000	1
2789	C	70.86839	76.23776	71.10321	0.00000	0.00000	0.00000	1
2790	C	72.35340	75.89469	71.70667	0.00000	0.00000	0.00000	1
2791	O	73.30010	75.89840	70.95289	0.00000	0.00000	0.00000	1
2792	C	70.99878	77.71081	70.51418	0.00000	0.00000	0.00000	1
2793	C	71.57927	77.57386	69.07701	0.00000	0.00000	0.00000	1
2794	C	70.42572	76.89095	68.20205	0.00000	0.00000	0.00000	1
2795	N	70.79229	77.15654	66.87763	0.00000	0.00000	0.00000	1
2796	C	70.06056	76.91294	65.86671	0.00000	0.00000	0.00000	1
2797	N	68.80874	76.33015	66.09596	0.00000	0.00000	0.00000	1
2798	N	70.69269	77.30382	64.67768	0.00000	0.00000	0.00000	1
2799	H	69.93272	76.83740	72.96597	0.00000	0.00000	0.00000	1
2800	H	70.48585	75.48722	70.37016	0.00000	0.00000	0.00000	1
2801	H	70.01521	78.23174	70.50432	0.00000	0.00000	0.00000	1
2802	H	71.66507	78.33086	71.15620	0.00000	0.00000	0.00000	1
2803	H	71.86662	78.56564	68.66202	0.00000	0.00000	0.00000	1

2804	H	72.51091	76.95816	69.08724	0.00000	0.00000	0.00000	1
2805	H	70.33396	75.78084	68.31477	0.00000	0.00000	0.00000	1
2806	H	69.40406	77.32671	68.32861	0.00000	0.00000	0.00000	1
2807	H	71.70036	77.56837	66.73096	0.00000	0.00000	0.00000	1
2808	H	68.37452	76.04969	66.97432	0.00000	0.00000	0.00000	1
2809	H	68.13438	76.09294	65.36802	0.00000	0.00000	0.00000	1
2810	H	71.61393	77.70609	64.51230	0.00000	0.00000	0.00000	1
2811	H	70.27523	77.17942	63.75471	0.00000	0.00000	0.00000	1
2812	N	72.32377	75.70265	73.01888	0.00000	0.00000	0.00000	1
2813	C	73.50779	75.32195	73.70342	0.00000	0.00000	0.00000	1
2814	C	73.15860	73.94312	74.49215	0.00000	0.00000	0.00000	1
2815	O	72.51445	73.06830	73.95577	0.00000	0.00000	0.00000	1
2816	C	73.94531	76.50087	74.69439	0.00000	0.00000	0.00000	1
2817	C	74.09963	77.83212	73.93881	0.00000	0.00000	0.00000	1
2818	C	74.65565	77.87203	72.62457	0.00000	0.00000	0.00000	1
2819	C	73.71301	79.04862	74.57699	0.00000	0.00000	0.00000	1
2820	C	74.77529	79.09766	71.96596	0.00000	0.00000	0.00000	1
2821	C	73.85803	80.25217	73.88575	0.00000	0.00000	0.00000	1
2822	C	74.38165	80.33049	72.56261	0.00000	0.00000	0.00000	1
2823	O	74.49659	81.57950	71.89827	0.00000	0.00000	0.00000	1
2824	H	71.41444	75.70339	73.47821	0.00000	0.00000	0.00000	1
2825	H	74.22773	75.18062	72.86409	0.00000	0.00000	0.00000	1
2826	H	73.20302	76.61563	75.51594	0.00000	0.00000	0.00000	1
2827	H	74.91010	76.24136	75.18799	0.00000	0.00000	0.00000	1
2828	H	74.96798	76.93965	72.11755	0.00000	0.00000	0.00000	1
2829	H	73.31499	79.03912	75.60652	0.00000	0.00000	0.00000	1
2830	H	75.19118	79.10028	70.94312	0.00000	0.00000	0.00000	1
2831	H	73.55713	81.18873	74.38643	0.00000	0.00000	0.00000	1
2832	H	74.90981	81.28160	71.05342	0.00000	0.00000	0.00000	1
2833	N	73.82569	73.87072	75.64864	0.00000	0.00000	0.00000	1
2834	C	73.45156	72.82605	76.55326	0.00000	0.00000	0.00000	1
2835	C	72.32431	73.37079	77.59010	0.00000	0.00000	0.00000	1
2836	O	71.67307	74.37702	77.41054	0.00000	0.00000	0.00000	1
2837	C	74.78242	72.30468	77.26401	0.00000	0.00000	0.00000	1
2838	O	74.58270	71.14634	78.14682	0.00000	0.00000	0.00000	1
2839	C	75.41211	73.56465	77.94454	0.00000	0.00000	0.00000	1
2840	H	74.27259	74.72186	75.98143	0.00000	0.00000	0.00000	1
2841	H	73.00926	72.07245	75.85755	0.00000	0.00000	0.00000	1
2842	H	75.50151	71.95772	76.47664	0.00000	0.00000	0.00000	1
2843	H	75.19319	70.51713	77.72847	0.00000	0.00000	0.00000	1
2844	H	76.35025	73.30523	78.49074	0.00000	0.00000	0.00000	1
2845	H	74.71330	74.02856	78.68282	0.00000	0.00000	0.00000	1
2846	H	75.67419	74.35368	77.20208	0.00000	0.00000	0.00000	1
2847	N	72.18446	72.46043	78.54708	0.00000	0.00000	0.00000	1
2848	C	71.27333	72.73454	79.60046	0.00000	0.00000	0.00000	1
2849	C	72.05025	73.39715	80.88239	0.00000	0.00000	0.00000	1
2850	O	71.41350	73.84947	81.80654	0.00000	0.00000	0.00000	1
2851	C	70.76507	71.35382	80.20619	0.00000	0.00000	0.00000	1
2852	C	69.89044	70.55166	79.19278	0.00000	0.00000	0.00000	1
2853	C	68.37986	71.00225	79.32110	0.00000	0.00000	0.00000	1
2854	C	68.14372	72.31029	78.53081	0.00000	0.00000	0.00000	1
2855	N	66.60231	72.58238	78.54142	0.00000	0.00000	0.00000	1
2856	H	72.81511	71.64647	78.58427	0.00000	0.00000	0.00000	1
2857	H	70.50142	73.41061	79.16700	0.00000	0.00000	0.00000	1
2858	H	71.65045	70.74333	80.49405	0.00000	0.00000	0.00000	1
2859	H	70.20026	71.52962	81.14871	0.00000	0.00000	0.00000	1
2860	H	70.26536	70.68232	78.15264	0.00000	0.00000	0.00000	1
2861	H	69.97119	69.46297	79.41244	0.00000	0.00000	0.00000	1
2862	H	67.70900	70.20370	78.92923	0.00000	0.00000	0.00000	1
2863	H	68.09626	71.12861	80.39139	0.00000	0.00000	0.00000	1
2864	H	68.58622	73.22220	78.97805	0.00000	0.00000	0.00000	1
2865	H	68.40368	72.25153	77.45466	0.00000	0.00000	0.00000	1

2866	H	65.95750	71.77677	78.29195	0.00000	0.00000	0.00000	1
2867	H	66.28607	73.32719	77.85602	0.00000	0.00000	0.00000	1
2868	H	66.17636	72.93621	79.44694	0.00000	0.00000	0.00000	1
2869	N	73.36608	73.18348	80.81489	0.00000	0.00000	0.00000	1
2870	C	74.19380	73.98650	81.66593	0.00000	0.00000	0.00000	1
2871	C	74.56233	75.36632	80.88765	0.00000	0.00000	0.00000	1
2872	O	73.96321	75.78059	79.92492	0.00000	0.00000	0.00000	1
2873	C	75.49055	73.13412	81.99430	0.00000	0.00000	0.00000	1
2874	C	75.71245	73.14648	83.54125	0.00000	0.00000	0.00000	1
2875	C	74.95608	71.91657	84.18655	0.00000	0.00000	0.00000	1
2876	C	73.42328	72.07687	84.06213	0.00000	0.00000	0.00000	1
2877	N	72.77751	70.81180	84.72246	0.00000	0.00000	0.00000	1
2878	H	73.71470	72.78610	79.94331	0.00000	0.00000	0.00000	1
2879	H	73.52735	74.17103	82.54094	0.00000	0.00000	0.00000	1
2880	H	75.39155	72.09220	81.61630	0.00000	0.00000	0.00000	1
2881	H	76.37471	73.56256	81.47005	0.00000	0.00000	0.00000	1
2882	H	76.79934	73.07796	83.77073	0.00000	0.00000	0.00000	1
2883	H	75.36812	74.10547	83.98958	0.00000	0.00000	0.00000	1
2884	H	75.28335	70.96713	83.70433	0.00000	0.00000	0.00000	1
2885	H	75.23633	71.81595	85.26032	0.00000	0.00000	0.00000	1
2886	H	72.99987	72.93269	84.62499	0.00000	0.00000	0.00000	1
2887	H	73.03445	72.07720	83.02328	0.00000	0.00000	0.00000	1
2888	H	73.03453	70.60717	85.73195	0.00000	0.00000	0.00000	1
2889	H	72.96069	69.87591	84.25633	0.00000	0.00000	0.00000	1
2890	H	71.71831	70.81501	84.77464	0.00000	0.00000	0.00000	1
2891	N	75.53957	75.97654	81.56518	0.00000	0.00000	0.00000	1
2892	C	76.11022	77.24991	81.08850	0.00000	0.00000	0.00000	1
2893	C	76.85469	76.95246	79.65505	0.00000	0.00000	0.00000	1
2894	O	77.61729	76.00951	79.53347	0.00000	0.00000	0.00000	1
2895	C	77.11274	77.70729	82.13204	0.00000	0.00000	0.00000	1
2896	C	77.88251	78.93365	81.67642	0.00000	0.00000	0.00000	1
2897	C	76.44997	77.97822	83.47051	0.00000	0.00000	0.00000	1
2898	H	75.93126	75.45453	82.34666	0.00000	0.00000	0.00000	1
2899	H	75.22232	77.91506	80.98246	0.00000	0.00000	0.00000	1
2900	H	77.84862	76.88406	82.27665	0.00000	0.00000	0.00000	1
2901	H	78.70223	79.20089	82.40250	0.00000	0.00000	0.00000	1
2902	H	78.37872	78.76428	80.67687	0.00000	0.00000	0.00000	1
2903	H	77.21686	79.83498	81.57662	0.00000	0.00000	0.00000	1
2904	H	75.93002	77.06402	83.86904	0.00000	0.00000	0.00000	1
2905	H	77.19524	78.30517	84.24671	0.00000	0.00000	0.00000	1
2906	H	75.67453	78.78893	83.39062	0.00000	0.00000	0.00000	1
2907	N	76.55921	77.89982	78.76308	0.00000	0.00000	0.00000	1
2908	C	77.12438	77.86262	77.44381	0.00000	0.00000	0.00000	1
2909	C	78.68209	78.36829	77.57556	0.00000	0.00000	0.00000	1
2910	O	79.01967	79.48825	77.28943	0.00000	0.00000	0.00000	1
2911	C	76.19693	78.84959	76.62612	0.00000	0.00000	0.00000	1
2912	C	75.82509	79.90881	77.71230	0.00000	0.00000	0.00000	1
2913	C	75.62410	78.99265	78.99417	0.00000	0.00000	0.00000	1
2914	H	77.06362	76.78980	77.15712	0.00000	0.00000	0.00000	1
2915	H	76.70785	79.29102	75.74023	0.00000	0.00000	0.00000	1
2916	H	75.29175	78.32840	76.24399	0.00000	0.00000	0.00000	1
2917	H	76.66056	80.62963	77.85985	0.00000	0.00000	0.00000	1
2918	H	74.92403	80.51124	77.45747	0.00000	0.00000	0.00000	1
2919	H	75.87179	79.47913	79.96598	0.00000	0.00000	0.00000	1
2920	H	74.62131	78.51236	79.06711	0.00000	0.00000	0.00000	1
2921	N	79.39461	77.36081	78.06637	0.00000	0.00000	0.00000	1
2922	C	80.81330	77.50703	78.09633	0.00000	0.00000	0.00000	1
2923	C	81.39750	76.94557	76.67942	0.00000	0.00000	0.00000	1
2924	O	80.72143	76.85312	75.68294	0.00000	0.00000	0.00000	1
2925	C	81.31707	76.65606	79.33805	0.00000	0.00000	0.00000	1
2926	C	82.43215	77.43577	80.09878	0.00000	0.00000	0.00000	1
2927	C	81.69896	78.38479	81.12453	0.00000	0.00000	0.00000	1

2928	O	80.51608	78.31141	81.34930	0.00000	0.00000	0.00000	1
2929	N	82.58489	79.21630	81.70975	0.00000	0.00000	0.00000	1
2930	H	78.92632	76.48186	78.36976	0.00000	0.00000	0.00000	1
2931	H	80.92817	78.61252	78.19352	0.00000	0.00000	0.00000	1
2932	H	80.46834	76.44409	80.03172	0.00000	0.00000	0.00000	1
2933	H	81.69149	75.66414	78.99700	0.00000	0.00000	0.00000	1
2934	H	83.10854	76.73566	80.63680	0.00000	0.00000	0.00000	1
2935	H	83.09674	78.00703	79.41407	0.00000	0.00000	0.00000	1
2936	H	83.59943	79.26767	81.55805	0.00000	0.00000	0.00000	1
2937	H	82.35863	79.89218	82.44718	0.00000	0.00000	0.00000	1
2938	N	82.69631	76.65881	76.80600	0.00000	0.00000	0.00000	1
2939	C	83.51500	76.28367	75.65000	0.00000	0.00000	0.00000	1
2940	C	83.20501	74.72193	75.18156	0.00000	0.00000	0.00000	1
2941	O	83.74743	74.28718	74.19312	0.00000	0.00000	0.00000	1
2942	C	84.99180	76.31288	75.98872	0.00000	0.00000	0.00000	1
2943	C	85.54345	77.72477	76.05723	0.00000	0.00000	0.00000	1
2944	C	85.30905	75.56488	77.27033	0.00000	0.00000	0.00000	1
2945	H	83.09294	76.84126	77.72466	0.00000	0.00000	0.00000	1
2946	H	83.20907	77.00772	74.85777	0.00000	0.00000	0.00000	1
2947	H	85.51957	75.79126	75.15559	0.00000	0.00000	0.00000	1
2948	H	85.03161	78.32955	76.85588	0.00000	0.00000	0.00000	1
2949	H	86.64500	77.72804	76.28791	0.00000	0.00000	0.00000	1
2950	H	85.40423	78.27234	75.08395	0.00000	0.00000	0.00000	1
2951	H	84.73704	74.59754	77.33282	0.00000	0.00000	0.00000	1
2952	H	86.40317	75.31414	77.34622	0.00000	0.00000	0.00000	1
2953	H	85.04285	76.16811	78.18155	0.00000	0.00000	0.00000	1
2954	N	82.45451	74.06507	76.05951	0.00000	0.00000	0.00000	1
2955	C	81.87671	72.84059	75.63369	0.00000	0.00000	0.00000	1
2956	C	80.25170	73.02909	75.70035	0.00000	0.00000	0.00000	1
2957	O	79.69109	73.32055	76.72829	0.00000	0.00000	0.00000	1
2958	C	82.33361	71.78422	76.74881	0.00000	0.00000	0.00000	1
2959	O	81.91883	70.41492	76.53221	0.00000	0.00000	0.00000	1
2960	H	82.07615	74.62763	76.81932	0.00000	0.00000	0.00000	1
2961	H	82.28604	72.63521	74.61659	0.00000	0.00000	0.00000	1
2962	H	83.44222	71.89586	76.87228	0.00000	0.00000	0.00000	1
2963	H	81.87415	72.14168	77.71078	0.00000	0.00000	0.00000	1
2964	H	82.71997	70.06590	76.09998	0.00000	0.00000	0.00000	1
2965	N	79.74666	72.81683	74.49790	0.00000	0.00000	0.00000	1
2966	C	78.33104	72.84603	74.29850	0.00000	0.00000	0.00000	1
2967	C	78.21228	71.99898	72.93588	0.00000	0.00000	0.00000	1
2968	O	79.23666	71.71398	72.34574	0.00000	0.00000	0.00000	1
2969	C	77.82597	74.36950	74.07634	0.00000	0.00000	0.00000	1
2970	O	78.40336	75.08102	72.97737	0.00000	0.00000	0.00000	1
2971	C	78.00921	75.00401	75.50089	0.00000	0.00000	0.00000	1
2972	H	80.28928	72.54942	73.65619	0.00000	0.00000	0.00000	1
2973	H	77.87042	72.39215	75.20550	0.00000	0.00000	0.00000	1
2974	H	76.72324	74.32857	73.84875	0.00000	0.00000	0.00000	1
2975	H	77.62599	75.19269	72.38972	0.00000	0.00000	0.00000	1
2976	H	79.08258	75.26273	75.69026	0.00000	0.00000	0.00000	1
2977	H	77.68269	74.31240	76.31584	0.00000	0.00000	0.00000	1
2978	H	77.42284	75.94667	75.60081	0.00000	0.00000	0.00000	1
2979	N	76.94700	71.69166	72.63822	0.00000	0.00000	0.00000	1
2980	C	76.60958	71.08354	71.38414	0.00000	0.00000	0.00000	1
2981	C	76.52285	72.23939	70.22388	0.00000	0.00000	0.00000	1
2982	O	75.93312	73.27837	70.39170	0.00000	0.00000	0.00000	1
2983	C	75.15205	70.52346	71.65534	0.00000	0.00000	0.00000	1
2984	C	74.58946	71.58622	72.64960	0.00000	0.00000	0.00000	1
2985	C	75.85018	71.79729	73.59244	0.00000	0.00000	0.00000	1
2986	H	77.39224	70.32169	71.16783	0.00000	0.00000	0.00000	1
2987	H	74.54684	70.43040	70.72525	0.00000	0.00000	0.00000	1
2988	H	75.18173	69.51180	72.11803	0.00000	0.00000	0.00000	1
2989	H	74.31860	72.52916	72.12030	0.00000	0.00000	0.00000	1

2990	H	73.67905	71.25264	73.19956	0.00000	0.00000	0.00000	1
2991	H	75.89378	72.78049	74.11545	0.00000	0.00000	0.00000	1
2992	H	76.01550	70.98149	74.33568	0.00000	0.00000	0.00000	1
2993	N	77.10613	71.77180	69.12788	0.00000	0.00000	0.00000	1
2994	C	76.97453	72.48477	67.91192	0.00000	0.00000	0.00000	1
2995	C	75.81564	71.72190	67.03251	0.00000	0.00000	0.00000	1
2996	O	76.07199	70.97786	66.11617	0.00000	0.00000	0.00000	1
2997	C	78.40813	72.40163	67.18383	0.00000	0.00000	0.00000	1
2998	O	79.00319	71.09798	67.09820	0.00000	0.00000	0.00000	1
2999	C	79.19702	73.46780	68.02667	0.00000	0.00000	0.00000	1
3000	H	77.55973	70.85909	69.11384	0.00000	0.00000	0.00000	1
3001	H	76.65627	73.50294	68.23457	0.00000	0.00000	0.00000	1
3002	H	78.28365	72.77640	66.13175	0.00000	0.00000	0.00000	1
3003	H	78.87580	70.89158	66.14931	0.00000	0.00000	0.00000	1
3004	H	78.70133	74.46647	68.00715	0.00000	0.00000	0.00000	1
3005	H	80.23683	73.60264	67.64833	0.00000	0.00000	0.00000	1
3006	H	79.27129	73.15465	69.09552	0.00000	0.00000	0.00000	1
3007	N	74.61615	71.99640	67.54608	0.00000	0.00000	0.00000	1
3008	C	73.52815	72.12660	66.39365	0.00000	0.00000	0.00000	1
3009	C	73.74474	73.22929	65.47880	0.00000	0.00000	0.00000	1
3010	O	73.92188	74.12854	64.73131	0.00000	0.00000	0.00000	1
3011	C	72.11894	72.31699	67.21780	0.00000	0.00000	0.00000	1
3012	C	70.98666	71.97195	66.31186	0.00000	0.00000	0.00000	1
3013	C	70.73352	70.46783	66.30758	0.00000	0.00000	0.00000	1
3014	C	69.71797	72.70137	66.74419	0.00000	0.00000	0.00000	1
3015	H	74.65529	72.69274	68.28642	0.00000	0.00000	0.00000	1
3016	H	73.66827	71.12196	65.92203	0.00000	0.00000	0.00000	1
3017	H	72.11589	71.68499	68.13418	0.00000	0.00000	0.00000	1
3018	H	72.04206	73.36899	67.57478	0.00000	0.00000	0.00000	1
3019	H	71.24010	72.29948	65.27682	0.00000	0.00000	0.00000	1
3020	H	70.42661	70.09964	67.31980	0.00000	0.00000	0.00000	1
3021	H	71.64818	69.89354	66.01137	0.00000	0.00000	0.00000	1
3022	H	69.91851	70.18630	65.59313	0.00000	0.00000	0.00000	1
3023	H	68.84337	72.42735	66.10101	0.00000	0.00000	0.00000	1
3024	H	69.83933	73.81375	66.68246	0.00000	0.00000	0.00000	1
3025	H	69.44208	72.45631	67.80170	0.00000	0.00000	0.00000	1
3026		273						
3027		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	5.5500 22200
		0.2500	300.00	0.00	0.00	0.00	-1291.4707	0.0000 0.0000
3028	N	68.28674	77.46674	77.67093	0.00000	0.00000	0.00000	1
3029	C	68.90259	77.45802	76.45629	0.00000	0.00000	0.00000	1
3030	C	68.26919	76.13234	75.58950	0.00000	0.00000	0.00000	1
3031	O	67.96150	75.08236	76.09826	0.00000	0.00000	0.00000	1
3032	C	70.50762	77.08260	76.66746	0.00000	0.00000	0.00000	1
3033	C	71.08846	77.99003	77.68443	0.00000	0.00000	0.00000	1
3034	C	72.40373	77.41146	78.20282	0.00000	0.00000	0.00000	1
3035	C	71.30911	79.39542	77.13277	0.00000	0.00000	0.00000	1
3036	H	68.28276	76.58146	78.14358	0.00000	0.00000	0.00000	1
3037	H	68.73069	78.46955	76.00592	0.00000	0.00000	0.00000	1
3038	H	70.61567	76.01127	76.99810	0.00000	0.00000	0.00000	1
3039	H	71.04751	77.15567	75.69792	0.00000	0.00000	0.00000	1
3040	H	70.38269	78.05075	78.54654	0.00000	0.00000	0.00000	1
3041	H	73.22605	77.49362	77.44886	0.00000	0.00000	0.00000	1
3042	H	72.30263	76.32045	78.46455	0.00000	0.00000	0.00000	1
3043	H	72.74612	77.93981	79.12820	0.00000	0.00000	0.00000	1
3044	H	72.20093	79.88973	77.59516	0.00000	0.00000	0.00000	1
3045	H	70.42675	80.05633	77.32702	0.00000	0.00000	0.00000	1
3046	H	71.46767	79.38637	76.02538	0.00000	0.00000	0.00000	1
3047	N	68.31485	76.46464	74.31161	0.00000	0.00000	0.00000	1
3048	C	67.77189	75.60418	73.27703	0.00000	0.00000	0.00000	1
3049	C	68.84020	75.46010	72.00698	0.00000	0.00000	0.00000	1
3050	O	68.57043	74.71774	71.09238	0.00000	0.00000	0.00000	1

3051	C	66.50808	76.20341	72.66519	0.00000	0.00000	0.00000	1
3052	C	65.33164	76.11861	73.61741	0.00000	0.00000	0.00000	1
3053	C	66.71215	77.63150	72.20123	0.00000	0.00000	0.00000	1
3054	H	68.59675	77.43199	74.17256	0.00000	0.00000	0.00000	1
3055	H	67.59070	74.64576	73.82361	0.00000	0.00000	0.00000	1
3056	H	66.25817	75.58985	71.76971	0.00000	0.00000	0.00000	1
3057	H	65.11234	75.05416	73.91252	0.00000	0.00000	0.00000	1
3058	H	65.53132	76.69116	74.56634	0.00000	0.00000	0.00000	1
3059	H	64.39314	76.54064	73.16000	0.00000	0.00000	0.00000	1
3060	H	65.82287	78.01502	71.62688	0.00000	0.00000	0.00000	1
3061	H	66.87252	78.32799	73.07093	0.00000	0.00000	0.00000	1
3062	H	67.61214	77.72302	71.52998	0.00000	0.00000	0.00000	1
3063	N	69.88813	76.25901	72.13064	0.00000	0.00000	0.00000	1
3064	C	70.86845	76.23764	71.10333	0.00000	0.00000	0.00000	1
3065	C	72.35353	75.89478	71.70673	0.00000	0.00000	0.00000	1
3066	O	73.30026	75.89869	70.95288	0.00000	0.00000	0.00000	1
3067	C	70.99856	77.71075	70.51435	0.00000	0.00000	0.00000	1
3068	C	71.57908	77.57400	69.07718	0.00000	0.00000	0.00000	1
3069	C	70.42578	76.89072	68.20210	0.00000	0.00000	0.00000	1
3070	N	70.79233	77.15603	66.87751	0.00000	0.00000	0.00000	1
3071	C	70.06095	76.91248	65.86688	0.00000	0.00000	0.00000	1
3072	N	68.80931	76.33001	66.09594	0.00000	0.00000	0.00000	1
3073	N	70.69299	77.30293	64.67810	0.00000	0.00000	0.00000	1
3074	H	69.93305	76.83671	72.96645	0.00000	0.00000	0.00000	1
3075	H	70.48602	75.48710	70.37028	0.00000	0.00000	0.00000	1
3076	H	70.01487	78.23143	70.50452	0.00000	0.00000	0.00000	1
3077	H	71.66471	78.33093	71.15639	0.00000	0.00000	0.00000	1
3078	H	71.86609	78.56587	68.66220	0.00000	0.00000	0.00000	1
3079	H	72.51085	76.95872	69.08723	0.00000	0.00000	0.00000	1
3080	H	70.33423	75.78062	68.31510	0.00000	0.00000	0.00000	1
3081	H	69.40402	77.32630	68.32850	0.00000	0.00000	0.00000	1
3082	H	71.70059	77.56773	66.73109	0.00000	0.00000	0.00000	1
3083	H	68.37461	76.04957	66.97435	0.00000	0.00000	0.00000	1
3084	H	68.13465	76.09262	65.36804	0.00000	0.00000	0.00000	1
3085	H	71.61448	77.70514	64.51240	0.00000	0.00000	0.00000	1
3086	H	70.27578	77.17854	63.75479	0.00000	0.00000	0.00000	1
3087	N	72.32394	75.70228	73.01891	0.00000	0.00000	0.00000	1
3088	C	73.50807	75.32167	73.70335	0.00000	0.00000	0.00000	1
3089	C	73.15884	73.94300	74.49235	0.00000	0.00000	0.00000	1
3090	O	72.51467	73.06802	73.95615	0.00000	0.00000	0.00000	1
3091	C	73.94556	76.50059	74.69436	0.00000	0.00000	0.00000	1
3092	C	74.09983	77.83191	73.93890	0.00000	0.00000	0.00000	1
3093	C	74.65592	77.87202	72.62470	0.00000	0.00000	0.00000	1
3094	C	73.71306	79.04827	74.57724	0.00000	0.00000	0.00000	1
3095	C	74.77538	79.09776	71.96624	0.00000	0.00000	0.00000	1
3096	C	73.85788	80.25193	73.88612	0.00000	0.00000	0.00000	1
3097	C	74.38149	80.33046	72.56299	0.00000	0.00000	0.00000	1
3098	O	74.49621	81.57955	71.89879	0.00000	0.00000	0.00000	1
3099	H	71.41464	75.70265	73.47820	0.00000	0.00000	0.00000	1
3100	H	74.22798	75.18032	72.86402	0.00000	0.00000	0.00000	1
3101	H	73.20324	76.61525	75.51589	0.00000	0.00000	0.00000	1
3102	H	74.91035	76.24105	75.18795	0.00000	0.00000	0.00000	1
3103	H	74.96864	76.93989	72.11776	0.00000	0.00000	0.00000	1
3104	H	73.31510	79.03860	75.60678	0.00000	0.00000	0.00000	1
3105	H	75.19133	79.10056	70.94342	0.00000	0.00000	0.00000	1
3106	H	73.55682	81.18838	74.38690	0.00000	0.00000	0.00000	1
3107	H	74.90946	81.28181	71.05389	0.00000	0.00000	0.00000	1
3108	N	73.82583	73.87095	75.64891	0.00000	0.00000	0.00000	1
3109	C	73.45183	72.82633	76.55363	0.00000	0.00000	0.00000	1
3110	C	72.32456	73.37097	77.59047	0.00000	0.00000	0.00000	1
3111	O	71.67339	74.37730	77.41107	0.00000	0.00000	0.00000	1
3112	C	74.78282	72.30527	77.26441	0.00000	0.00000	0.00000	1

3113	O	74.58327	71.14698	78.14719	0.00000	0.00000	0.00000	1
3114	C	75.41216	73.56545	77.94491	0.00000	0.00000	0.00000	1
3115	H	74.27271	74.72217	75.98155	0.00000	0.00000	0.00000	1
3116	H	73.00964	72.07261	75.85797	0.00000	0.00000	0.00000	1
3117	H	75.50202	71.95854	76.47704	0.00000	0.00000	0.00000	1
3118	H	75.19370	70.51775	77.72872	0.00000	0.00000	0.00000	1
3119	H	76.35029	73.30630	78.49125	0.00000	0.00000	0.00000	1
3120	H	74.71316	74.02927	78.68305	0.00000	0.00000	0.00000	1
3121	H	75.67417	74.35446	77.20241	0.00000	0.00000	0.00000	1
3122	N	72.18457	72.46049	78.54730	0.00000	0.00000	0.00000	1
3123	C	71.27336	72.73461	79.60061	0.00000	0.00000	0.00000	1
3124	C	72.05034	73.39691	80.88265	0.00000	0.00000	0.00000	1
3125	O	71.41366	73.84891	81.80701	0.00000	0.00000	0.00000	1
3126	C	70.76469	71.35398	80.20620	0.00000	0.00000	0.00000	1
3127	C	69.89036	70.55182	79.19253	0.00000	0.00000	0.00000	1
3128	C	68.37973	71.00236	79.32037	0.00000	0.00000	0.00000	1
3129	C	68.14384	72.31062	78.53036	0.00000	0.00000	0.00000	1
3130	N	66.60249	72.58303	78.54104	0.00000	0.00000	0.00000	1
3131	H	72.81523	71.64654	78.58446	0.00000	0.00000	0.00000	1
3132	H	70.50166	73.41091	79.16712	0.00000	0.00000	0.00000	1
3133	H	71.64990	70.74341	80.49444	0.00000	0.00000	0.00000	1
3134	H	70.19955	71.52990	81.14850	0.00000	0.00000	0.00000	1
3135	H	70.26560	70.68249	78.15250	0.00000	0.00000	0.00000	1
3136	H	69.97107	69.46313	79.41221	0.00000	0.00000	0.00000	1
3137	H	67.70903	70.20391	78.92804	0.00000	0.00000	0.00000	1
3138	H	68.09571	71.12843	80.39058	0.00000	0.00000	0.00000	1
3139	H	68.58651	73.22232	78.97783	0.00000	0.00000	0.00000	1
3140	H	68.40381	72.25207	77.45419	0.00000	0.00000	0.00000	1
3141	H	65.95757	71.77794	78.29019	0.00000	0.00000	0.00000	1
3142	H	66.28659	73.32894	77.85669	0.00000	0.00000	0.00000	1
3143	H	66.17640	72.93558	79.44700	0.00000	0.00000	0.00000	1
3144	N	73.36619	73.18343	80.81491	0.00000	0.00000	0.00000	1
3145	C	74.19393	73.98645	81.66594	0.00000	0.00000	0.00000	1
3146	C	74.56208	75.36647	80.88783	0.00000	0.00000	0.00000	1
3147	O	73.96257	75.78098	79.92544	0.00000	0.00000	0.00000	1
3148	C	75.49080	73.13415	81.99402	0.00000	0.00000	0.00000	1
3149	C	75.71287	73.14635	83.54094	0.00000	0.00000	0.00000	1
3150	C	74.95625	71.91662	84.18628	0.00000	0.00000	0.00000	1
3151	C	73.42348	72.07707	84.06164	0.00000	0.00000	0.00000	1
3152	N	72.77743	70.81217	84.72203	0.00000	0.00000	0.00000	1
3153	H	73.71477	72.78630	79.94320	0.00000	0.00000	0.00000	1
3154	H	73.52757	74.17077	82.54106	0.00000	0.00000	0.00000	1
3155	H	75.39184	72.09227	81.61590	0.00000	0.00000	0.00000	1
3156	H	76.37486	73.56273	81.46970	0.00000	0.00000	0.00000	1
3157	H	76.79977	73.07752	83.77030	0.00000	0.00000	0.00000	1
3158	H	75.36885	74.10540	83.98935	0.00000	0.00000	0.00000	1
3159	H	75.28345	70.96708	83.70421	0.00000	0.00000	0.00000	1
3160	H	75.23634	71.81607	85.26009	0.00000	0.00000	0.00000	1
3161	H	73.00008	72.93302	84.62431	0.00000	0.00000	0.00000	1
3162	H	73.03478	72.07728	83.02274	0.00000	0.00000	0.00000	1
3163	H	73.03396	70.60784	85.73171	0.00000	0.00000	0.00000	1
3164	H	72.96085	69.87615	84.25625	0.00000	0.00000	0.00000	1
3165	H	71.71820	70.81539	84.77369	0.00000	0.00000	0.00000	1
3166	N	75.53946	75.97664	81.56524	0.00000	0.00000	0.00000	1
3167	C	76.11023	77.24986	81.08840	0.00000	0.00000	0.00000	1
3168	C	76.85451	76.95227	79.65485	0.00000	0.00000	0.00000	1
3169	O	77.61698	76.00916	79.53327	0.00000	0.00000	0.00000	1
3170	C	77.11291	77.70716	82.13179	0.00000	0.00000	0.00000	1
3171	C	77.88284	78.93339	81.67602	0.00000	0.00000	0.00000	1
3172	C	76.45034	77.97827	83.47032	0.00000	0.00000	0.00000	1
3173	H	75.93153	75.45435	82.34635	0.00000	0.00000	0.00000	1
3174	H	75.22240	77.91514	80.98239	0.00000	0.00000	0.00000	1

3175	H	77.84870	76.88383	82.27638	0.00000	0.00000	0.00000	1
3176	H	78.70256	79.20066	82.40211	0.00000	0.00000	0.00000	1
3177	H	78.37912	78.76382	80.67653	0.00000	0.00000	0.00000	1
3178	H	77.21727	79.83476	81.57608	0.00000	0.00000	0.00000	1
3179	H	75.93009	77.06424	83.86883	0.00000	0.00000	0.00000	1
3180	H	77.19579	78.30491	84.24648	0.00000	0.00000	0.00000	1
3181	H	75.67520	78.78926	83.39052	0.00000	0.00000	0.00000	1
3182	N	76.55916	77.89960	78.76277	0.00000	0.00000	0.00000	1
3183	C	77.12420	77.86249	77.44379	0.00000	0.00000	0.00000	1
3184	C	78.68192	78.36796	77.57540	0.00000	0.00000	0.00000	1
3185	O	79.01945	79.48799	77.28909	0.00000	0.00000	0.00000	1
3186	C	76.19689	78.84927	76.62604	0.00000	0.00000	0.00000	1
3187	C	75.82509	79.90862	77.71212	0.00000	0.00000	0.00000	1
3188	C	75.62414	78.99249	78.99403	0.00000	0.00000	0.00000	1
3189	H	77.06345	76.78956	77.15699	0.00000	0.00000	0.00000	1
3190	H	76.70769	79.29072	75.74003	0.00000	0.00000	0.00000	1
3191	H	75.29159	78.32818	76.24393	0.00000	0.00000	0.00000	1
3192	H	76.66059	80.62942	77.85961	0.00000	0.00000	0.00000	1
3193	H	74.92402	80.51109	77.45732	0.00000	0.00000	0.00000	1
3194	H	75.87194	79.47902	79.96581	0.00000	0.00000	0.00000	1
3195	H	74.62127	78.51235	79.06709	0.00000	0.00000	0.00000	1
3196	N	79.39455	77.36063	78.06637	0.00000	0.00000	0.00000	1
3197	C	80.81314	77.50687	78.09642	0.00000	0.00000	0.00000	1
3198	C	81.39747	76.94561	76.67952	0.00000	0.00000	0.00000	1
3199	O	80.72148	76.85329	75.68291	0.00000	0.00000	0.00000	1
3200	C	81.31699	76.65600	79.33808	0.00000	0.00000	0.00000	1
3201	C	82.43214	77.43557	80.09877	0.00000	0.00000	0.00000	1
3202	C	81.69914	78.38480	81.12444	0.00000	0.00000	0.00000	1
3203	O	80.51626	78.31134	81.34950	0.00000	0.00000	0.00000	1
3204	N	82.58508	79.21661	81.70923	0.00000	0.00000	0.00000	1
3205	H	78.92621	76.48168	78.36979	0.00000	0.00000	0.00000	1
3206	H	80.92806	78.61233	78.19369	0.00000	0.00000	0.00000	1
3207	H	80.46830	76.44401	80.03183	0.00000	0.00000	0.00000	1
3208	H	81.69133	75.66399	78.99706	0.00000	0.00000	0.00000	1
3209	H	83.10844	76.73541	80.63687	0.00000	0.00000	0.00000	1
3210	H	83.09686	78.00668	79.41404	0.00000	0.00000	0.00000	1
3211	H	83.59958	79.26814	81.55736	0.00000	0.00000	0.00000	1
3212	H	82.35881	79.89263	82.44653	0.00000	0.00000	0.00000	1
3213	N	82.69630	76.65877	76.80607	0.00000	0.00000	0.00000	1
3214	C	83.51501	76.28355	75.65024	0.00000	0.00000	0.00000	1
3215	C	83.20501	74.72184	75.18186	0.00000	0.00000	0.00000	1
3216	O	83.74749	74.28696	74.19350	0.00000	0.00000	0.00000	1
3217	C	84.99170	76.31308	75.98893	0.00000	0.00000	0.00000	1
3218	C	85.54302	77.72510	76.05762	0.00000	0.00000	0.00000	1
3219	C	85.30916	75.56503	77.27047	0.00000	0.00000	0.00000	1
3220	H	83.09282	76.84111	77.72484	0.00000	0.00000	0.00000	1
3221	H	83.20896	77.00752	74.85791	0.00000	0.00000	0.00000	1
3222	H	85.51972	75.79169	75.15579	0.00000	0.00000	0.00000	1
3223	H	85.03101	78.32966	76.85633	0.00000	0.00000	0.00000	1
3224	H	86.64458	77.72867	76.28830	0.00000	0.00000	0.00000	1
3225	H	85.40366	78.27275	75.08440	0.00000	0.00000	0.00000	1
3226	H	84.73833	74.59695	77.33228	0.00000	0.00000	0.00000	1
3227	H	86.40355	75.31564	77.34697	0.00000	0.00000	0.00000	1
3228	H	85.04164	76.16761	78.18175	0.00000	0.00000	0.00000	1
3229	N	82.45430	74.06506	76.05973	0.00000	0.00000	0.00000	1
3230	C	81.87631	72.84069	75.63379	0.00000	0.00000	0.00000	1
3231	C	80.25130	73.02928	75.70063	0.00000	0.00000	0.00000	1
3232	O	79.69075	73.32066	76.72866	0.00000	0.00000	0.00000	1
3233	C	82.33321	71.78414	76.74875	0.00000	0.00000	0.00000	1
3234	O	81.91828	70.41489	76.53202	0.00000	0.00000	0.00000	1
3235	H	82.07595	74.62768	76.81948	0.00000	0.00000	0.00000	1
3236	H	82.28550	72.63536	74.61666	0.00000	0.00000	0.00000	1

3237	H	83.44184	71.89566	76.87209	0.00000	0.00000	0.00000	1
3238	H	81.87389	72.14153	77.71081	0.00000	0.00000	0.00000	1
3239	H	82.71935	70.06587	76.09967	0.00000	0.00000	0.00000	1
3240	N	79.74623	72.81720	74.49816	0.00000	0.00000	0.00000	1
3241	C	78.33059	72.84613	74.29875	0.00000	0.00000	0.00000	1
3242	C	78.21198	71.99879	72.93629	0.00000	0.00000	0.00000	1
3243	O	79.23643	71.71359	72.34636	0.00000	0.00000	0.00000	1
3244	C	77.82529	74.36948	74.07615	0.00000	0.00000	0.00000	1
3245	O	78.40202	75.08045	72.97647	0.00000	0.00000	0.00000	1
3246	C	78.00952	75.00470	75.50023	0.00000	0.00000	0.00000	1
3247	H	80.28886	72.54966	73.65651	0.00000	0.00000	0.00000	1
3248	H	77.87004	72.39242	75.20586	0.00000	0.00000	0.00000	1
3249	H	76.72242	74.32838	73.84929	0.00000	0.00000	0.00000	1
3250	H	77.62438	75.19145	72.38905	0.00000	0.00000	0.00000	1
3251	H	79.08311	75.26294	75.68896	0.00000	0.00000	0.00000	1
3252	H	77.68297	74.31372	76.31572	0.00000	0.00000	0.00000	1
3253	H	77.42381	75.94780	75.59987	0.00000	0.00000	0.00000	1
3254	N	76.94674	71.69152	72.63846	0.00000	0.00000	0.00000	1
3255	C	76.60958	71.08337	71.38431	0.00000	0.00000	0.00000	1
3256	C	76.52281	72.23927	70.22409	0.00000	0.00000	0.00000	1
3257	O	75.93283	73.27812	70.39194	0.00000	0.00000	0.00000	1
3258	C	75.15205	70.52314	71.65527	0.00000	0.00000	0.00000	1
3259	C	74.58920	71.58587	72.64941	0.00000	0.00000	0.00000	1
3260	C	75.84973	71.79722	73.59243	0.00000	0.00000	0.00000	1
3261	H	77.39236	70.32164	71.16808	0.00000	0.00000	0.00000	1
3262	H	74.54701	70.42999	70.72508	0.00000	0.00000	0.00000	1
3263	H	75.18177	69.51150	72.11800	0.00000	0.00000	0.00000	1
3264	H	74.31827	72.52874	72.12002	0.00000	0.00000	0.00000	1
3265	H	73.67877	71.25216	73.19923	0.00000	0.00000	0.00000	1
3266	H	75.89316	72.78053	74.11527	0.00000	0.00000	0.00000	1
3267	H	76.01497	70.98159	74.33587	0.00000	0.00000	0.00000	1
3268	N	77.10638	71.77186	69.12816	0.00000	0.00000	0.00000	1
3269	C	76.97461	72.48473	67.91216	0.00000	0.00000	0.00000	1
3270	C	75.81552	71.72182	67.03294	0.00000	0.00000	0.00000	1
3271	O	76.07166	70.97769	66.11677	0.00000	0.00000	0.00000	1
3272	C	78.40807	72.40159	67.18386	0.00000	0.00000	0.00000	1
3273	O	79.00312	71.09793	67.09809	0.00000	0.00000	0.00000	1
3274	C	79.19710	73.46772	68.02665	0.00000	0.00000	0.00000	1
3275	H	77.56013	70.85921	69.11415	0.00000	0.00000	0.00000	1
3276	H	76.65639	73.50295	68.23472	0.00000	0.00000	0.00000	1
3277	H	78.28343	72.77641	66.13182	0.00000	0.00000	0.00000	1
3278	H	78.87549	70.89154	66.14923	0.00000	0.00000	0.00000	1
3279	H	78.70131	74.46634	68.00742	0.00000	0.00000	0.00000	1
3280	H	80.23679	73.60272	67.64803	0.00000	0.00000	0.00000	1
3281	H	79.27170	73.15441	69.09543	0.00000	0.00000	0.00000	1
3282	N	74.61617	71.99651	67.54676	0.00000	0.00000	0.00000	1
3283	C	73.52800	72.12722	66.39439	0.00000	0.00000	0.00000	1
3284	C	73.74513	73.23033	65.47964	0.00000	0.00000	0.00000	1
3285	O	73.92221	74.12913	64.73222	0.00000	0.00000	0.00000	1
3286	C	72.11894	72.31746	67.21818	0.00000	0.00000	0.00000	1
3287	C	70.98680	71.97250	66.31183	0.00000	0.00000	0.00000	1
3288	C	70.73362	70.46811	66.30747	0.00000	0.00000	0.00000	1
3289	C	69.71774	72.70182	66.74434	0.00000	0.00000	0.00000	1
3290	H	74.65541	72.69291	68.28684	0.00000	0.00000	0.00000	1
3291	H	73.66838	71.12261	65.92207	0.00000	0.00000	0.00000	1
3292	H	72.11574	71.68535	68.13440	0.00000	0.00000	0.00000	1
3293	H	72.04196	73.36936	67.57512	0.00000	0.00000	0.00000	1
3294	H	71.24026	72.30015	65.27701	0.00000	0.00000	0.00000	1
3295	H	70.42693	70.09992	67.31968	0.00000	0.00000	0.00000	1
3296	H	71.64829	69.89412	66.01099	0.00000	0.00000	0.00000	1
3297	H	69.91853	70.18689	65.59310	0.00000	0.00000	0.00000	1
3298	H	68.84342	72.42769	66.10096	0.00000	0.00000	0.00000	1

3299	H	69.83920	73.81411	66.68268	0.00000	0.00000	0.00000	1
3300	H	69.44194	72.45651	67.80173	0.00000	0.00000	0.00000	1

2 control - SCM's ReaxFF Input

Input file for the energy minimization within SCM's ReaxFF.

Listing 130: control emin

```

1 # General parameters
2     0 itrans      1: Translate atoms back into unit cell
3     1 icobo
4     1 icentr      0: off, 1: put center of mass at center of cube, 2: put com at
      origin
5     1 imetho      0: Normal MD-run 1: Energy minimisation 2:MD-energy minimisation
6     1 igeofo      0:xyz-input geometry 1: Biograf input geometry 2: xmol-input geometry
7 150.0 axis1      a cell axis
8 150.0 axis2      b cell axis
9 150.0 axis3      c cell axis
10 90.000 angle1    cell angle alpha
11 90.000 angle2    cell angle beta
12 90.000 angle3    cell angle gamma
13 0.0050 cutof2    B0-cutoff for valency angles and torsion angles
14 25 irecon        Frequency of reading control-file
15 1 ixmolo         0: only x,y,z-coordinates in xmolout  1: x,y,z + velocities + molnr.
      in xmolout
16 00001 ichupd     Charge update frequency
17 4 icharg         Charges. 1:EEM 2:- 3: Shielded EEM (default for crystals) 4: Full
      system EEM 5: Fixed (unit 26) 6: Fragment EEM
18 1 iappen        1: Append fort.7 and fort.8
19 # MD-parameters
20 0300.00 mdtemp    1st MD-temperature
21 000.25 tdamp1     1st Berendsen/Anderson temperature damping constant (fs)
22 0 nrstep
23 1 imdmet         MD-method. 1:Velocity Verlet+Berendsen 2:Hoover-Nose;3:NVE 4: NPT
24 0.250 tstep      MD-time step (fs)
25 0000.00 mdpres    MD-pressure (MPa)
26 00100.0 pdamp1    Berendsen pressure damping constant (fs)
27 0 inpt          0: Change all cell parameters in NPT-run  1: fixed x 2: fixed y 3:
      fixed z
28 0004000 nmdit     Number of MD-iterations
29 000000 nmdeqi     Number of MD-equilibrium iterations
30 100 iout1         Output to unit 71 and unit 73
31 1000 iout2        Save coordinates (xmolout)
32 1 iout3          0: create moldyn.xxxx-files 1: do not create moldyn.xxxx-files
33 0 ivels          1:Set vels and accels from moldyn.vel to zero
34 001000 iout6      Save velocity file (restart-files)
35 50 iout7         Frequency of reaxout.kf writing
36 500000 irten      Frequency of removal of rotational and translational energy
37 0 npreit         Nr. of iterations in previous runs
38 0.00 range        Range for back-translation of atoms
39 # MM-parameters
40 03.0000 endmm      End point criterium for MM energy minimisation
41 500 imaxmo        Maximum movement (1/1D6 A) during minimisation 0: Conjugate gradient
42 11101 imaxit      Maximum number of iterations
43 1 iout4           Frequency of structure output during minimisation
44 0 iout5           1:Remove fort.57 and fort.58 files
45 0 icelop          0: No cell parameter optimisation 1:Cell parameter optimisation
46 1.00050 celopt     Cell parameter change
47 0 icelo2          Change all cell parameters (0) or only x/y/z axis (1/2/3)

```

3 MD - CXCR4 + EPI-X4

Shortend Trajectory of CXCR4 and EPI-X4 (every 2000th image)

Listing 131: control emin

1	5463							
2	150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	0.0000	0
	0.2500	400.00	0.00	0.00	0.00 -25768.3435	0.3525	400.0000	
3	N	65.31100	109.69780	59.77190	-637.81715	-537.95505	128.31970	1
4	H	65.94100	108.87480	59.68890	1815.64688	2133.64569	-1431.50574	1
5	H	64.42200	109.47580	60.26290	298.67448	-1303.95025	-2847.58380	1
6	H	65.74600	110.46680	60.31990	1607.41886	-2678.28120	375.81997	1
7	C	65.07300	110.23980	58.36890	250.52454	841.36837	246.55166	1
8	H	65.99500	110.60580	57.94090	81.33623	1897.04725	2508.54986	1
9	C	64.57200	109.07580	57.46690	378.68866	758.52905	-335.67780	1
10	H	63.72300	108.60380	58.00590	-498.82673	2902.04710	1107.93536	1
11	H	65.36700	108.31580	57.30390	1825.83454	2064.81780	-1516.93174	1
12	C	64.06900	109.37880	56.07290	569.42849	633.03860	-326.28872	1
13	H	64.86000	109.98680	55.58490	2832.62222	-576.14906	-1241.98625	1
14	H	63.10100	109.92380	56.09390	240.20186	-1139.12498	2922.82801	1
15	S	63.78400	107.89480	55.05890	505.57229	85.68365	219.69429	1
16	C	63.35500	108.83480	53.50190	-869.87204	226.92678	-152.57087	1
17	H	64.24900	109.35680	53.09790	946.70162	2998.88790	-93.02501	1
18	H	63.14400	108.16180	52.64390	1455.09290	-2266.57970	-1625.89893	1
19	H	62.46700	109.49880	53.57490	-1499.80430	1526.46630	-2306.23371	1
20	C	64.20700	111.41880	58.36390	-837.25650	297.34736	205.02954	1
21	O	63.25100	111.43480	59.17690	610.52612	-475.02150	-158.86996	1
22	N	64.43500	112.38880	57.48690	-110.29444	533.17298	645.16199	1
23	H	65.13300	112.24580	56.78990	654.61939	-2669.33879	1531.12053	1
24	C	63.48300	113.49880	57.31190	-317.53438	-97.62167	-849.17191	1
25	H	63.22500	113.92180	58.27090	-2319.28714	-2091.15589	-382.36165	1
26	C	64.12400	114.66180	56.54490	-909.20212	-1.05087	-69.29212	1
27	H	64.28200	114.38580	55.47990	593.09351	1181.77544	-2854.79826	1
28	H	63.34000	115.43580	56.68990	-2443.96997	1875.26019	-639.24661	1
29	C	65.44500	115.15480	57.20390	-431.18422	-477.77421	645.95896	1
30	H	66.25700	114.45680	56.90490	2131.92792	-1679.03260	1591.84142	1
31	H	65.31200	115.17380	58.30590	1763.64081	2163.75555	1451.19236	1
32	C	65.89500	116.52780	56.78890	193.56188	-730.46210	-510.30375	1
33	O	66.39800	116.65480	55.61890	474.69686	138.46776	615.72461	1
34	O	65.78200	117.48080	57.60290	-395.05638	-545.62127	-412.13483	1
35	C	62.20400	113.11580	56.57590	-200.00050	-838.02099	298.61618	1
36	O	62.22500	112.31380	55.66790	203.33457	-560.10405	-188.23329	1
37	N	61.04700	113.70880	56.97790	-568.19059	621.99226	54.38174	1
38	H	61.04300	114.23080	57.82690	-2785.32528	281.84288	1435.53263	1
39	C	59.73700	113.42980	56.36590	-18.47557	-71.45658	-908.84741	1
40	H	59.91800	113.26680	55.31290	-2082.03596	-2298.40051	529.81848	1
41	H	58.98400	114.16080	56.62090	-2323.67413	613.98655	-2030.21804	1
42	C	59.19200	112.14780	56.93090	505.91605	-645.40307	398.69139	1
43	O	59.31000	111.77580	58.08890	-620.78190	-451.33913	-185.87642	1
44	N	58.56200	111.40380	55.94890	508.80851	-220.57079	636.50194	1
45	H	58.47400	111.82980	55.05190	707.31680	2430.51482	1868.29518	1
46	C	57.87500	110.13780	56.01090	-431.12889	800.07626	73.87060	1
47	H	57.76700	109.95980	54.95090	1935.73757	-2415.68363	561.79966	1
48	C	58.62000	108.94680	56.58990	399.27872	604.82924	553.36163	1
49	H	58.96700	109.18380	57.61890	2196.73043	2189.76815	526.79890	1
50	C	57.74600	107.62980	56.62790	-739.43343	-533.41251	12.66079	1
51	H	56.88400	107.77680	57.31390	2379.97955	-1864.14277	871.14596	1
52	H	58.49600	106.91780	57.03390	610.90176	3086.24411	11.07053	1
53	H	57.25700	107.46180	55.64490	2407.74805	-1121.89555	1685.91991	1
54	C	59.89200	108.69180	55.73090	552.37139	-499.13420	526.49967	1
55	H	60.46000	107.93180	56.30790	-2853.36259	-621.31981	1170.68777	1
56	H	60.53800	109.58580	55.60090	-948.64980	2042.34479	-2197.07022	1

57	C	59.57500	108.00080	54.36190	-589.39940	679.02636	-151.59995	1
58	H	60.54100	107.88380	53.82490	2279.89638	516.73247	-2105.53706	1
59	H	58.78200	108.53880	53.79990	2485.54959	-1895.59912	356.33331	1
60	H	59.27100	106.95080	54.55890	-2071.75806	2361.21377	175.25495	1
61	C	56.48300	110.35280	56.48890	-626.74106	33.22444	661.47017	1
62	O	56.23200	110.72880	57.61390	-494.78213	-211.96420	-577.83133	1
63	N	55.51000	110.10980	55.59990	298.36158	668.28082	-420.77714	1
64	H	55.68700	109.79380	54.67090	1423.02840	-842.07996	2676.58696	1
65	C	54.13200	110.46880	55.93890	-562.06457	-551.34409	459.95012	1
66	H	54.18500	111.42780	56.43490	367.93292	2298.15833	-2116.91282	1
67	C	53.21700	110.89980	54.75590	-598.43326	431.78225	-535.62368	1
68	H	52.16900	111.09380	55.06890	2577.16638	-1046.48916	-1470.13609	1
69	H	53.67400	111.80280	54.29990	2055.88982	-626.19471	2297.69960	1
70	O	53.16900	109.82880	53.75190	175.88709	681.05106	358.97133	1
71	H	52.74300	109.09380	54.19890	-1791.22073	2401.81507	959.70771	1
72	C	53.33100	109.55880	56.84290	-741.01262	21.30884	530.93995	1
73	O	52.32800	109.92080	57.43390	361.55453	601.33889	362.34941	1
74	N	53.81900	108.32080	57.03090	-717.28209	-420.93005	144.90197	1
75	H	54.63200	108.03380	56.52990	-2511.73549	-1395.42995	1281.47817	1
76	C	53.27600	107.22980	57.84390	-315.38428	-845.70486	-129.48762	1
77	H	53.71100	106.35180	57.38890	-947.43436	-2973.43547	399.09381	1
78	C	53.68500	107.21180	59.33890	-582.37724	648.99036	266.64444	1
79	H	53.02300	106.46180	59.82190	2256.70610	-2141.09507	-470.33575	1
80	C	55.10400	106.60980	59.52090	-755.53303	-364.16236	357.78013	1
81	H	55.25900	106.34180	60.58690	2376.76960	1712.36305	-1147.60850	1
82	H	55.24300	105.66880	58.94590	-2497.24019	-1899.87062	-229.14903	1
83	H	55.91800	107.29780	59.20490	-1519.26996	-1970.50533	-1925.39704	1
84	C	53.49000	108.57480	60.04890	792.13528	-325.73872	312.83700	1
85	H	52.61700	109.17680	59.71690	2424.57460	2000.36678	-134.89620	1
86	H	54.39300	109.19080	59.84990	-2030.60966	-1897.44686	-1474.63422	1
87	C	53.42500	108.40480	61.55690	322.74875	-757.74522	-391.28818	1
88	H	54.39100	108.06980	61.99090	-967.26387	-626.45216	-2927.48775	1
89	H	53.08300	109.37180	61.98490	-2366.39255	-1817.64686	-997.28253	1
90	H	52.80700	107.56480	61.93990	-2735.93884	1477.94169	-478.07244	1
91	C	51.74800	107.04180	57.69290	534.29515	298.97215	675.71840	1
92	O	51.26900	106.49380	56.68990	-421.98068	-475.88817	-468.07050	1
93	N	50.96400	107.43080	58.69590	738.64120	-175.29094	369.26218	1
94	H	51.44500	107.82480	59.47590	-2187.84852	1830.83186	1326.49907	1
95	C	49.51000	107.15480	58.80290	-480.09988	-52.79815	773.41287	1
96	H	49.24000	106.29580	58.20690	-797.98833	478.74135	-3005.36979	1
97	C	49.13800	106.74880	60.22390	626.63504	627.89309	211.02084	1
98	H	48.04800	106.59680	60.36990	-2541.19385	-1032.01872	1541.26487	1
99	H	49.52600	107.52080	60.92290	1500.63915	2715.49669	-521.90620	1
100	C	49.80200	105.42880	60.66190	156.34109	646.39906	623.84030	1
101	C	49.51100	104.24580	59.97190	-782.69746	-359.48071	-299.34814	1
102	H	48.82300	104.26580	59.13890	-2292.15100	-415.77080	2114.56962	1
103	C	49.99500	102.99780	60.39790	-893.96840	-137.06794	116.12013	1
104	H	49.67200	102.07880	59.93090	-1364.88315	-1990.13725	2018.58217	1
105	C	50.83600	102.89980	61.52590	-431.14538	361.32335	-717.64204	1
106	O	51.34200	101.66280	61.93590	-711.72147	-201.17784	276.78016	1
107	H	52.07400	101.77080	62.54690	2162.07263	-2262.59015	-323.03864	1
108	C	50.70100	105.34680	61.77690	74.96514	-403.36374	814.32728	1
109	H	50.99900	106.23980	62.30790	1737.80775	-2267.04501	1318.61949	1
110	C	51.19500	104.07880	62.11790	10.73246	-670.48962	617.88307	1
111	H	51.89600	104.05880	62.93890	-2374.85852	2036.45887	333.32946	1
112	C	48.66600	108.33480	58.25590	594.88125	603.38902	336.88127	1
113	O	47.44300	108.33480	58.50390	446.05914	-325.05626	564.79811	1
114	N	49.33000	109.34580	57.52190	-594.75174	394.55488	-450.85375	1
115	H	50.32600	109.32880	57.49590	-2406.65710	-1578.70913	1270.39573	1
116	C	48.70200	110.35780	56.73590	-865.48018	165.35998	234.62978	1
117	H	49.51800	111.06180	56.67490	-1970.01195	1495.38084	-1944.50901	1
118	C	48.32200	110.06680	55.26590	562.88804	-149.74036	-701.55960	1

119	H	48.01000	111.02580	54.79990	-1723.78248	-713.98499	2533.18488	1
120	O	47.28400	109.07980	55.22090	-363.06735	320.35793	-623.84303	1
121	H	46.60800	109.42880	55.80590	681.71193	993.43412	-2906.30069	1
122	C	49.48500	109.62180	54.37090	692.33013	-61.54088	590.20565	1
123	H	49.16200	109.70980	53.31190	3051.93252	134.09191	-752.29878	1
124	H	50.28600	110.34180	54.64090	-2609.05251	-1278.02176	1207.36555	1
125	H	49.70100	108.55280	54.58190	-2941.40876	1020.30552	453.11958	1
126	C	47.57700	111.10780	57.38490	650.16682	436.16239	467.43607	1
127	O	46.39300	110.89080	57.12090	-301.20932	-317.28978	657.44001	1
128	N	47.88200	112.03280	58.27090	-572.15517	-554.48258	-279.03372	1
129	H	48.83600	112.25780	58.45390	-2186.62039	2104.46012	-829.55718	1
130	C	46.81200	112.72280	58.99690	406.02563	-749.60925	323.54314	1
131	H	46.01700	112.92780	58.29590	-1448.90481	1449.80297	-2386.83314	1
132	C	46.15500	111.80380	60.08690	128.82578	636.50492	640.09094	1
133	H	45.48300	111.07380	59.58590	-1735.30460	616.43085	-2550.87380	1
134	H	47.00000	111.26880	60.57090	-283.59024	-2574.19557	1786.42660	1
135	O	45.43200	112.47680	61.08990	-500.20041	-427.14734	-437.00334	1
136	H	44.56000	112.09380	61.21190	-2158.82516	-539.63033	2224.07267	1
137	C	47.30300	114.07380	59.45890	616.14077	-592.13650	318.11305	1
138	O	48.42400	114.32380	59.86690	-126.46106	-321.69902	-710.03139	1
139	N	46.33200	114.98980	59.38090	-779.80526	20.00679	322.76272	1
140	H	45.47600	114.82980	58.89590	-2001.26457	-420.68031	-2390.85642	1
141	C	46.40900	116.36480	59.86390	465.58388	-772.37405	134.61417	1
142	H	47.26700	116.76780	59.34590	2014.79584	1503.24460	1891.84556	1
143	C	45.16300	117.20380	59.51090	-223.72262	-832.29354	-297.80306	1
144	H	45.19100	118.23680	59.92090	-770.12187	2981.20109	-646.20320	1
145	H	44.26900	116.67380	59.90090	-471.38089	-1709.58465	-2598.72018	1
146	C	44.82600	117.37080	58.03290	-297.40929	700.79008	501.88841	1
147	O	45.71600	117.07080	57.16090	-405.38803	224.61790	639.40173	1
148	O	43.78100	117.95980	57.71290	-263.78280	29.70124	-743.74976	1
149	C	46.82400	116.53780	61.30190	-606.07194	274.25726	-623.62710	1
150	O	47.50400	117.48180	61.75190	522.30663	-346.84740	-480.12487	1
151	N	46.49000	115.47180	62.10190	-562.05691	-415.49385	473.42282	1
152	H	45.90500	114.76980	61.70290	2894.62860	-1120.26444	-514.15862	1
153	C	46.81200	115.30180	63.49290	395.52060	-152.00027	-807.40967	1
154	H	46.41100	116.13880	64.04490	1365.81931	-1338.74614	-2498.10380	1
155	C	46.28400	113.95680	64.09990	397.16889	-799.40098	-186.18796	1
156	H	46.69400	113.83180	65.12490	1346.92975	2286.75763	1689.59937	1
157	H	46.70100	113.18980	63.41290	2408.00873	1695.41184	-1106.93219	1
158	C	44.81000	113.88480	64.02690	-417.50990	-758.78581	285.27283	1
159	O	44.22800	114.89880	63.63190	-388.52591	-553.56476	-407.72651	1
160	N	44.13400	112.78080	64.44390	-517.37619	-376.10424	-550.94443	1
161	H	43.13400	112.74780	64.46190	-1865.44274	2237.93649	1187.42995	1
162	H	44.63200	112.12380	65.00990	1946.08158	-1647.35193	1843.15608	1
163	C	48.27100	115.34780	63.66390	-71.33377	-715.66557	560.52234	1
164	O	48.75500	115.84680	64.69590	549.50417	174.39701	539.68331	1
165	N	49.09400	114.78180	62.71890	582.33452	-16.87225	-610.96164	1
166	H	48.76200	114.38980	61.86490	1566.89667	-2026.72431	1826.32133	1
167	C	50.53500	114.78580	62.77090	-249.36110	604.67021	635.32982	1
168	H	50.99700	114.55180	63.71790	1755.56054	-2218.92294	1375.72323	1
169	C	51.15000	113.64380	61.82790	643.60234	644.35876	-45.04254	1
170	H	50.78900	113.78680	60.78690	-554.62476	3092.45672	-165.31494	1
171	H	52.25900	113.70180	61.85990	2230.28325	1351.73538	1759.79383	1
172	C	50.82300	112.26880	62.31090	-371.01252	526.00669	-645.84648	1
173	C	51.69800	111.63680	63.23690	-320.89938	699.21388	489.46352	1
174	H	52.60400	112.12780	63.56090	709.66459	719.95863	-2979.30562	1
175	C	51.44700	110.35180	63.72190	451.18329	-783.68514	-117.14196	1
176	H	52.13100	109.96180	64.46090	-1122.87261	-1267.21102	2651.70880	1
177	C	50.40700	109.57580	63.20790	378.75399	828.44739	-40.88212	1
178	O	50.05200	108.37980	63.75790	555.01495	184.17046	530.72297	1
179	H	50.65900	108.15080	64.46590	891.02809	-2484.26089	1712.52533	1
180	C	49.82500	111.46180	61.76290	394.55542	-470.90609	-673.81339	1

181	H	49.07500	111.91980	61.13690	2016.91856	-1060.71859	2169.13388	1
182	C	49.60600	110.15880	62.27290	344.37401	-390.78512	-748.42804	1
183	H	48.69600	109.66080	61.97190	-1062.72377	2749.37317	-1099.90525	1
184	C	51.20200	116.03480	62.27090	627.94011	-345.68922	563.59664	1
185	O	52.28700	116.46380	62.68990	-546.04755	-567.93889	53.89537	1
186	N	50.51400	116.67680	61.33390	-738.20959	-311.93525	265.35880	1
187	H	49.65700	116.22980	61.08790	-368.92311	2669.21390	-1624.01328	1
188	C	50.91600	117.85280	60.57690	-342.65727	206.31415	819.43363	1
189	H	51.92000	117.69080	60.21190	1327.71152	-1813.42467	-2201.56747	1
190	C	50.01500	118.20880	59.38790	847.18615	-230.12949	-246.50974	1
191	H	49.02300	118.57080	59.73390	933.03089	-2405.24345	1800.68974	1
192	O	49.75800	117.08080	58.61790	-614.36626	415.48690	-271.20465	1
193	H	49.30700	117.45980	57.85990	-2509.95781	-1890.29593	-158.49082	1
194	C	50.71300	119.22280	58.45690	-170.66794	-523.72999	726.65697	1
195	H	50.36900	119.10080	57.40790	1374.00483	1957.08783	2044.54009	1
196	H	51.80600	119.02380	58.44690	-973.61161	-2425.18650	-1751.79254	1
197	H	50.63100	120.26780	58.82490	-2646.48056	-714.85490	1543.81001	1
198	C	50.96000	119.06580	61.54390	725.95815	-443.54152	-328.18697	1
199	O	51.87600	119.93180	61.48590	-694.73977	295.08999	-232.13310	1
200	N	50.00500	119.13780	62.47790	-162.22679	-765.05259	-317.88250	1
201	H	49.35900	118.38080	62.53090	2666.42016	1472.94964	-786.66962	1
202	C	49.99000	119.99780	63.65990	500.53767	198.19477	735.95644	1
203	H	50.16900	121.00080	63.30190	-2922.49830	83.05115	1162.03805	1
204	C	48.61300	120.03080	64.30690	660.59545	-453.60954	-435.08970	1
205	H	48.18100	119.03180	64.53290	2742.37084	-1160.78399	-1014.99208	1
206	H	48.66100	120.58280	65.26990	306.20586	1694.38815	2633.15647	1
207	C	47.57200	120.77580	63.45990	-470.86725	-759.15118	182.82373	1
208	H	47.54400	120.23480	62.48890	-119.77742	1736.51799	2620.76036	1
209	H	46.55800	120.69780	63.90690	-586.14818	1720.20645	-2568.17957	1
210	C	47.92400	122.23580	63.23490	-311.61999	531.66622	672.06772	1
211	O	48.09300	122.64780	62.07790	-353.65294	-610.86611	-354.11781	1
212	O	48.15800	122.93180	64.26690	441.55324	-396.12869	521.28689	1
213	C	51.05000	119.71080	64.68690	673.96832	-396.07191	-469.40893	1
214	O	51.30200	118.56080	64.97790	-497.09315	-196.37468	-581.34552	1
215	N	51.58900	120.75180	65.34890	-341.36189	484.42081	-601.23276	1
216	H	51.26000	121.67180	65.15190	1080.25693	-713.16287	2867.51982	1
217	C	52.56100	120.67980	66.43190	495.67658	707.96741	-290.75398	1
218	H	53.39500	120.09880	66.06790	470.41975	2054.41744	2335.87253	1
219	C	52.95500	122.14780	66.82590	-71.04859	-818.84628	-394.83397	1
220	H	51.97800	122.56380	67.15390	1548.16084	-1183.96184	2469.74869	1
221	H	53.25100	122.70680	65.91290	-1302.68703	-929.34644	2708.79086	1
222	C	54.10700	122.27280	67.87790	-796.76535	81.70128	-435.82207	1
223	H	53.80100	122.02580	68.91790	2354.64088	1869.45184	926.84540	1
224	H	54.82700	121.47980	67.58490	1549.01585	2732.48118	-179.78523	1
225	C	54.75900	123.65480	67.87090	-213.95449	616.86018	636.52023	1
226	O	55.63000	123.91080	67.02390	-126.35229	559.39788	542.89625	1
227	O	54.43000	124.46180	68.79590	-46.70079	175.24499	-768.59317	1
228	C	52.04700	119.94880	67.69290	-355.15677	-823.77917	-163.40913	1
229	O	51.02000	120.34680	68.24990	-668.48005	312.12958	281.66784	1
230	N	52.81100	118.90280	68.20390	246.93134	805.76383	-49.41510	1
231	H	53.56100	118.54280	67.65390	-2566.95031	-1063.01005	1476.14429	1
232	C	52.46000	118.03280	69.30690	-590.07812	690.83456	-77.50114	1
233	H	51.59900	117.45380	69.00690	2347.61703	-1081.23772	1793.83542	1
234	C	53.52300	116.85980	69.48290	725.56606	-538.36511	-123.15805	1
235	H	53.07200	116.10880	70.16590	1045.02487	1576.21006	-2514.30131	1
236	H	53.66200	116.37380	68.49390	1802.35862	28.44178	-2578.55012	1
237	C	54.91600	117.26480	70.10790	-576.90308	-482.24756	-515.82083	1
238	H	54.77000	117.43580	71.19590	484.51933	2308.86716	-2081.48978	1
239	H	55.36700	118.17980	69.66690	1920.70502	-2092.24524	-1353.37663	1
240	S	56.23900	115.97180	69.95690	-389.45599	-398.53009	-26.61590	1
241	C	55.37600	114.58580	70.80290	-338.31655	255.68040	807.23011	1
242	H	56.12900	113.76980	70.83190	1429.41716	-2795.35621	202.42652	1

243	H	54.53900	114.22880	70.16590	-1978.97674	-1763.88412	-1694.28159	1
244	H	55.02300	114.75580	71.84190	1916.28562	1481.53445	2007.76775	1
245	C	52.20000	118.71080	70.64890	388.42660	-807.59821	168.40699	1
246	O	52.91500	119.64880	70.97790	-735.37882	145.34206	248.43692	1
247	N	51.21600	118.21080	71.41490	-343.82757	52.86089	-769.19478	1
248	H	50.67800	117.48480	70.99390	-2893.61153	-922.24024	-821.40825	1
249	C	50.81400	118.79680	72.69490	-563.05869	-533.54968	479.31270	1
250	H	51.33000	119.69580	72.99790	2941.25425	717.96157	855.44188	1
251	H	49.79700	119.14380	72.58690	-2315.51239	132.70742	-2125.79805	1
252	C	50.93000	117.84780	73.85490	454.70767	790.17509	-17.75587	1
253	O	51.01900	118.16680	75.05290	412.95350	517.46571	-430.49492	1
254	N	50.99800	116.54480	73.59190	393.11431	-41.91803	745.90637	1
255	H	51.07400	116.21780	72.65290	-1765.31676	1682.88637	1987.40445	1
256	C	51.24700	115.58080	74.58990	-706.47776	568.76657	94.04665	1
257	H	50.61700	115.77180	75.44690	1296.16369	2197.79699	1840.61792	1
258	C	50.83800	114.13280	74.24690	660.48385	-461.28193	427.11950	1
259	H	51.10000	113.42080	75.05790	551.73321	2652.20567	1599.88181	1
260	H	49.73600	114.04180	74.13690	67.47395	-3100.03367	-532.41409	1
261	O	51.41100	113.59580	73.06890	473.88069	551.27384	308.48252	1
262	H	52.36200	113.53980	73.18990	-2259.60099	-127.99613	-2185.41680	1
263	C	52.74000	115.47980	75.09390	-59.75506	136.22552	899.62378	1
264	O	53.67700	115.65280	74.29690	-781.17088	-7.65142	115.50214	1
265	N	52.96000	115.23580	76.43190	-567.73238	390.44269	487.75685	1
266	H	52.13300	115.20480	76.98790	-2069.41889	1915.25038	-1395.54566	1
267	C	54.25700	114.86280	77.04290	656.85015	21.44070	-632.09111	1
268	H	55.10700	115.30180	76.54190	2759.74565	83.51715	-1508.32857	1
269	H	54.22100	115.03380	78.10890	42.15724	1061.40532	2961.39625	1
270	C	54.41600	113.39880	76.98090	-370.53267	-710.73057	434.76270	1
271	O	53.59300	112.69380	76.37590	154.37836	11.90406	-774.37255	1
272	N	55.57900	112.83980	77.40290	138.65499	-257.46323	791.93419	1
273	H	56.36100	113.40180	77.66290	1510.69631	2107.38219	1781.84264	1
274	C	55.75500	111.46880	77.54390	359.55564	-395.40116	-738.80218	1
275	H	55.39900	111.03980	76.61890	-2235.52476	1880.24405	-1168.47661	1
276	C	57.26800	111.09280	77.55690	727.87086	-543.79823	-77.06159	1
277	H	57.66800	111.68780	76.70790	-2661.00559	-1401.00435	-924.37129	1
278	H	57.36000	109.99780	77.39790	-1641.30559	2515.02322	937.55022	1
279	C	58.03100	111.60080	78.77190	-306.07235	848.25066	135.06126	1
280	O	59.25200	111.30280	78.87290	188.40035	-593.20694	486.04327	1
281	O	57.51600	112.46380	79.53090	676.45332	-224.35251	340.15302	1
282	C	54.85100	110.75880	78.66790	-463.98191	-296.47116	726.82642	1
283	O	54.46200	111.36580	79.65890	70.35126	538.02814	-573.76271	1
284	N	54.49300	109.47880	78.36290	-435.46505	130.40193	-711.36335	1
285	H	54.67700	109.08680	77.46490	841.87018	-2082.59627	2202.78769	1
286	C	53.76800	108.54880	79.17990	430.14130	617.90026	514.42077	1
287	H	52.81700	109.00280	79.41590	-235.35062	3037.49624	785.14516	1
288	C	53.38200	107.31980	78.25890	413.69700	-168.95326	794.83369	1
289	H	54.34200	107.04580	77.77190	-379.89386	2391.19881	2008.99853	1
290	H	52.70000	107.65380	77.44790	1198.39067	2164.37903	-1943.59189	1
291	C	52.81800	106.16380	79.07090	421.18946	-694.55628	414.29701	1
292	C	53.41400	104.92580	79.23390	-240.58022	869.62901	131.59613	1
293	H	54.42500	104.85180	78.86090	-2190.44871	1793.59299	1372.29183	1
294	C	52.72300	103.84880	79.87090	-551.89627	449.85556	569.64154	1
295	H	53.13500	102.84980	79.87490	-2692.99508	1559.27435	463.32193	1
296	C	51.39200	104.10480	80.26790	206.54373	376.10785	-804.57043	1
297	O	50.59800	103.10580	80.83390	433.58136	-410.12556	517.13776	1
298	H	49.86400	103.55080	81.26490	1588.46795	-1898.21374	1942.10720	1
299	C	51.47800	106.36080	79.45290	-711.47028	525.73618	-221.04867	1
300	H	50.93600	107.28580	79.31990	-2879.60782	1239.71328	-263.05137	1
301	C	50.76400	105.33380	80.04890	-648.21613	586.79076	258.73433	1
302	H	49.79000	105.62980	80.40890	-924.48069	2514.60475	-1649.34067	1
303	C	54.31600	108.18180	80.56890	-561.52673	-372.13036	-614.53863	1
304	O	53.62700	108.14980	81.56290	497.91119	467.53260	396.38989	1

305	N	55.68800	107.92880	80.57790	-433.23298	20.15064	-724.27579	1
306	H	56.10600	107.80480	79.68190	2502.00501	32.77674	1907.12424	1
307	C	56.44100	107.71180	81.79290	-739.65208	-463.49025	263.70929	1
308	H	55.98600	108.43680	82.45190	1095.79596	-2129.61372	-2040.14776	1
309	C	56.29100	106.15780	82.24090	-419.31983	549.92603	-594.30905	1
310	H	55.20700	105.98880	82.41890	2722.18904	-774.90780	1373.83805	1
311	H	56.67400	105.44380	81.47990	-2157.12055	-1448.33524	1774.08630	1
312	C	56.99500	105.84580	83.54390	-102.20739	590.69776	687.08137	1
313	O	57.19800	104.63480	83.81990	629.73890	356.53000	316.13685	1
314	O	57.36300	106.74580	84.32990	-300.27440	426.76794	-592.73235	1
315	C	57.82100	108.16680	81.61990	-226.44491	-449.70442	-760.22341	1
316	O	58.33300	109.17280	82.17690	567.06529	-17.23705	-549.33330	1
317	N	58.56500	107.53480	80.70590	-809.43081	-148.67963	188.11810	1
318	H	58.26400	106.72480	80.20790	-2156.34980	-1029.24040	2046.71590	1
319	C	59.85300	108.03280	80.26890	-468.54051	-606.73866	-493.74992	1
320	H	59.71000	109.10180	80.20890	-1515.33597	1004.83514	-2567.54542	1
321	C	61.08800	107.57880	81.06890	428.62307	-692.38599	410.28638	1
322	H	61.97600	107.81280	80.44490	2751.26827	423.56343	-1466.06383	1
323	H	60.96100	106.48180	81.19490	-1815.08318	-2532.30611	437.17849	1
324	O	61.18400	108.26280	82.33390	672.19713	-382.33209	160.00130	1
325	H	60.66900	107.78380	82.98790	601.70700	1837.84543	2481.63234	1
326	C	60.05000	107.53880	78.82690	-74.26237	794.17176	-441.84535	1
327	O	59.94300	106.33880	78.50090	-668.67814	385.70393	166.52103	1
328	N	60.38400	108.47080	78.00190	393.85757	675.08060	-319.08413	1
329	H	60.19400	109.41180	78.26890	-1816.30563	1555.16773	-2044.67929	1
330	C	60.67400	108.12380	76.60790	904.18788	-46.95501	108.12265	1
331	H	60.04800	107.29280	76.32090	1819.62955	1861.18503	-1767.24781	1
332	C	60.20800	109.28180	75.58590	-43.10306	886.67973	208.30792	1
333	H	60.43500	108.91680	74.56190	2372.41933	1942.46578	704.75488	1
334	H	59.11400	109.34780	75.77190	-89.95310	-2268.14834	-2178.44848	1
335	C	60.77400	110.64280	75.95290	429.65920	-624.06885	507.32834	1
336	H	60.26100	111.39580	75.31790	-1432.79834	-1665.51231	2251.97333	1
337	H	60.57500	110.97880	76.99390	1122.33026	1486.73055	-2535.39608	1
338	S	62.55100	110.85680	75.67090	438.60939	134.25516	-317.50270	1
339	C	62.43900	111.03380	73.84490	369.89737	388.36231	-737.42908	1
340	H	63.38500	111.51080	73.50790	1116.47799	1665.51419	-2424.41036	1
341	H	62.50200	110.05080	73.32990	-2985.47745	-966.87288	224.29326	1
342	H	61.55400	111.65080	73.58090	-1988.06635	-1042.73197	2204.20699	1
343	C	62.06900	107.56380	76.30990	269.07769	-4.42747	-871.22247	1
344	O	63.03500	107.93580	76.95290	475.07566	109.62868	-621.21807	1
345	N	62.16100	106.58480	75.43990	517.09379	-171.34958	644.92296	1
346	H	61.40400	106.33880	74.84090	-2349.22886	1504.74288	1454.33795	1
347	C	63.41000	105.90980	75.13290	-624.18257	-478.01165	-461.90041	1
348	H	64.14600	106.06280	75.90790	-2342.21064	-159.10473	2094.50740	1
349	C	63.16600	104.40980	74.87990	602.97994	-604.65315	319.78236	1
350	H	62.45500	104.32780	74.02990	-2585.93458	1654.64169	687.98944	1
351	H	64.13300	103.91480	74.64490	2435.74999	1954.99822	-378.58972	1
352	C	62.53200	103.69180	76.04290	-330.93251	-799.17625	288.53424	1
353	H	61.66000	104.23780	76.46090	-1519.66182	1835.76983	-2053.97257	1
354	H	63.23400	103.66580	76.90290	20.29495	-2237.00862	-2212.14980	1
355	C	62.25800	102.19480	75.76290	-452.73765	-785.92160	93.84494	1
356	H	61.54400	102.17580	74.91190	-1697.49561	-1934.24538	-1809.81482	1
357	H	61.77700	101.70080	76.63490	-2067.60589	1805.09650	-1537.80972	1
358	C	63.46800	101.44780	75.28890	-583.69775	-683.59205	-153.13343	1
359	H	64.24800	101.46280	76.07990	1887.23045	2290.58395	-1043.94091	1
360	H	63.89700	101.89080	74.36490	1516.45135	-2146.38012	-1729.63982	1
361	N	63.12400	100.07280	74.98990	739.34801	-388.98777	121.34792	1
362	H	62.54300	99.89180	74.14690	-1919.35125	1386.69995	2071.56469	1
363	H	63.89900	99.38180	74.93190	2628.20852	-1698.71606	-324.20660	1
364	H	62.54400	99.71080	75.77390	-86.97828	-2787.29733	-1456.58319	1
365	C	64.06300	106.52780	73.93390	-611.58936	460.20818	-495.59852	1
366	O	63.56800	106.44980	72.81290	497.95718	580.16888	-197.66119	1

367	N	65.20700	107.25280	74.15290	630.71635	-210.79508	520.03328	1
368	H	65.59800	107.30980	75.06890	-2464.37488	1447.43124	-1315.30434	1
369	C	65.85000	107.87280	72.97490	69.82670	663.52994	-621.53299	1
370	H	65.63600	107.23580	72.12990	-1593.95325	1287.62804	-2387.37372	1
371	C	65.38700	109.28680	72.58690	173.50623	-722.80134	528.11439	1
372	H	64.30700	109.23580	72.32990	1774.50095	2329.86017	1149.40167	1
373	H	65.40200	109.96080	73.47090	-913.49335	1201.49647	2760.46416	1
374	C	66.04100	110.06580	71.42790	872.02946	115.05480	-240.37057	1
375	H	65.55700	109.78380	70.46790	-2232.87896	106.22793	2213.86391	1
376	H	67.05200	109.61780	71.32090	-789.06758	613.78790	-2983.09621	1
377	C	65.97100	111.59280	71.60190	-607.49360	-341.83178	-587.83805	1
378	O	65.06100	112.23780	70.97590	724.00339	1.76245	-315.34619	1
379	O	66.75900	112.17680	72.38990	548.19796	348.25432	-449.24954	1
380	C	67.35200	107.73080	73.03590	218.52958	-425.89927	-776.08352	1
381	O	67.83700	106.97580	72.19790	536.53107	-393.48506	-425.36002	1
382	N	68.22200	108.25380	73.96990	-450.68827	240.63929	672.04546	1
383	C	67.88700	109.31680	74.86890	-498.93459	-179.94217	-741.71160	1
384	H	66.91900	109.13480	75.38190	1404.55301	-1948.91199	2031.55092	1
385	H	67.69700	110.19280	74.21090	-1578.69783	-2556.31178	933.38602	1
386	C	69.65900	108.01880	74.03690	-459.64308	699.39143	-361.98187	1
387	H	70.07900	108.16480	73.05290	-1241.71990	1151.77913	-2651.36998	1
388	C	70.14800	109.25780	74.86290	-668.03733	307.02304	-539.36443	1
389	H	70.28000	110.09880	74.14990	2888.19205	-1003.91282	-740.76446	1
390	H	71.15000	109.03480	75.28890	2006.58822	1460.18518	1933.82759	1
391	C	69.04400	109.50680	75.87390	-737.48456	505.55391	178.83729	1
392	H	69.09000	110.54880	76.25790	2232.27236	1666.11546	1462.61602	1
393	H	69.12200	108.76480	76.69690	3076.67406	-597.46055	274.48831	1
394	C	70.08700	106.61680	74.57190	-667.00086	-614.09358	97.21074	1
395	O	71.25500	106.47080	74.96990	486.63680	-427.53607	-451.69100	1
396	N	69.19600	105.56580	74.56890	605.89723	583.20402	-73.71506	1
397	H	68.36100	105.61180	74.02590	-2426.72247	-431.88383	-1955.17790	1
398	C	69.48600	104.28380	75.21390	-800.59421	-385.74731	204.20317	1
399	H	69.77300	104.39880	76.24890	2046.73852	90.54925	-2387.65335	1
400	C	68.21500	103.35380	75.28190	30.03648	-0.37494	-911.34443	1
401	H	67.84500	103.20280	74.24490	-1825.93331	-209.09434	2553.52175	1
402	H	68.48900	102.35480	75.68390	-1890.28550	27.38608	-2514.81549	1
403	S	66.88000	104.12080	76.21390	195.65999	327.39544	-407.11178	1
404	C	70.55400	103.47180	74.55290	-41.53492	-598.87998	686.34439	1
405	O	70.50800	103.20580	73.35790	-272.53787	-556.54031	489.50303	1
406	N	71.52600	102.95180	75.35490	-478.74045	-482.18673	500.97487	1
407	H	71.48700	103.20280	76.31890	-228.40112	1667.45140	2658.13186	1
408	C	72.33200	101.85280	75.04890	-204.90218	881.08175	114.72162	1
409	H	72.03800	101.35280	74.13890	886.33756	150.73731	3014.94780	1
410	C	73.81400	102.26780	74.93190	77.25381	644.14506	640.74956	1
411	H	74.39600	101.32180	74.90890	-1150.89139	-2849.28212	674.73450	1
412	H	74.14900	102.95580	75.73790	-2581.63378	1080.72853	-1437.15659	1
413	C	73.94900	103.02380	73.66090	598.72907	687.12798	28.80354	1
414	C	74.30600	102.35780	72.44890	-224.18917	817.90129	-335.00403	1
415	H	74.29800	101.27780	72.45890	-2316.16460	123.57426	2125.63807	1
416	C	74.70200	103.04680	71.29590	401.78273	-557.21131	599.61420	1
417	H	74.89000	102.53680	70.36190	119.45646	2952.82235	-1079.25740	1
418	C	74.81400	104.45080	71.38890	360.96702	-28.26743	-836.87201	1
419	H	75.24600	104.96280	70.54190	-1743.04270	666.48540	-2532.94800	1
420	C	73.98600	104.42880	73.64890	458.23108	637.35358	-463.95657	1
421	H	73.78100	104.96380	74.56490	-3069.02688	-685.04438	100.07198	1
422	C	74.45500	105.11980	72.52590	38.98743	631.38976	656.71756	1
423	H	74.60000	106.18980	72.51690	-1784.05118	-1635.43488	2010.15929	1
424	C	72.21300	100.84580	76.15190	-763.57979	150.34859	-475.17598	1
425	O	71.68300	101.16780	77.20590	-690.90603	163.90978	-345.55705	1
426	N	72.53700	99.58580	75.86190	467.85121	-101.71349	695.29986	1
427	H	72.87100	99.41180	74.93890	2104.70849	1048.27536	2090.34618	1
428	C	72.58100	98.56180	76.81190	900.02218	-134.67921	-57.20650	1

429	H	71.71300	98.59980	77.45290	2864.58880	291.91619	1267.73111	1
430	C	72.54400	97.15380	76.13090	-294.84409	-709.86159	490.52470	1
431	H	72.71300	96.34080	76.86890	-2364.97392	1292.53496	-1623.10750	1
432	H	73.25700	97.11580	75.27990	-1460.95230	-1595.98307	2284.00583	1
433	C	71.15900	97.00780	75.56090	-85.27762	-638.77948	-645.08876	1
434	H	70.31600	97.24980	76.24290	2369.92782	853.57037	-1884.96312	1
435	H	71.13100	97.73280	74.71890	-2548.07914	-233.03401	1830.63216	1
436	C	70.94100	95.54280	75.00690	-668.66546	248.40500	568.00745	1
437	H	71.06100	94.85480	75.87090	2509.11451	1648.34279	941.02957	1
438	H	71.71300	95.43180	74.21590	-1860.00457	2536.65173	63.30279	1
439	N	69.55900	95.45880	74.44790	390.41094	337.20349	-668.24052	1
440	H	68.95100	96.25180	74.49390	-2564.56482	-1434.85597	-1123.57549	1
441	C	68.96900	94.33980	74.12190	234.50530	375.01418	797.38487	1
442	N	69.66000	93.24180	73.94590	577.41225	-600.07732	-138.47233	1
443	H	70.65800	93.29780	73.98490	1034.06525	-185.93057	-2965.52948	1
444	H	69.18800	92.38480	73.73990	1609.12958	-1418.95934	-2301.19156	1
445	N	67.64900	94.26480	73.96590	-113.33767	-726.22360	-415.24226	1
446	H	67.06000	95.03580	74.20890	-1565.39657	-2236.71637	1563.60471	1
447	H	67.26300	93.35580	73.80890	1525.50127	-1948.68861	1942.59744	1
448	C	73.74800	98.68280	77.74690	755.96089	475.62491	-183.72556	1
449	O	73.63900	98.24680	78.83690	463.22655	615.70376	173.08168	1
450	N	74.84600	99.31480	77.33590	-790.76865	-206.10640	211.84281	1
451	H	74.88600	99.55780	76.36990	-2516.14661	-1888.33412	-37.77206	1
452	C	76.06300	99.48080	78.09590	-676.30911	-517.34974	326.19970	1
453	H	76.77600	99.87080	77.38390	3093.13872	370.72935	-439.63492	1
454	C	75.87900	100.65680	79.10690	-2.47182	-361.65621	-837.04820	1
455	H	74.92800	100.55580	79.67290	2293.57654	-2009.15854	-775.25148	1
456	H	76.66200	100.74080	79.88990	-1042.32021	1903.85729	2277.52547	1
457	C	75.60300	102.01980	78.43190	463.06484	644.11096	-449.60319	1
458	H	74.71700	101.89880	77.77190	1711.81835	-593.77103	-2572.03035	1
459	H	76.44600	102.35880	77.79190	1553.07480	2650.84665	677.64071	1
460	C	75.26700	103.23980	79.28090	-392.01105	573.27873	590.87210	1
461	O	74.10200	103.50380	79.64390	-687.88794	387.46435	17.57214	1
462	O	76.23400	103.93280	79.71990	722.93122	-317.28029	18.19079	1
463	C	76.72800	98.22480	78.72090	-494.92821	-120.37527	-756.31135	1
464	O	76.23600	97.10980	78.65890	-436.21647	586.06331	-299.78695	1
465	N	77.86900	98.38280	79.40690	240.36755	-539.61408	603.08571	1
466	H	78.16300	99.31580	79.59790	-1646.26057	1759.18637	-2023.19442	1
467	C	78.75500	97.37880	79.91690	93.74012	-237.27461	-875.42250	1
468	H	78.24500	96.43280	79.81790	-1164.93251	1606.90261	2441.11091	1
469	C	80.00100	97.35880	78.99090	368.91637	-593.35085	585.90655	1
470	H	80.84600	97.00080	79.61690	-1678.32018	2496.80112	-920.57144	1
471	H	80.19900	98.40480	78.67290	-2063.05746	-2245.50344	-774.42523	1
472	C	79.83000	96.53980	77.68790	-537.31659	225.99264	701.19128	1
473	H	80.86500	96.35380	77.32790	581.12542	-1687.83623	2590.70035	1
474	H	79.16200	97.11380	77.01190	-2651.36805	-1539.47471	706.03917	1
475	C	79.13700	95.18980	77.86590	734.41092	149.37853	-519.40125	1
476	O	79.56700	94.36780	78.71590	-684.63631	-165.06219	357.28816	1
477	O	78.32600	94.90780	76.96890	-293.37082	-594.43953	429.18811	1
478	C	79.11700	97.51380	81.41390	13.86330	-661.35695	627.58728	1
479	O	79.60500	98.53980	81.90390	-203.26659	753.77743	-118.86762	1
480	N	78.81900	96.47680	82.28590	-128.43913	562.37264	-616.37058	1
481	H	78.31700	95.69580	81.92190	-2750.95225	255.50441	1505.05994	1
482	C	79.20300	96.47480	83.67590	274.93315	650.36456	576.96508	1
483	H	79.11900	97.48380	84.05190	-1512.59960	456.75187	2720.59670	1
484	C	78.30400	95.58880	84.57390	-279.92943	-685.49286	-532.15605	1
485	H	78.37100	94.58480	84.10390	-2810.92677	851.15893	1128.02720	1
486	H	77.26300	95.94780	84.42690	-1630.68225	2061.54193	-1728.91483	1
487	C	78.83000	95.41580	85.95590	328.23710	-639.86951	-560.60541	1
488	O	79.81200	94.70780	86.27390	578.37715	-175.01029	-508.40781	1
489	N	78.20900	96.11780	86.93990	-9.69508	212.88791	-816.85802	1
490	H	77.67900	96.92680	86.68390	-264.20800	645.91936	3067.76931	1

491	H	78.67300	96.06480	87.82390	1469.95309	2140.74062	-1776.14575	1
492	C	80.69000	96.04180	83.75490	378.24319	-22.34042	-829.38773	1
493	O	81.10400	95.04180	83.13390	161.73252	483.74341	-602.87820	1
494	N	81.45100	96.92680	84.40990	497.23555	395.97537	-555.54711	1
495	H	81.08100	97.69580	84.92590	1670.81636	1976.32021	-1789.06605	1
496	C	82.84600	96.66980	84.72090	205.86799	-780.04324	424.97284	1
497	H	83.24900	95.99880	83.97690	1594.82121	1338.03133	2358.90731	1
498	C	83.58400	98.04180	84.88990	40.63712	-406.66264	815.12277	1
499	H	84.67900	97.92480	85.02990	-1012.27326	2706.09389	1245.22485	1
500	H	83.40100	98.55980	83.92390	1781.41214	-878.82307	2439.76782	1
501	H	83.07200	98.64180	85.67190	2364.33775	2074.56491	65.67828	1
502	C	83.00800	95.84680	86.00290	500.78592	11.64795	761.92440	1
503	O	83.77400	94.88980	86.04690	552.42643	-507.04756	247.69951	1
504	N	82.40400	96.36780	87.13390	-46.17366	-659.23202	525.31270	1
505	H	81.78200	97.14680	87.11390	-1807.89452	2510.97374	569.87236	1
506	C	82.83500	96.10880	88.51090	236.86674	864.31394	-168.24557	1
507	H	83.91500	96.11680	88.48190	-1207.86809	110.73305	2902.93285	1
508	C	82.44500	97.30480	89.36290	188.71149	-121.75925	883.74977	1
509	H	82.84500	98.22480	88.88690	-1307.07613	-1974.16178	-2071.82612	1
510	H	82.87500	97.21880	90.38390	-242.68203	2433.26362	-1979.53526	1
511	C	80.92300	97.56480	89.56490	450.39606	542.97537	-577.73016	1
512	O	80.11000	96.84580	88.98890	-604.38440	232.86764	-451.79574	1
513	N	80.55400	98.59480	90.38390	297.64192	-781.70590	114.09411	1
514	H	81.14700	98.87580	91.13890	1748.42026	-2146.87973	-1494.04159	1
515	H	79.59800	98.88580	90.35990	716.09906	-2173.24149	2159.27066	1
516	C	82.40200	94.79380	89.05990	-411.57009	-620.27723	-526.60917	1
517	O	82.89700	94.33280	90.08190	-403.43707	349.49488	-581.99578	1
518	N	81.51000	94.10480	88.38990	-662.67971	-516.80321	80.26415	1
519	H	81.16800	94.55480	87.56790	-366.96978	2473.50813	1909.27130	1
520	C	81.12400	92.75780	88.70090	584.80035	558.93828	-420.77019	1
521	H	81.62000	92.33280	89.56190	-1513.99996	1695.63418	-2175.05289	1
522	C	79.64100	92.55580	89.08290	-510.77412	670.29164	-348.23831	1
523	H	78.94900	92.91080	88.29090	1613.17726	-690.35458	2611.37816	1
524	H	79.48000	93.19280	89.97990	-1092.29596	-2124.44132	2047.40441	1
525	C	79.23800	91.16380	89.48190	-625.69741	646.88214	-146.61940	1
526	C	79.93400	90.37880	90.42390	97.96293	43.84402	905.50095	1
527	H	80.74300	90.81880	90.98890	-3054.85671	-701.24759	272.63258	1
528	C	79.52800	89.06080	90.67690	420.97657	806.39842	62.85955	1
529	H	80.04400	88.47980	91.42690	1632.60506	-1493.96721	2236.26674	1
530	C	78.39300	88.54880	90.02890	748.84000	-445.00395	-269.55731	1
531	H	78.14700	87.53080	90.29090	-2056.48829	-2287.47847	660.69993	1
532	C	78.16600	90.60380	88.79290	-370.80497	121.68960	-824.10334	1
533	H	77.64300	91.20280	88.06190	-2144.51173	-1945.56929	1230.46976	1
534	C	77.70400	89.30980	89.05490	-231.67402	515.88356	-715.29176	1
535	H	76.95400	88.81680	88.45390	332.09743	1906.94858	-2480.21866	1
536	C	81.44200	91.76880	87.58190	-225.36693	731.28835	495.86097	1
537	O	82.25000	90.81680	87.70090	-643.66273	-407.57298	-207.86963	1
538	N	80.77800	91.92480	86.40090	763.66915	155.92721	-324.29680	1
539	H	80.15600	92.68380	86.22890	1025.71397	2467.62668	1660.40828	1
540	C	80.86900	90.98080	85.33390	-840.15650	310.08258	-171.57174	1
541	H	80.38800	90.05880	85.62390	-2963.51925	788.38558	-703.01358	1
542	C	80.14800	91.45480	83.98090	-837.29747	9.18433	-360.97036	1
543	H	80.41000	90.71080	83.19890	1720.06170	-2073.01539	1625.49106	1
544	H	80.51500	92.46580	83.70290	-1118.67406	2323.36364	-1802.43612	1
545	C	78.63300	91.53180	84.15290	-251.15276	674.99988	-559.23918	1
546	O	78.15100	91.93080	85.23790	333.03720	460.58310	-548.24872	1
547	N	77.82300	90.99780	83.19090	245.91157	396.30012	703.66612	1
548	H	78.28200	90.77880	82.32990	1387.92430	1734.74334	2227.67994	1
549	H	76.85700	90.84880	83.40290	2142.26967	-264.31098	2288.89637	1
550	C	82.29900	90.64080	84.91590	-864.04073	-82.37831	-279.46098	1
551	O	82.69200	89.49280	85.00890	596.34707	433.12300	-283.55224	1
552	N	83.18700	91.60280	84.66990	-841.12656	-28.23182	-66.19183	1

553	H	83.00200	92.58180	84.64290	2092.06009	-2260.51354	-641.55230	1
554	C	84.54300	91.32680	84.26490	577.97959	-410.42098	-573.53746	1
555	H	84.50800	90.45280	83.63190	-1178.71085	2855.54929	-595.57131	1
556	C	85.05300	92.48880	83.38590	496.57895	-746.06880	168.05265	1
557	H	86.14700	92.44080	83.19790	1429.62827	2477.58113	-1309.95456	1
558	H	84.83900	93.51380	83.75890	2515.32733	-1503.79632	-1144.53103	1
559	C	84.53300	92.34280	81.91890	652.00081	-614.35052	170.05698	1
560	H	83.45200	92.09780	81.83390	631.47272	-2234.96461	2122.35757	1
561	H	85.11200	91.48080	81.52490	-2859.93487	1309.98493	54.20537	1
562	C	84.94100	93.63080	81.17690	119.35182	-602.48810	673.95418	1
563	H	85.97200	93.97180	81.40990	-723.70638	-2972.33312	-734.65033	1
564	H	84.26000	94.40880	81.58290	-1877.78583	-1693.98437	1871.51371	1
565	C	84.90400	93.63080	79.66090	718.00822	551.18195	110.06205	1
566	H	84.83100	94.69680	79.35490	2123.84623	-539.05247	-2257.63723	1
567	H	85.84700	93.24380	79.21990	-1783.51678	968.23568	-2404.12433	1
568	N	83.68900	93.01780	79.12490	726.34632	74.75630	-423.68008	1
569	H	82.82700	93.53580	79.39090	-1652.40631	2575.37043	-731.60562	1
570	H	83.77400	93.03380	78.08890	-1184.51832	2465.45591	1554.56416	1
571	H	83.55000	92.05080	79.48290	-2364.80403	-1584.09949	-1340.35702	1
572	C	85.52300	91.00780	85.37090	678.67410	-589.11183	-154.27156	1
573	O	86.73000	90.88980	85.12690	-65.23234	659.02925	-430.17719	1
574	N	84.97100	90.73280	86.52890	-55.59608	461.02311	-705.00997	1
575	H	83.98200	90.80380	86.63890	-1999.45745	-1560.20085	-1861.76514	1
576	C	85.69000	90.07680	87.63190	621.76741	580.63698	-328.20268	1
577	H	86.74100	89.99580	87.40090	-3081.23309	491.69876	403.06477	1
578	C	85.64700	90.95180	88.97890	447.05882	339.67515	718.47770	1
579	H	84.65000	91.44080	88.94490	-928.95370	-1505.89169	-2601.45372	1
580	C	85.84700	90.02680	90.24690	-496.35257	420.61418	638.88093	1
581	H	86.83700	89.57380	90.02490	2295.62206	-1244.98294	-1754.52645	1
582	H	85.06000	89.24180	90.25090	-1464.35575	-2582.34347	-1041.82085	1
583	H	85.79200	90.62080	91.18390	-2871.62139	1035.06178	762.01308	1
584	C	86.75100	91.99180	88.80390	-716.39392	535.48603	177.44145	1
585	H	87.73100	91.55880	89.09590	-2011.16270	2048.01054	-1288.06197	1
586	H	86.82900	92.25180	87.72690	2457.98221	-237.79132	1949.36015	1
587	C	86.61200	93.21980	89.72990	-119.13341	-521.82628	738.21106	1
588	H	85.58000	93.61480	89.85090	1408.95346	2034.93532	1942.19325	1
589	H	86.93100	92.85080	90.72790	1278.85214	2395.67008	1588.56171	1
590	H	87.37500	93.98980	89.48690	-898.17563	2184.36499	-2078.47452	1
591	C	85.13000	88.64980	87.81490	91.30633	-177.55752	889.71202	1
592	O	85.88500	87.65180	87.82690	-406.60415	484.58626	472.73296	1
593	N	83.82600	88.54680	87.90990	-583.72278	491.60631	360.91998	1
594	H	83.15600	89.27680	88.01690	1523.98348	2666.37650	682.74223	1
595	C	83.13400	87.29780	87.98890	-321.45261	16.93891	853.13088	1
596	H	83.56400	86.79980	88.84590	2383.81824	1623.71770	-1256.65336	1
597	C	81.61900	87.60380	88.25290	-782.70833	-466.30006	-37.18784	1
598	H	81.05200	88.01580	87.39090	2448.72210	848.45015	1783.84938	1
599	H	81.37000	88.24980	89.12090	-1517.31044	-1926.54470	1970.89340	1
600	C	80.84400	86.27080	88.50390	-280.52934	-801.38958	-332.45907	1
601	C	80.09000	85.49180	87.61190	-216.95295	693.80286	550.47253	1
602	H	80.05300	85.86080	86.59690	2512.33038	1476.61981	-1185.75554	1
603	C	79.40000	84.34180	88.00890	148.59986	-886.08935	-155.61086	1
604	H	78.84100	83.76780	87.28590	-323.95670	-2958.00140	1021.52142	1
605	C	79.47800	83.93480	89.35490	-638.99266	453.47035	-466.37326	1
606	H	78.96900	83.02580	89.64090	-632.11128	-440.06841	3050.41003	1
607	C	80.99400	85.82380	89.86490	147.11343	574.65893	-692.51409	1
608	H	81.73600	86.29080	90.49590	375.29028	2769.09652	-1445.50611	1
609	C	80.30600	84.65280	90.26790	24.69251	-623.90608	-664.51674	1
610	H	80.48200	84.28180	91.26690	-2373.94869	-1191.52542	-1686.07859	1
611	C	83.37800	86.39580	86.79090	269.15974	594.81189	-636.55546	1
612	O	83.72200	85.26080	86.90890	-588.88055	232.47149	-472.02112	1
613	N	83.32200	86.93180	85.55290	467.42489	-452.35475	538.10914	1
614	H	83.05500	87.89180	85.50190	-1158.83148	-275.13268	-2911.98177	1

615	C	83.49600	86.13280	84.35290	-854.23097	277.96686	-156.44445	1
616	H	82.75300	85.35980	84.48090	-1017.99525	2707.72351	-1236.99041	1
617	C	83.02400	86.92280	83.11790	-720.42085	-222.03127	512.97847	1
618	H	83.30700	86.48280	82.13790	1304.37913	1937.54573	-2107.78032	1
619	H	83.52300	87.91480	83.07890	370.04228	-2122.64552	2292.52501	1
620	C	81.48800	87.26180	83.25690	-13.27654	-406.21188	816.25158	1
621	H	81.22000	87.74480	84.22190	-1339.38095	-1926.95232	2095.50463	1
622	C	81.14900	88.28680	82.18890	466.39389	-539.38801	-568.32062	1
623	H	80.07300	88.55480	82.11890	2044.95439	1783.84312	-1591.94582	1
624	H	81.51800	88.03180	81.17190	-2324.15467	-1537.60860	1460.23665	1
625	H	81.73000	89.23080	82.27090	-866.54331	-1806.49143	2425.67880	1
626	C	80.56500	86.01080	83.06190	-512.64853	721.31371	-219.88410	1
627	H	79.57800	86.23780	82.60590	-2614.91104	-1706.75049	384.01720	1
628	H	80.43400	85.42780	83.99890	2290.23109	2149.66023	178.96556	1
629	H	81.08700	85.32580	82.36090	-2005.39683	40.57786	2423.83234	1
630	C	84.85900	85.42580	84.17190	271.76028	-679.43556	544.02636	1
631	O	84.87300	84.21580	83.92590	489.99464	-232.86132	573.85372	1
632	N	86.02000	85.99180	84.34990	772.49265	-247.84400	-233.45395	1
633	C	86.16700	87.45380	84.22290	-38.02327	44.67794	909.95006	1
634	H	85.56100	88.17180	84.81690	1477.02567	-2701.09055	-648.63797	1
635	H	86.09600	87.77680	83.16190	1173.35413	-582.73564	-2860.39953	1
636	C	87.30000	85.35580	84.29190	-371.85486	768.91243	-319.29397	1
637	H	87.36000	84.75980	83.39390	-1951.11782	-1726.41590	-1763.76122	1
638	C	88.32200	86.47380	84.15590	578.83747	135.71660	-691.36039	1
639	H	88.60700	86.61280	83.09090	-733.56839	2603.64339	1606.59414	1
640	H	89.29100	86.34080	84.68290	2568.40441	-489.15501	1749.92926	1
641	C	87.63700	87.74680	84.70290	-594.20144	671.88998	164.13258	1
642	H	87.58900	87.64080	85.80790	2328.10660	1640.07163	1337.27743	1
643	H	88.00100	88.74580	84.37890	-1949.71798	-1214.24786	-2149.98329	1
644	C	87.49300	84.44880	85.47990	485.99674	-771.15644	-23.99827	1
645	O	88.17500	83.43780	85.31690	667.02038	338.23839	-253.58595	1
646	N	86.94800	84.79480	86.61690	-351.21097	360.46375	-677.78243	1
647	H	86.51700	85.69380	86.61590	2658.87252	-910.42782	-1414.12317	1
648	C	86.99100	84.05980	87.81290	752.58343	418.51104	-299.86278	1
649	H	88.04200	83.90580	88.00490	-1282.28310	1354.76212	-2533.49480	1
650	C	86.54200	84.90880	89.03390	422.30738	559.35235	-583.29447	1
651	H	85.51300	85.29680	88.87390	-2247.22178	599.70292	-2118.62619	1
652	O	87.43800	86.02880	89.13590	470.83428	633.93561	8.24303	1
653	H	87.11700	86.76680	88.61390	265.48626	1743.24994	-2605.53698	1
654	C	86.58800	84.13880	90.31390	-280.22500	861.65118	102.38256	1
655	H	86.42200	84.88380	91.12190	-1792.57882	1437.36362	2149.15640	1
656	H	87.58000	83.65880	90.45790	-432.47922	1218.71390	2868.08723	1
657	H	85.87300	83.28880	90.33790	850.54544	-2923.52327	792.34485	1
658	C	86.28000	82.71080	87.71290	352.70556	-609.86529	-578.89043	1
659	O	86.82200	81.66680	88.07090	491.28648	-367.68551	-497.06357	1
660	N	85.01900	82.70380	87.12790	152.03866	116.75225	-822.14685	1
661	H	84.59100	83.60380	87.13890	-2670.47446	1533.40975	-644.55172	1
662	C	84.34600	81.49680	86.73990	-169.54950	895.80157	-15.60477	1
663	H	84.30700	80.75780	87.52590	2630.13013	725.45100	-1566.64054	1
664	C	82.88500	81.78680	86.44690	476.61807	489.67358	603.74332	1
665	H	82.91900	82.67580	85.78090	-1563.19923	-1396.76035	2345.99551	1
666	C	82.17700	80.62380	85.67890	-681.83180	-555.91392	-239.82518	1
667	H	81.07800	80.71880	85.54690	602.73017	-2089.52721	-2273.50360	1
668	H	82.70400	80.35880	84.73790	465.57596	2498.61775	-1854.28546	1
669	H	82.32100	79.72080	86.31090	1408.56024	-2171.16793	1788.91422	1
670	C	82.07000	82.12980	87.72690	833.83245	-259.28105	262.57912	1
671	H	81.10200	82.37580	87.23990	2009.33983	-1845.03907	-1567.35782	1
672	H	82.53400	83.06080	88.11890	2001.44440	-772.01096	2301.40079	1
673	C	81.94500	81.05480	88.81990	-711.29367	296.77117	-487.27733	1
674	H	82.88100	80.59980	89.20790	-587.70429	3052.00527	-487.94852	1
675	H	81.31400	80.20680	88.47790	2819.11105	-507.83191	1301.13253	1
676	H	81.40000	81.55980	89.64590	-694.54622	-1642.16649	2592.12673	1

677	C	85.05200	80.71580	85.59890	-4.22895	117.73405	-904.19678	1
678	O	85.24900	79.52680	85.71490	33.01373	785.75877	71.55753	1
679	N	85.49400	81.43280	84.53190	-389.96503	-638.06614	-391.75397	1
680	H	85.40200	82.42480	84.48490	-912.91230	-3006.00745	-169.51857	1
681	C	86.03100	80.79380	83.32290	-680.12736	-510.63371	328.83277	1
682	H	85.31500	80.12480	82.86790	2092.89870	-1750.34149	1566.62246	1
683	C	86.55300	81.83280	82.24690	-280.07891	679.12645	-540.17967	1
684	H	87.16500	81.34780	81.45690	-401.43550	1247.37788	2860.26646	1
685	H	87.19100	82.46680	82.89890	-1414.90619	-2747.45996	589.68677	1
686	C	85.50700	82.73980	81.58390	-381.73017	-518.08598	-646.00309	1
687	C	84.15500	82.39380	81.53690	13.98738	736.61994	537.25824	1
688	H	83.79200	81.55280	82.10890	-1971.37046	-504.49935	-2399.45934	1
689	C	83.21100	83.32080	80.93390	-807.86256	349.76018	-237.64869	1
690	H	82.15600	83.09880	80.98090	2041.51106	1767.43141	-1614.51077	1
691	C	83.64600	84.52480	80.37890	778.54054	-29.86410	473.74442	1
692	O	82.63200	85.34680	79.76390	-233.59847	-567.07109	497.48303	1
693	H	81.83700	84.81180	79.82390	-1073.70180	-2324.00967	1828.76181	1
694	C	85.92600	83.94280	80.96390	12.02304	-905.25558	-108.71426	1
695	H	86.96400	84.21780	81.07890	2835.24504	-600.94536	-1224.12273	1
696	C	84.98800	84.82180	80.36790	-671.76561	494.51852	-368.28440	1
697	H	85.38700	85.78680	80.09090	2233.26708	-634.59033	2123.21443	1
698	C	87.28100	79.90080	83.70090	-597.77310	657.57265	-204.24626	1
699	O	87.52500	78.85780	83.08590	-544.70164	560.35624	113.70242	1
700	N	88.11400	80.46780	84.61090	647.50288	512.31416	-175.91620	1
701	H	87.81200	81.38580	84.85490	559.06666	2850.33201	1208.83337	1
702	C	89.22100	79.75680	85.24590	-797.62956	436.77539	66.82327	1
703	H	89.95300	79.50280	84.49390	-1460.06880	-2547.55562	1129.77241	1
704	C	89.96200	80.65580	86.28690	-454.18283	-344.00928	711.91753	1
705	H	90.83200	80.05380	86.62590	2287.01729	-336.87369	-2134.07926	1
706	H	89.32800	80.96580	87.14490	935.25630	2256.94615	-1982.35111	1
707	O	90.43900	81.84080	85.66990	614.75734	91.34602	487.19252	1
708	H	89.67500	82.42080	85.62090	2373.53990	-1179.91475	1694.79668	1
709	C	88.73400	78.47380	85.93690	-905.12227	101.27148	44.14489	1
710	O	89.25800	77.41880	85.68690	455.97762	479.88502	430.60655	1
711	N	87.62200	78.53080	86.72490	-698.23013	282.60942	-381.15468	1
712	H	87.11900	79.38180	86.85290	1749.77418	2397.46164	-1043.40512	1
713	C	87.01300	77.34680	87.36090	-109.87209	694.32003	580.77433	1
714	H	87.78600	76.78980	87.87090	2154.73553	2267.17444	339.50120	1
715	C	85.83700	77.64780	88.31690	-570.15198	-362.84637	-612.14396	1
716	H	85.15200	78.26580	87.69790	2173.88273	954.33054	2064.39176	1
717	C	85.23200	76.35180	88.91690	-581.57871	629.52021	-311.32219	1
718	H	84.85900	75.70780	88.09290	1916.25287	867.57994	-2339.55257	1
719	H	85.99500	75.79680	89.50290	-1845.52259	-1492.04024	2065.45117	1
720	H	84.35600	76.61180	89.54990	-672.14676	3070.81391	128.63473	1
721	C	86.39100	78.49780	89.48490	356.99775	773.14505	-325.96063	1
722	H	87.06500	79.27980	89.07290	1431.02713	-2197.52367	-1738.18218	1
723	H	87.08200	77.89680	90.11390	-988.36040	-1147.52745	2757.63498	1
724	C	85.32100	79.24980	90.26490	550.97854	-644.36010	-335.66904	1
725	H	85.66100	79.80480	91.16590	-1836.89018	-1093.54418	2308.29413	1
726	H	84.50800	78.55480	90.56390	2591.63684	369.16478	-1745.09658	1
727	H	84.81600	79.99880	89.61990	946.08171	-1654.16507	-2503.37643	1
728	C	86.59100	76.33380	86.29590	40.75260	705.04492	-576.80317	1
729	O	86.87600	75.13580	86.32990	266.79178	-247.24634	-700.94124	1
730	N	85.94400	76.86980	85.20790	-711.83126	-4.55967	453.81467	1
731	H	85.63800	77.81680	85.14890	842.37471	1784.07581	-2450.65391	1
732	C	85.54400	75.97380	84.09090	-585.75515	55.87593	-696.57719	1
733	H	84.97100	75.16780	84.52390	-586.97010	-2292.83159	-2072.82793	1
734	C	84.70500	76.68680	83.02590	816.47427	-154.59043	-375.39655	1
735	H	85.34800	77.43880	82.51990	-2027.81144	-1170.43123	-2101.49893	1
736	C	84.27500	75.71480	81.91990	390.62822	-9.12547	823.87943	1
737	H	85.09700	75.06980	81.54390	-1043.18891	1845.65843	-2324.54901	1
738	H	83.47900	75.04880	82.31590	-1130.74826	2166.20224	1981.71705	1

739	H	83.83700	76.40380	81.16690	-1216.70776	-1778.85079	-2292.05984	1
740	C	83.45000	77.48980	83.55590	419.46463	384.39946	712.55700	1
741	H	82.97200	77.88180	82.63290	2756.57425	499.32282	1431.85241	1
742	H	83.89400	78.25780	84.22490	-2550.79173	-1013.73960	-1537.53692	1
743	C	82.33100	76.72480	84.30590	-569.19555	-645.58374	-301.14624	1
744	H	81.47300	77.36780	84.59690	625.84537	408.42952	3056.09704	1
745	H	82.01000	75.87880	83.66190	-2554.73294	-333.43172	1805.65477	1
746	H	82.78500	76.35380	85.24990	1986.33564	2424.54117	-272.57487	1
747	C	86.82000	75.33080	83.39190	637.84342	6.19652	651.58912	1
748	O	86.93000	74.10180	83.14490	-599.14387	513.65301	28.53841	1
749	N	87.87300	76.12580	83.05390	-663.86913	290.65683	-432.97653	1
750	H	87.78700	77.10580	83.21590	969.26659	2388.87271	1803.34014	1
751	C	89.14600	75.69580	82.51290	630.94474	149.00597	-641.21522	1
752	H	88.77200	75.17380	81.64490	1623.04462	-2062.26052	-1735.23311	1
753	C	89.90200	76.92480	82.03590	429.36837	562.65273	-574.90495	1
754	H	89.27500	77.50780	81.32890	-1806.21469	1033.38445	2359.64643	1
755	H	90.24800	77.70980	82.74190	968.87177	-2107.61869	2125.43106	1
756	C	91.23100	76.59480	81.38190	335.66772	-777.81997	337.30443	1
757	C	91.21500	76.27080	80.01490	-23.36967	907.47043	86.03647	1
758	H	90.34000	76.17680	79.38890	-467.53920	-1960.65393	-2415.67164	1
759	C	92.38300	75.83580	79.33690	124.29451	103.54849	897.37372	1
760	H	92.23500	75.47680	78.32890	1781.61946	-2563.46973	-390.74451	1
761	C	93.59700	75.74780	79.99190	629.41964	-214.97680	-623.75227	1
762	H	94.46100	75.44580	79.41890	-281.46604	2946.36560	1066.73935	1
763	C	92.48600	76.63880	82.03490	851.84921	315.37290	-79.64839	1
764	H	92.45700	76.91580	83.07890	1218.97345	-2335.50035	1719.81629	1
765	C	93.65300	76.24480	81.37190	120.85959	619.33722	658.22896	1
766	H	94.58100	76.33180	81.91690	2968.31632	-683.86815	787.17776	1
767	C	89.91100	74.63880	83.25790	-899.20530	-97.73742	115.44797	1
768	O	90.31700	73.58680	82.77890	113.37404	592.87936	-509.18329	1
769	N	90.07200	74.84380	84.60690	-64.86282	763.94033	-353.35574	1
770	H	89.75100	75.72580	84.94490	-1902.98710	2503.37145	99.98835	1
771	C	90.99200	74.14780	85.47890	176.20601	833.55186	324.95190	1
772	H	91.87600	73.95580	84.88990	-1938.84985	1230.85296	2150.36938	1
773	C	91.44100	74.96580	86.68890	173.02299	894.91988	-25.14875	1
774	H	90.54900	75.39680	87.18990	1719.42224	-1244.72462	-2322.17011	1
775	H	91.98500	74.47680	87.52490	-140.95733	3113.86396	-426.85887	1
776	C	92.29500	76.20180	86.29890	-749.23088	-254.34103	453.22702	1
777	H	91.81200	76.81980	85.51190	2493.22330	789.70012	-1748.83891	1
778	C	92.49600	77.08680	87.49090	615.93485	-41.19508	671.10225	1
779	H	93.34000	76.67480	88.08490	-644.39557	2184.95975	-2170.00725	1
780	H	92.75900	78.11980	87.17690	-2280.25586	-592.01586	-2085.22821	1
781	H	91.62000	77.10680	88.17290	-2013.59702	1687.69269	1730.70698	1
782	C	93.63900	75.80880	85.71290	-662.53911	-597.98125	186.84578	1
783	H	94.39500	76.62280	85.73390	2425.53471	-1273.93938	-1546.63701	1
784	H	94.08800	74.94380	86.24590	218.14437	-1964.51532	2447.71706	1
785	H	93.51200	75.52980	84.64590	2280.59240	1358.96732	-1688.29274	1
786	C	90.49500	72.83780	85.92890	-810.95123	-84.95218	408.15712	1
787	O	91.27500	71.96380	86.38890	-129.50298	-269.20414	731.01665	1
788	N	89.19100	72.60280	85.69690	-251.93515	121.47951	796.51974	1
789	H	88.59100	73.30280	85.31790	43.31501	-3145.28314	-59.53133	1
790	C	88.45900	71.35680	85.94490	726.48390	-372.36520	406.22199	1
791	H	89.12800	70.64180	86.40090	2333.32560	-2080.92148	351.54472	1
792	C	87.22600	71.64880	86.78490	631.74897	106.00902	648.92706	1
793	H	86.71000	70.67580	86.92890	-1829.54859	1647.60973	1958.66290	1
794	O	86.29500	72.52080	86.19690	722.07675	-294.97409	123.38023	1
795	H	86.60700	73.42780	86.23990	272.75475	493.84464	-3095.14920	1
796	C	87.61600	72.22880	88.17090	-735.97154	-495.50351	-210.41188	1
797	H	86.73200	72.42180	88.81590	-1085.15946	2935.96839	317.40318	1
798	H	88.12700	73.21380	88.10690	-35.06783	-1908.79420	2500.70014	1
799	H	88.25200	71.51380	88.73390	1027.51984	2137.29586	-2067.46115	1
800	C	88.17800	70.69480	84.65590	-47.19641	571.30404	-709.10874	1

801	O	88.41700	69.53780	84.41390	235.50712	-361.22663	-661.57309	1
802	N	87.69700	71.45480	83.66790	-641.78769	345.94488	-425.56196	1
803	H	87.49600	72.42580	83.77290	2623.53799	492.24444	1665.22373	1
804	C	87.33000	70.99180	82.32790	-514.93006	-529.73946	-534.48494	1
805	H	86.87200	71.79880	81.77690	-1048.08217	-1588.60383	2505.21214	1
806	H	86.53900	70.25880	82.39390	3137.72187	-193.95131	123.73591	1
807	C	88.38800	70.38780	81.46990	-130.35224	-889.90919	-150.06972	1
808	O	88.07800	69.34780	80.89690	-369.07184	-568.54953	405.17236	1
809	N	89.50700	71.10180	81.21690	-378.33265	-574.17396	489.75602	1
810	H	89.71200	71.85980	81.82990	-620.69684	-1577.17562	2650.56197	1
811	C	90.54000	70.62380	80.30890	-321.64006	682.06396	512.62797	1
812	H	90.04700	70.37080	79.38190	2550.62627	-1531.66824	1022.99769	1
813	C	91.49700	71.77680	80.00190	-684.88866	-170.05872	577.45871	1
814	H	90.87200	72.69580	80.01990	-275.26504	2904.80995	-1176.66246	1
815	C	92.63800	71.97780	81.09890	362.06379	824.28792	144.60375	1
816	H	93.11400	72.96780	80.93290	-1446.05167	-651.16070	2717.19534	1
817	H	93.41500	71.18380	81.09390	-1775.22326	-144.94800	-2593.41448	1
818	H	92.18000	72.00080	82.11090	2936.47914	-377.82875	1064.21893	1
819	C	92.06200	71.74980	78.55590	282.82799	-290.71302	816.66717	1
820	H	91.23500	71.68480	77.81690	-1767.79188	2090.98319	1549.49263	1
821	H	92.43600	72.79180	78.45790	-1695.32947	2126.98507	1581.14475	1
822	C	93.19900	70.75380	78.20890	626.50407	-561.61670	-351.46882	1
823	H	94.09500	70.93880	78.83990	-2524.82516	385.19354	-1837.14727	1
824	H	93.64100	70.73480	77.18990	902.56296	-2279.38943	1971.79871	1
825	H	92.87200	69.72480	78.47090	-2537.52079	633.89517	1748.53978	1
826	C	91.19200	69.33780	80.85890	-845.85400	40.75214	338.11430	1
827	O	91.46200	68.34780	80.13890	-212.93731	675.59238	-349.08432	1
828	N	91.48600	69.32480	82.18790	-413.14054	594.69609	-433.96284	1
829	H	91.23100	70.17480	82.64090	2768.65843	-1191.23536	902.06154	1
830	C	91.91500	68.12480	82.90290	674.76662	-4.89852	-613.28380	1
831	H	92.79300	67.74880	82.39990	1137.05328	2474.96393	1574.76652	1
832	C	92.25100	68.54980	84.34890	-623.70194	-217.42377	628.62850	1
833	H	91.36300	68.83680	84.95190	2031.03728	-2134.16384	-1103.83808	1
834	C	92.93000	67.35280	85.13090	-38.21424	545.58213	729.61004	1
835	H	93.39500	67.66780	86.08990	2816.88312	785.42742	-1160.38765	1
836	H	93.59900	66.86780	84.38790	683.50592	2165.82641	2177.20965	1
837	H	92.08600	66.72380	85.48590	-1297.42712	-2085.69786	-1965.90273	1
838	C	93.12200	69.81780	84.36490	-82.64499	-713.48418	-561.74829	1
839	H	92.59100	70.79080	84.28690	418.05189	-1824.98671	-2528.41499	1
840	H	93.47800	69.79780	85.41690	-1799.71518	611.07834	-2507.15671	1
841	H	93.92400	69.74080	83.59990	-2110.06411	-1558.22569	-1737.17828	1
842	C	90.88500	67.01480	82.85490	-556.90750	641.70428	-330.93904	1
843	O	91.19100	65.97680	82.31990	578.50465	275.09237	-461.82658	1
844	N	89.59800	67.27880	83.21290	527.47058	507.40287	420.70109	1
845	H	89.33800	68.17280	83.56890	-3101.06471	-449.88638	281.47141	1
846	C	88.50800	66.28280	83.31090	-543.31176	554.50542	478.31693	1
847	H	87.63400	66.81180	83.66190	-1058.56279	-2935.79372	398.47993	1
848	H	88.77800	65.52880	84.03490	13.31072	2345.67527	2096.62981	1
849	C	88.13700	65.55880	82.06790	314.14467	-561.63813	-646.00831	1
850	O	88.04400	64.34280	82.03790	301.13903	-577.45636	446.63929	1
851	N	87.94300	66.29480	80.94490	-133.31966	640.18901	-533.90653	1
852	H	88.08700	67.28080	80.99990	-2812.65001	978.91141	-1014.37598	1
853	C	87.72000	65.63780	79.67190	413.69976	-526.35060	-619.07879	1
854	H	87.02600	64.82080	79.79990	1059.06714	206.50054	2955.32748	1
855	C	86.96700	66.60780	78.71390	-92.17659	171.75748	-890.76026	1
856	H	87.46400	67.58080	78.50890	3104.91925	80.66297	501.19475	1
857	H	86.78100	66.01880	77.79090	2249.29314	359.21715	-2170.22340	1
858	C	85.61000	66.79680	79.39290	257.20112	777.19145	-401.58690	1
859	O	84.83300	65.81480	79.48890	41.48806	742.67780	265.20870	1
860	N	85.34400	67.99780	79.87490	293.16062	776.53241	154.03428	1
861	H	86.08300	68.66580	79.96190	-2086.18902	-1479.44611	1832.28840	1
862	H	84.39500	68.15680	80.14790	-3074.19845	130.00965	656.22221	1

863	C	88.89800	64.98780	79.03490	729.59863	376.10731	-397.08957	1
864	O	88.72200	64.04280	78.34190	-693.58536	354.52459	-129.91881	1
865	N	90.14400	65.40080	79.46790	210.13862	-791.79120	-203.91357	1
866	H	90.25700	66.25580	79.96790	-1062.04363	2020.92879	-2164.74858	1
867	C	91.31700	64.73480	79.05890	97.70485	515.88956	745.49495	1
868	H	91.30700	64.62180	77.98490	-2927.03199	1151.10278	-75.31504	1
869	H	92.21500	65.29480	79.27790	1062.09970	-1925.40192	2250.11064	1
870	C	91.40100	63.43180	79.75790	310.82975	-796.83060	-316.06465	1
871	O	91.82500	62.42080	79.26990	-577.07887	332.13922	424.60658	1
872	N	91.02800	63.38680	81.05790	661.05041	154.45958	-501.82356	1
873	H	90.80500	64.21680	81.56290	-2517.52490	1601.70543	-997.41382	1
874	C	90.91800	62.15580	81.79590	275.37986	-734.86526	-464.31669	1
875	H	91.86200	61.64080	81.70190	-1066.15996	2389.99152	1746.27308	1
876	C	90.82800	62.40680	83.27890	331.56885	-794.75202	299.80382	1
877	H	90.54300	61.55180	83.92790	1677.69666	2644.70176	298.51762	1
878	H	89.92600	63.04680	83.38890	-2285.97755	-1673.79653	1367.82238	1
879	C	92.01900	63.17780	83.96190	-507.29365	-341.32403	-676.46291	1
880	H	92.39400	64.07880	83.43090	2371.87763	457.82649	2015.64324	1
881	C	91.67700	63.61180	85.38990	-427.74577	655.48410	467.78751	1
882	H	91.21000	62.80180	85.98990	-2952.71904	-361.96864	-1024.03866	1
883	H	92.58900	63.86880	85.96890	1883.89389	-747.97171	-2406.18128	1
884	H	90.99500	64.48680	85.45990	-1863.27798	1324.56257	-2161.47065	1
885	C	93.24800	62.26580	83.90690	395.64209	142.65578	809.05356	1
886	H	93.04800	61.32980	84.47190	2319.96381	-1501.10801	1504.21703	1
887	H	94.12500	62.84280	84.26990	-1438.91126	1875.01864	-2076.55140	1
888	H	93.55700	61.98580	82.87690	1529.33518	1892.55504	1994.39103	1
889	C	89.83700	61.22880	81.39190	-670.64914	389.97123	-479.16926	1
890	O	90.05200	60.01880	81.38790	781.35197	-104.16432	47.60376	1
891	N	88.67800	61.73480	81.04490	330.59139	-215.15975	746.38322	1
892	H	88.46700	62.70780	81.09490	-1221.30094	-2124.56655	1973.03503	1
893	C	87.67100	60.85880	80.39390	540.49009	460.58516	571.99894	1
894	H	87.32000	60.08580	81.06090	-2109.82119	420.31282	-2295.69552	1
895	C	86.36900	61.62080	80.15290	437.16704	378.29483	705.14467	1
896	H	86.66700	62.53680	79.59990	-931.64399	-1905.93439	2323.29073	1
897	C	85.41000	60.79180	79.24990	-40.18690	139.68571	-900.17994	1
898	H	85.78800	60.71980	78.20790	-337.71721	2233.51169	2189.88558	1
899	H	84.42100	61.27980	79.11590	-2232.42026	1456.66377	1671.12438	1
900	H	85.21300	59.82180	79.75490	-1555.71342	-964.44593	-2558.87202	1
901	C	85.66900	62.05280	81.46790	59.94967	164.68914	894.83771	1
902	H	84.86800	62.78280	81.22090	2288.98316	-975.36532	-1925.47262	1
903	H	85.26400	61.20280	82.05790	1418.49257	-211.68327	-2800.23128	1
904	H	86.41700	62.61580	82.06690	1686.79616	1795.69322	-1956.63763	1
905	C	88.14800	60.21080	79.10090	-460.61643	407.85428	673.00698	1
906	O	87.98300	59.02080	78.84890	-678.66037	361.86766	-179.16229	1
907	N	88.93200	60.97080	78.26790	603.21865	-484.47884	-337.75701	1
908	H	88.88200	61.95180	78.43890	950.00296	-2010.56634	-2225.61084	1
909	C	89.63900	60.42180	77.09990	725.26411	366.18609	413.94532	1
910	H	88.99200	59.82980	76.46890	-2637.04200	-778.25505	-1529.23341	1
911	C	90.13200	61.55680	76.21090	-245.39354	328.56694	-814.41806	1
912	H	90.77500	62.20780	76.84090	2388.04920	1975.44820	-541.34249	1
913	C	91.04800	61.07380	75.04890	-454.31315	-405.65078	-678.60004	1
914	H	91.94600	60.50580	75.37390	-1639.17125	-2672.23587	265.51703	1
915	H	91.50200	61.91580	74.48490	2378.32481	2035.61491	313.16012	1
916	H	90.55600	60.35680	74.35590	-884.49316	-328.70926	-3001.30776	1
917	C	89.00800	62.48180	75.66090	7.02713	567.02539	714.06151	1
918	H	88.47400	61.93980	74.85190	2612.78447	-1684.72838	-482.98432	1
919	H	88.14100	62.60780	76.34490	-2631.13738	-1490.45271	-868.27012	1
920	C	89.53000	63.78780	75.11390	-553.20240	-415.10246	594.22895	1
921	H	90.19400	63.52080	74.26490	942.90686	-3000.78915	66.46305	1
922	H	88.68400	64.35180	74.66590	-2106.33165	2266.34950	-570.30969	1
923	H	89.97900	64.42080	75.90890	-2572.36207	1655.35637	-735.50996	1
924	C	90.77300	59.45680	77.46190	332.79423	-609.46388	-590.97613	1

925	O	90.96700	58.38780	76.89490	-33.13991	738.45028	277.88517	1
926	N	91.47500	59.73380	78.58890	-205.99053	-461.63039	676.11949	1
927	H	91.42900	60.64380	78.99590	1676.62045	1711.55738	2039.05405	1
928	C	92.46700	58.82380	79.17890	-724.88543	-475.55518	-282.55864	1
929	H	93.13400	58.59180	78.36190	-2154.49200	2198.57070	-650.13636	1
930	C	93.39400	59.54580	80.25190	-727.45292	-66.62977	545.73229	1
931	H	93.67500	58.93680	81.13790	-477.43093	1900.27554	2461.55211	1
932	H	92.68800	60.32980	80.60090	-1885.56164	2439.64756	-625.30258	1
933	C	94.60100	60.20980	79.64990	0.07779	136.16699	-901.61497	1
934	H	94.23900	60.46180	78.62990	-1494.27344	2209.19348	-1668.78317	1
935	C	95.06300	61.43480	80.47190	181.28753	817.11273	-361.81848	1
936	H	95.28300	61.04180	81.48790	-1711.81780	-2403.28153	1091.85344	1
937	H	94.26400	62.20680	80.47790	-1638.91079	-1988.92275	-1804.54535	1
938	H	96.00300	61.82780	80.02690	789.63194	-1754.67722	2489.13951	1
939	C	95.76500	59.20580	79.52190	-723.88704	514.99269	205.47768	1
940	H	96.08900	58.91780	80.54590	-2579.66576	1679.81506	649.43986	1
941	H	95.53700	58.21280	79.07790	1397.94009	-2453.65391	1386.92906	1
942	H	96.53300	59.68580	78.87890	591.89494	-2907.09292	1047.23319	1
943	C	91.86500	57.57880	79.69390	-582.56779	-303.19306	-632.56600	1
944	O	92.42900	56.49880	79.48290	535.77260	-24.90168	-579.61613	1
945	N	90.65400	57.56080	80.28190	-381.42184	-696.43704	286.64460	1
946	H	90.21300	58.42780	80.50190	-2074.13190	2027.32988	-1219.07205	1
947	C	89.92200	56.39580	80.60690	-269.30077	-32.73197	-870.54966	1
948	H	90.56100	55.73180	81.16890	2609.90647	-683.93234	-1618.28644	1
949	C	88.72200	56.64380	81.52490	-255.95642	818.20196	-310.61692	1
950	H	88.11700	57.51680	81.19890	-2200.53987	-872.08249	2072.51602	1
951	C	87.81900	55.37180	81.65790	-270.06871	308.71118	-814.37786	1
952	H	87.24900	55.30580	80.70590	-1679.32935	2605.55697	537.72862	1
953	H	88.39100	54.44580	81.87890	2325.06348	1309.71624	-1666.41814	1
954	H	87.10100	55.43280	82.50390	1541.58712	-1896.34312	-1981.31727	1
955	C	89.30500	57.08480	82.90890	-335.17659	787.08053	-315.61352	1
956	H	89.91800	58.00280	82.78290	2332.24242	609.63530	-2021.68651	1
957	H	89.92900	56.23680	83.26390	-1968.73005	1708.57905	1761.55779	1
958	H	88.39800	57.27180	83.52290	-1980.23295	-1726.76671	-1730.65895	1
959	C	89.44700	55.63980	79.32990	-359.27848	576.33568	608.44652	1
960	O	89.89800	54.49180	79.18290	-449.67866	648.30608	33.39991	1
961	N	88.71500	56.24380	78.37590	-687.55598	361.92186	-330.07821	1
962	H	88.39800	57.18380	78.48190	-1682.32476	-210.17816	-2650.25183	1
963	C	88.13600	55.43780	77.35890	481.60797	-515.20904	-577.98305	1
964	H	87.98700	54.42380	77.69790	2167.44450	1544.81508	-1677.48530	1
965	C	86.80000	55.99480	76.89190	518.43415	-69.51995	746.88955	1
966	H	86.79700	57.04880	76.53890	-1143.95498	2795.22945	-881.07069	1
967	H	86.30400	55.48680	76.03690	1254.94298	2533.45344	-1380.20217	1
968	C	85.67600	55.90280	77.97190	-484.48634	-150.54762	757.66708	1
969	H	86.01400	56.61080	78.75890	1871.95387	1227.76250	2210.56875	1
970	H	85.62800	54.90080	78.44890	-2218.83620	1002.44526	1992.50988	1
971	S	83.95900	56.24880	77.57990	-404.97605	-144.73323	355.32703	1
972	C	84.12800	58.00880	77.20090	-197.22130	-509.73989	-729.87671	1
973	H	83.24300	58.67880	77.24590	-414.07682	-2980.23816	919.21005	1
974	H	84.54900	58.20380	76.19090	411.47298	2082.84638	-2321.78103	1
975	H	84.85200	58.45580	77.91490	2087.45348	1033.17280	-2115.02202	1
976	C	89.02800	55.25480	76.12090	452.00509	-403.62784	-681.34204	1
977	O	88.67300	54.33880	75.34490	-482.40885	216.79530	-586.43732	1
978	N	90.17100	55.99680	75.92590	-667.46038	-222.59038	466.50022	1
979	H	90.45000	56.78180	76.47390	1347.87838	2726.98930	-803.10612	1
980	C	91.03600	55.84080	74.74190	-889.83329	191.54029	-54.40627	1
981	H	91.33000	56.77180	74.28090	-1586.87762	296.94965	-2700.34564	1
982	H	90.59400	55.18780	74.00390	-572.29216	2941.77648	957.42313	1
983	C	92.32500	55.26980	75.05690	636.94938	-640.72478	123.36225	1
984	O	92.92800	54.78180	74.07790	-199.28590	-698.80068	309.17628	1
985	N	92.85900	55.28180	76.31390	-420.26493	-726.64527	89.64558	1
986	H	92.39700	55.80080	77.02990	-2179.54868	-321.32446	2246.00632	1

987	C	94.18600	54.76780	76.54990	-516.28029	736.80378	-148.41107	1
988	H	94.42000	54.19980	75.66190	2046.46465	2181.63635	-975.02384	1
989	C	95.24000	55.87480	76.84190	-403.38982	768.94288	-278.30649	1
990	H	96.23400	55.39980	76.97990	1643.87484	994.04106	-2491.54252	1
991	H	94.96800	56.43880	77.75990	1807.35693	-538.28990	-2518.31911	1
992	C	95.32500	56.83880	75.67490	658.83343	599.46334	-195.02109	1
993	C	94.57400	58.04680	75.56990	735.77653	-405.26549	354.74468	1
994	H	93.81100	58.35680	76.26890	1625.72964	-2631.85930	573.18932	1
995	C	94.76300	58.89280	74.47790	-420.74497	-268.55247	-763.08862	1
996	H	94.19800	59.78980	74.27190	-2210.21796	872.57426	2061.98374	1
997	C	95.64700	58.60780	73.44990	417.26536	581.36110	565.11937	1
998	O	95.87200	59.44180	72.41690	-555.02119	-364.40461	427.53712	1
999	H	96.32200	59.00280	71.69190	1960.54608	-1695.32460	1783.35632	1
1000	C	96.26800	56.58880	74.66090	-707.17336	-527.74710	-229.86917	1
1001	H	96.92000	55.72780	74.64290	-1392.07536	228.65270	-2812.12915	1
1002	C	96.40200	57.42980	73.55890	243.88306	-863.32614	-163.21773	1
1003	H	97.07000	57.15380	72.75690	1815.36562	1085.64151	-2328.96037	1
1004	C	94.25100	53.70880	77.63690	517.31090	682.10256	-313.96900	1
1005	O	94.75800	52.60880	77.40090	-416.13956	-623.25887	-249.00497	1
1006	N	93.66100	53.96080	78.80590	256.79754	-672.06997	441.64383	1
1007	H	93.27600	54.86780	78.95390	-1234.01676	-2604.29812	1262.16487	1
1008	C	93.44100	53.00680	79.89090	-599.56266	600.82935	-333.13618	1
1009	H	94.35700	52.47780	80.10790	1827.87857	1575.23439	2018.84194	1
1010	C	92.94400	53.62880	81.25290	445.77242	-396.55549	-689.55181	1
1011	H	92.05600	54.20480	80.91490	1528.57417	1902.28294	1985.70059	1
1012	H	92.64800	52.84180	81.97990	1217.80572	896.89466	2758.75976	1
1013	C	93.94700	54.46080	82.04690	-393.38206	815.68796	106.55845	1
1014	H	94.47900	55.07880	81.29190	-1516.57166	-2750.17328	186.50351	1
1015	H	94.64500	53.84780	82.65590	2442.85213	-1927.82729	462.79762	1
1016	C	93.27700	55.39580	83.02990	-567.21803	42.86215	712.65528	1
1017	O	92.47900	54.97380	83.85390	278.53089	-654.64459	342.76557	1
1018	N	93.52300	56.72180	82.88790	-587.28231	-86.24744	600.27756	1
1019	H	94.41900	57.02380	82.56290	-2097.16996	45.48301	-2344.78905	1
1020	H	92.86000	57.35880	83.28190	1729.79074	364.51200	-2602.53362	1
1021	C	92.57700	51.86780	79.50590	309.23997	595.98626	616.94572	1
1022	O	92.78500	50.65780	79.79990	-586.64018	395.11844	-351.22919	1
1023	N	91.47300	52.18080	78.75590	361.09023	362.27129	671.59932	1
1024	H	91.20800	53.14080	78.70990	2028.97080	263.32461	2390.01337	1
1025	C	90.61600	51.17280	78.07990	625.30084	-488.83724	448.87417	1
1026	H	90.80800	50.23680	78.58390	-2144.40996	-1361.23221	-1856.55030	1
1027	C	89.08300	51.53180	78.20090	477.40451	-650.07167	425.37367	1
1028	H	88.90900	52.51580	77.71390	-2984.13350	-814.07351	574.85456	1
1029	H	88.49600	50.75480	77.66490	387.63192	2809.97985	1360.87507	1
1030	C	88.66600	51.54680	79.65090	-16.46731	727.72636	549.17591	1
1031	H	89.15400	52.39480	80.17690	1412.95289	2456.78161	-1366.02141	1
1032	H	89.07300	50.61780	80.10390	2470.71274	-1055.01199	-1637.30098	1
1033	C	87.13900	51.48180	79.68990	-432.57797	-796.00644	-103.44587	1
1034	H	86.76700	52.34880	79.10290	822.00885	-1659.18601	2543.54663	1
1035	H	86.88900	50.48680	79.26190	-2959.95700	805.02226	699.15660	1
1036	C	86.57500	51.74980	81.08890	626.28866	582.54457	-315.99896	1
1037	H	86.92000	52.73180	81.47690	-1470.60068	2538.39473	-1136.71109	1
1038	H	86.98500	50.92780	81.71390	428.27849	-2564.59065	-1771.34937	1
1039	N	85.12500	51.68880	81.07790	-325.89062	634.10551	-452.08162	1
1040	H	84.77400	50.75480	80.78390	2061.34753	2252.62626	-758.12104	1
1041	H	84.69900	52.02580	81.96490	-2254.09242	-2171.37274	-320.05317	1
1042	H	84.83800	52.34680	80.32490	2702.72499	846.95956	-1369.73113	1
1043	C	90.95300	50.94980	76.60790	-791.95575	415.04482	178.87113	1
1044	O	90.98900	51.89480	75.82090	-477.04654	-343.75641	-527.14833	1
1045	N	91.05100	49.72080	76.17790	-649.59839	398.10287	363.60462	1
1046	H	90.96200	48.97080	76.82890	1458.14370	2348.37727	-1502.38722	1
1047	C	91.29900	49.34780	74.85290	-196.54250	852.49423	257.05181	1
1048	H	91.82800	50.10280	74.28990	810.25378	-484.59869	-3001.14631	1

1049	C	92.38200	48.18380	74.82990	-232.57955	668.07899	-575.35052	1
1050	H	92.07000	47.34480	75.48790	1997.64510	893.54082	2260.35950	1
1051	H	92.30400	47.74580	73.81190	-1462.04695	-2629.60319	919.69126	1
1052	C	93.85500	48.62380	74.83190	-424.38912	617.07221	520.16032	1
1053	H	94.07900	49.05780	73.83490	-1533.42661	-1555.59845	-2264.27527	1
1054	H	94.46100	47.69280	74.87390	-1012.94100	-909.17038	-2836.47422	1
1055	C	94.33100	49.57380	75.99790	-123.48169	749.27765	504.76358	1
1056	H	93.81300	50.55380	75.93290	2516.78984	1864.77128	294.31821	1
1057	H	94.18600	49.06480	76.97490	-1086.76355	2939.52485	-276.34191	1
1058	C	95.82100	49.84980	75.84490	662.05657	334.81084	530.12621	1
1059	H	96.00100	50.55280	75.00390	1609.52510	-840.60521	2569.24854	1
1060	H	96.33200	48.90480	75.56290	-1866.05211	2255.16258	1153.39391	1
1061	N	96.36400	50.35680	77.12790	83.85254	-840.00723	-5.37561	1
1062	H	95.93900	49.92380	77.97290	366.75803	-1847.68540	-2519.87568	1
1063	H	96.24700	51.38080	77.26290	-212.69305	-2418.09462	-2001.45105	1
1064	H	97.39300	50.20580	77.11590	2220.86465	1037.98853	1971.94479	1
1065	C	90.00100	49.00580	74.10290	-646.14395	-433.52289	475.40183	1
1066	O	90.08300	48.49180	72.98190	-109.13754	630.33862	463.02208	1
1067	N	88.81000	49.29580	74.67490	645.30425	-291.62975	459.57241	1
1068	H	88.70200	49.78880	75.53390	-1336.66204	-690.57977	2763.08892	1
1069	C	87.55400	48.97680	74.08890	810.69662	332.42387	252.42102	1
1070	H	87.68600	49.00780	73.01690	1261.16373	-2809.95431	641.75465	1
1071	C	87.15200	47.53380	74.50490	195.68149	-372.14895	-809.11366	1
1072	H	87.00100	47.55280	75.60590	627.64980	-2730.86972	1430.60566	1
1073	H	88.03400	46.90580	74.25790	-294.96673	1838.16130	2536.21448	1
1074	C	85.88800	46.98380	73.78190	-514.60994	-676.19537	-330.73772	1
1075	H	85.04600	47.70380	73.87690	2159.55539	2127.79094	840.86413	1
1076	C	86.19700	46.73680	72.27590	513.37198	-390.36037	644.60763	1
1077	H	86.97300	45.94380	72.21590	757.55728	1552.81916	-2629.27478	1
1078	H	86.79000	47.58380	71.86990	-2370.02827	2.51577	2069.10268	1
1079	H	85.32100	46.35980	71.70490	1419.99629	2200.09975	-1743.96039	1
1080	C	85.44900	45.69380	74.43390	-572.82536	-688.13157	172.61823	1
1081	H	86.17400	44.86080	74.31090	-2596.52346	1295.27064	1215.96304	1
1082	H	84.50200	45.40480	73.93090	-2898.30672	-262.72757	-1195.41566	1
1083	H	85.30700	45.81980	75.52790	-2858.06058	-603.19043	1168.70751	1
1084	C	86.58300	49.95080	74.48290	470.41433	35.85679	780.30485	1
1085	O	86.54200	50.31480	75.64190	-588.56167	469.27101	-238.76160	1
1086	N	85.76300	50.38280	73.53390	74.47277	-813.32802	213.59687	1
1087	H	85.97600	50.05580	72.61690	1805.71083	1545.11727	2061.61278	1
1088	C	84.62100	51.21080	73.67290	-165.33727	-443.14724	-779.57367	1
1089	H	84.52300	51.36680	74.73690	-1667.06575	2602.13103	-589.94247	1
1090	C	84.88700	52.61880	73.07790	871.12257	223.68728	-150.20145	1
1091	H	83.94100	53.16780	72.88390	1370.99310	582.96801	2771.05620	1
1092	H	85.25400	52.43280	72.04590	-1938.95471	-86.65666	-2476.12025	1
1093	C	85.88700	53.42880	73.88690	645.13091	-641.00778	66.07680	1
1094	H	86.80800	52.87480	74.16590	-292.94778	2772.15421	-1458.61881	1
1095	H	85.38700	53.70380	74.83990	-220.80937	2915.27530	-1162.17013	1
1096	C	86.28500	54.67180	73.14490	-46.40004	-652.09192	-635.66828	1
1097	H	85.41500	55.31380	72.88890	972.19535	2320.72695	-1888.72678	1
1098	H	86.96800	55.30180	73.75390	1566.75036	2000.37395	1855.26914	1
1099	N	87.02500	54.16280	71.89790	-608.96999	352.30617	466.59212	1
1100	H	86.52100	54.27380	71.04090	2255.82456	2188.50576	-141.15364	1
1101	C	88.26400	53.66480	71.80990	-569.81877	363.39144	-612.13090	1
1102	N	89.10000	53.50980	72.82190	577.68006	610.17971	-81.47856	1
1103	H	88.79100	53.70980	73.75190	-327.84551	2636.03825	1685.83686	1
1104	H	90.04200	53.23980	72.62390	2824.26856	630.69254	1234.48785	1
1105	N	88.74400	53.35480	70.59690	243.88392	-464.76129	661.20335	1
1106	H	88.15000	53.32880	69.79290	593.76744	-1077.70321	-2895.55215	1
1107	H	89.71700	53.20780	70.42090	1555.41710	2697.84599	447.80674	1
1108	C	83.32200	50.61480	73.20590	-627.51682	-478.99942	-456.32576	1
1109	O	83.24600	50.07780	72.10590	158.13124	76.39803	769.92537	1
1110	N	82.30300	50.67980	74.02090	288.65807	-357.90700	-707.99109	1

1111	H	82.47000	51.01780	74.94390	-1317.19795	2080.32748	1958.43135	1
1112	C	80.90500	50.41080	73.69990	213.65388	861.83773	207.45781	1
1113	H	80.90700	49.61780	72.96590	2621.91957	1226.50582	1232.65870	1
1114	C	80.09800	49.91280	74.88890	891.07230	99.44429	165.98792	1
1115	H	80.65700	49.07480	75.35590	-610.32980	2738.34949	-1423.78574	1
1116	H	79.13500	49.50380	74.51390	-1334.15046	-2455.18096	-1445.80609	1
1117	O	79.93000	50.94380	75.84990	404.99634	677.47108	25.26136	1
1118	H	80.78600	51.10580	76.25190	2045.17830	-1934.17400	1405.14871	1
1119	C	80.20200	51.63780	73.09290	-290.77136	460.76193	731.16446	1
1120	O	80.82500	52.67380	72.89290	6.22925	-670.23758	417.57636	1
1121	N	78.90600	51.49280	72.63190	804.15742	-245.13745	76.88145	1
1122	H	78.46200	50.61780	72.45690	1966.48604	2031.87133	1379.36862	1
1123	C	78.10900	52.61380	72.12490	-38.80295	-523.18019	-745.80683	1
1124	H	78.62900	53.02480	71.27190	571.29205	3037.68164	586.80650	1
1125	C	76.74700	52.13880	71.62190	-1.64929	686.49319	600.14613	1
1126	H	76.16900	52.99880	71.21990	960.73814	-1454.63825	2619.01432	1
1127	H	76.18700	51.79780	72.51890	-1762.84482	-2491.16498	-764.65771	1
1128	C	76.84800	51.01580	70.56590	-675.82134	331.44193	514.64820	1
1129	H	75.93000	51.16180	69.95690	965.02650	1592.22819	2536.09138	1
1130	H	77.66100	51.23680	69.84290	2357.70359	464.66706	2030.65126	1
1131	S	76.94200	49.31380	71.19890	341.30531	408.22216	167.55883	1
1132	C	75.79700	48.59480	69.95690	827.16267	245.02624	295.32196	1
1133	H	75.35400	47.67380	70.39290	2064.85392	-2370.72865	-119.37418	1
1134	H	76.40800	48.33680	69.06590	-360.06608	-2325.14734	2088.60443	1
1135	H	75.08300	49.32480	69.51890	1737.04504	1346.82353	-2250.99248	1
1136	C	77.92300	53.80080	73.01490	-216.78428	637.19466	615.17358	1
1137	O	78.11000	54.94380	72.61990	511.66076	-576.12974	-172.93066	1
1138	N	77.71000	53.58280	74.34390	116.26666	-800.05617	243.03183	1
1139	H	77.59800	52.67680	74.74290	-1357.08445	-1232.82351	2556.69596	1
1140	C	77.68700	54.67680	75.33990	-678.35284	-109.41542	-599.43031	1
1141	H	76.94800	55.38980	75.00390	-1206.66008	2905.34747	33.96701	1
1142	C	77.20500	54.32980	76.79390	472.54445	10.69847	-779.76810	1
1143	H	77.72800	53.41580	77.14590	2373.67726	-1298.61513	-1605.45359	1
1144	O	75.76300	54.21780	76.78490	249.98320	-474.61047	-579.55201	1
1145	H	75.63300	53.42280	76.26290	3029.87441	-803.06926	-270.49405	1
1146	C	77.39900	55.42680	77.81890	-565.84948	425.25063	574.82803	1
1147	H	76.81700	55.15480	78.72490	2380.54261	2038.40372	275.95904	1
1148	H	78.42900	55.46880	78.23490	223.84325	3107.75120	-435.89326	1
1149	H	77.11100	56.36280	77.29590	-8.05197	-3029.05317	850.29306	1
1150	C	78.99300	55.41280	75.48290	701.70330	-576.93621	-78.79146	1
1151	O	79.01200	56.64380	75.52890	-59.21911	-775.59247	-136.29617	1
1152	N	80.04200	54.60680	75.54790	-398.63876	510.83580	-541.11571	1
1153	H	79.91100	53.62580	75.42390	-2349.11562	2066.51292	330.76636	1
1154	C	81.45000	55.05880	75.60490	206.95057	637.15206	-618.59495	1
1155	H	81.54600	55.60980	76.52890	632.20188	-642.48221	-3014.26004	1
1156	C	82.49400	53.85080	75.62690	598.64805	397.00326	-561.65820	1
1157	H	83.54200	54.17680	75.80090	-2232.34802	-1661.32334	-1467.94186	1
1158	H	82.40300	53.30880	74.66190	676.89204	2401.68197	-1916.23775	1
1159	C	82.13700	52.85880	76.75290	-370.00610	37.83435	-832.53531	1
1160	O	82.51800	51.66580	76.56390	-351.41515	21.40122	706.87807	1
1161	O	81.53100	53.20380	77.76190	286.97340	74.62546	731.91840	1
1162	C	81.81100	55.96680	74.36290	205.71236	700.87909	-545.80393	1
1163	O	82.31600	57.09180	74.51690	411.41298	417.00731	529.59560	1
1164	N	81.46000	55.58180	73.12090	230.67136	-741.50725	-331.10424	1
1165	H	80.97900	54.71980	72.97790	2577.54806	1047.01609	1469.09140	1
1166	C	81.68400	56.29980	71.95890	389.38357	-169.83255	-806.83848	1
1167	H	82.73300	56.54780	72.03390	-1969.42367	1749.85328	-1719.77037	1
1168	C	81.30300	55.39580	70.72990	-581.59895	323.43404	-623.36513	1
1169	H	81.29600	56.08680	69.85890	-2342.50797	-2032.69013	528.25512	1
1170	H	80.24900	55.09180	70.90490	-2701.29281	1283.89242	976.14733	1
1171	C	82.34400	54.32980	70.40590	45.24449	-679.72194	606.12047	1
1172	H	82.91800	54.03380	71.31090	-1064.36985	1985.27929	2196.36272	1

1173	H	83.11200	54.74680	69.71990	-611.85400	-2639.79983	1598.53612	1
1174	C	81.85800	53.05580	69.67590	660.61407	-567.71870	269.69526	1
1175	H	81.45300	53.35580	68.68590	-2517.02422	-608.94234	1786.61818	1
1176	H	81.02700	52.73880	70.34090	-286.32125	-1820.26254	-2550.07660	1
1177	C	82.96900	51.98280	69.53090	-514.95006	-516.07252	547.67380	1
1178	H	83.51800	51.86480	70.48990	1856.94857	1393.62275	2123.15423	1
1179	H	83.71600	52.20480	68.73890	1301.85931	-1533.97425	2418.74173	1
1180	N	82.51400	50.65680	69.16890	535.25158	528.00295	383.91525	1
1181	H	82.10400	50.74380	68.21690	-169.33332	2201.55980	-2241.13518	1
1182	H	83.32800	50.00980	69.15490	-692.77952	2016.47948	2313.45916	1
1183	H	81.81100	50.26080	69.82490	-1891.10716	-2335.74071	930.72835	1
1184	C	80.96500	57.63780	71.82890	831.35342	-336.52414	164.48099	1
1185	O	81.52700	58.63680	71.43890	528.41780	45.66680	-585.07812	1
1186	N	79.66900	57.69580	72.21290	67.36990	405.06377	-737.60215	1
1187	H	79.23700	56.80280	72.31390	1052.74506	-1323.30612	2653.07651	1
1188	C	78.91900	58.95380	72.34290	673.98104	4.29476	614.15154	1
1189	H	79.04000	59.54580	71.44790	-1796.10232	2269.58137	1233.38685	1
1190	C	77.45800	58.71880	72.77690	817.18460	-349.45788	-203.81249	1
1191	H	76.82600	59.62580	72.87990	-1459.46663	-662.24447	2707.32629	1
1192	H	77.44500	58.21880	73.76890	-2750.54998	1059.53428	1100.04007	1
1193	C	76.64300	57.82380	71.87090	570.71445	-85.92804	705.94079	1
1194	C	76.58300	58.10480	70.48090	196.61060	-845.10815	-280.33459	1
1195	H	77.12200	58.96280	70.10690	-2022.26458	1442.80133	-1930.54307	1
1196	C	75.81100	57.35880	69.59390	-620.67473	-144.62225	652.14898	1
1197	H	75.76500	57.60680	68.54390	-1774.85020	-1785.31973	-1886.99933	1
1198	C	75.22600	56.17080	70.00690	507.99053	-715.82818	246.95473	1
1199	O	74.53900	55.28780	69.16190	636.89690	24.24144	466.26378	1
1200	H	74.41500	54.44180	69.59890	-1229.13574	-2728.82755	-970.02668	1
1201	C	75.90500	56.70580	72.30390	-438.06824	-219.52237	768.99750	1
1202	H	75.83900	56.41280	73.34090	-1389.16845	2304.19206	1630.68580	1
1203	C	75.30900	55.81680	71.36490	-138.47807	486.79549	-758.48862	1
1204	H	74.94300	54.87280	71.74090	1875.29069	1905.15049	-1658.88899	1
1205	C	79.49600	59.91880	73.36590	314.93220	-626.23050	583.18443	1
1206	O	79.75100	61.08780	73.13790	166.40047	34.09026	-771.21720	1
1207	N	79.82100	59.45580	74.55290	-641.07289	-340.81376	-430.74798	1
1208	H	79.68400	58.49580	74.78390	2770.00984	-1453.88336	-333.90849	1
1209	C	80.44200	60.30880	75.56290	-729.93127	358.94081	-412.08353	1
1210	H	79.90500	61.24580	75.55490	-2787.83190	-900.98633	-1146.49167	1
1211	C	80.24100	59.73180	76.98690	332.98027	551.74550	-645.09848	1
1212	H	80.77400	60.48080	77.61190	2466.17135	124.53770	1949.54237	1
1213	H	80.74600	58.75980	77.17490	-1127.69053	2483.20785	-1568.50855	1
1214	C	78.72500	59.53680	77.40490	-655.38688	470.08820	-425.36587	1
1215	H	78.16700	60.42180	77.03090	2662.62756	1561.17670	-609.39974	1
1216	H	78.24300	58.62080	77.00190	-2099.73270	-1947.48585	1302.55430	1
1217	C	78.50600	59.36680	78.91590	31.97752	198.73558	889.34392	1
1218	H	78.94700	58.43680	79.33590	-74.44478	2293.05552	2152.80760	1
1219	H	77.42800	59.16480	79.09190	-1970.42781	-1072.69218	2205.66815	1
1220	N	79.05000	60.55680	79.71390	-229.64616	496.03660	643.33710	1
1221	H	79.41200	61.35180	79.22890	833.13704	-2924.64675	-806.56697	1
1222	C	79.10800	60.62180	81.05290	124.60381	-647.79417	-629.51379	1
1223	N	78.65600	59.79180	81.93890	-677.75721	-278.89576	418.96851	1
1224	H	78.00100	59.08680	81.66790	-1755.95806	-2224.39321	1366.35001	1
1225	H	78.68000	60.11080	82.88590	-1983.36234	-1569.63800	-1871.02555	1
1226	N	79.61200	61.72080	81.54490	-334.65245	-585.25440	-508.09184	1
1227	H	79.92100	62.44280	80.92490	-1562.22485	1491.63732	2287.50909	1
1228	H	79.73600	61.78780	82.53490	-1795.71036	1793.17424	-1859.61734	1
1229	C	81.91100	60.65180	75.26890	616.82672	440.14893	-507.19298	1
1230	O	82.34700	61.74380	75.64890	408.96491	673.97556	-46.17215	1
1231	N	82.63500	59.80580	74.56990	-190.24542	70.08760	-819.49173	1
1232	H	82.35300	58.85480	74.46790	-2529.63481	1462.88648	1165.82036	1
1233	C	83.96700	60.27580	74.06590	580.48783	-682.68440	168.60276	1
1234	H	84.51900	60.58080	74.94290	-2015.52347	-270.18547	2400.60225	1

1235	C	84.76500	59.15580	73.29790	807.44994	-162.97781	-391.04198	1
1236	H	84.27400	58.99080	72.31490	-1304.61225	1425.38317	-2482.84029	1
1237	H	84.62400	58.26080	73.94190	-1610.06251	2701.87052	76.29298	1
1238	C	86.25700	59.33680	73.14890	-736.82847	197.47386	499.53867	1
1239	H	86.42000	60.38280	72.81090	2282.69942	-2080.27261	-599.97954	1
1240	C	86.99400	59.10380	74.43890	-132.79600	758.65012	-488.12522	1
1241	H	88.03400	59.42780	74.21690	2316.28189	2059.60012	539.54772	1
1242	H	86.66200	59.73080	75.29390	1764.69691	-1722.13532	1954.05245	1
1243	H	86.94000	58.03480	74.73590	1618.11774	1947.21808	1867.68921	1
1244	C	86.78800	58.36680	72.08090	-33.05601	290.32281	863.75400	1
1245	H	86.63600	57.36080	72.52590	-1363.19630	2394.79000	-1518.19067	1
1246	H	87.88400	58.53880	72.02790	-262.56333	2650.23136	1674.98074	1
1247	H	86.34700	58.51580	71.07190	-2542.66483	1742.60188	629.61931	1
1248	C	83.83400	61.42680	73.15390	-349.49611	-412.57976	-734.22164	1
1249	O	84.63000	62.37580	73.26490	653.38230	407.13363	-175.95740	1
1250	N	82.85300	61.48880	72.22890	-696.62291	-443.72975	-174.62165	1
1251	H	82.23800	60.70680	72.16490	2557.02351	1717.87314	-639.35033	1
1252	C	82.51100	62.67080	71.40490	-174.66495	893.03350	-58.60317	1
1253	H	83.43700	63.02080	70.97290	2742.09203	936.70899	1225.45248	1
1254	C	81.45100	62.39580	70.30990	654.62704	631.74434	61.75378	1
1255	H	80.52300	61.97280	70.74890	-1124.67376	1215.25919	2675.15986	1
1256	H	81.11100	63.34480	69.84290	-1237.27166	-1033.78453	2701.60593	1
1257	N	83.07400	62.04880	68.49190	-65.61244	-824.28130	170.08128	1
1258	C	81.94000	61.60380	69.18490	553.72523	-722.80060	48.97612	1
1259	C	83.07900	61.30880	67.38090	-156.05578	800.76146	-407.28207	1
1260	H	83.93400	61.31080	66.70590	2707.28651	1600.97032	75.63083	1
1261	N	82.06700	60.43080	67.32990	27.73325	691.53841	-483.40230	1
1262	H	81.96900	59.68080	66.67590	2123.25559	2320.04986	-85.91020	1
1263	C	81.28500	60.67180	68.46190	751.95162	343.93963	-384.35049	1
1264	H	80.30900	60.21780	68.57990	2039.24247	190.54477	2388.18112	1
1265	C	81.99700	63.82580	72.29390	-160.21988	-892.31250	-97.77014	1
1266	O	82.45800	64.95180	72.13090	-742.17490	52.02864	-264.75775	1
1267	N	81.10700	63.58780	73.24290	-506.89933	-356.14508	573.48587	1
1268	H	80.64000	62.70880	73.29990	2261.43733	582.87510	-2108.17079	1
1269	C	80.62600	64.63480	74.15290	540.92378	420.08690	601.97962	1
1270	H	80.25900	65.41980	73.50690	1104.64224	2675.80596	-1232.09343	1
1271	C	79.51400	64.01580	75.02690	487.40404	679.16621	364.17243	1
1272	H	78.93200	63.32680	74.37890	1781.37923	-1451.21758	2149.15839	1
1273	H	80.05900	63.34980	75.72990	2047.54260	2138.23628	-1064.77281	1
1274	C	78.65200	64.92580	75.86790	150.99140	893.23266	-103.86534	1
1275	H	79.32500	65.43280	76.59190	1577.40469	-164.99908	-2717.13010	1
1276	C	77.84300	65.91680	75.11090	402.88510	394.90242	-716.37049	1
1277	H	78.40300	66.58380	74.41990	-2081.17384	-2130.37170	-1014.12924	1
1278	H	77.04300	65.37980	74.55790	1427.12257	-2280.78150	1630.82284	1
1279	H	77.34800	66.57180	75.85890	474.44067	676.84145	-3035.62480	1
1280	C	77.73700	63.96780	76.62590	178.26637	-636.12688	-628.50194	1
1281	H	78.25600	63.31880	77.36390	-2268.84858	-1446.41660	1630.46968	1
1282	H	77.23500	63.24180	75.95090	-2030.35526	-471.07066	-2356.68754	1
1283	H	77.01400	64.60180	77.18190	1036.87980	2968.51869	-104.89656	1
1284	C	81.76100	65.29180	74.99290	343.66896	299.69006	789.63822	1
1285	O	81.80900	66.50180	75.10190	447.19691	528.48600	379.92722	1
1286	N	82.73700	64.49880	75.49490	-433.79278	387.28297	-611.97060	1
1287	H	82.74800	63.51180	75.35190	2667.48998	-1434.27704	-851.80562	1
1288	C	84.02000	64.94880	76.06590	574.89745	-680.42524	194.84716	1
1289	H	83.77900	65.63080	76.86790	-1563.71622	1465.41777	2303.38199	1
1290	C	84.77200	63.73480	76.76590	595.79640	-682.68278	-102.08756	1
1291	H	85.81700	64.05580	76.96690	-1289.96943	2325.87140	1680.63301	1
1292	H	84.71000	62.84780	76.09990	2126.61121	2034.22205	-1112.51591	1
1293	O	84.15300	63.55380	78.01490	486.11575	-42.96009	-620.86483	1
1294	H	84.37800	64.25280	78.63390	-1787.26086	2063.96930	1563.31558	1
1295	C	84.93100	65.67980	75.13190	-663.49168	-288.52248	554.96358	1
1296	O	85.56500	66.64980	75.53790	-588.04176	-513.33378	-119.67683	1

1297	N	85.05100	65.29680	73.86190	-259.51888	742.08221	307.63002	1
1298	H	84.70800	64.42780	73.51290	-2106.68035	-139.62095	2332.51583	1
1299	C	85.69500	66.04380	72.82190	573.02431	366.65430	-607.17277	1
1300	H	86.70800	66.33380	73.05990	2764.78709	-1501.37226	-7.74138	1
1301	C	85.74100	65.15480	71.54090	-133.05896	-869.20207	-241.31740	1
1302	H	84.87900	64.46080	71.44990	148.62272	2088.94663	-2347.85849	1
1303	C	85.79600	65.94080	70.19390	454.61833	-363.57527	701.84486	1
1304	H	84.86900	66.50480	69.95490	2551.92878	-1366.56206	1232.23125	1
1305	H	85.96200	65.21880	69.36590	-1476.37308	-34.90144	-2778.00840	1
1306	H	86.63500	66.66980	70.17690	-1292.00135	2545.19150	1323.23807	1
1307	C	87.01400	64.26180	71.59490	-392.54470	622.82292	538.00676	1
1308	H	86.82200	63.39980	72.26990	-891.72079	-2485.89783	1709.78719	1
1309	H	87.92700	64.84480	71.84190	315.63313	-2973.12995	979.33663	1
1310	H	87.23900	63.84180	70.59090	-3023.59537	-818.79082	292.70952	1
1311	C	84.98600	67.39680	72.55390	-382.12363	-807.35395	-183.33613	1
1312	O	85.69000	68.41580	72.40690	210.25598	-515.88228	559.71879	1
1313	N	83.64700	67.48780	72.47490	216.00212	-314.44842	-753.08536	1
1314	H	83.09500	66.66380	72.57690	1593.33848	328.35976	2692.89409	1
1315	C	82.92000	68.76280	72.32790	-515.80784	257.10074	-706.60632	1
1316	H	83.22900	69.31680	71.45390	2024.47698	1690.93538	-1714.77600	1
1317	C	81.43200	68.40580	72.15790	648.50536	-302.09253	565.35997	1
1318	H	80.91900	69.33580	71.83390	-1725.51672	1315.79795	-2278.04610	1
1319	H	80.92200	68.18880	73.12090	-1757.06882	-1744.11894	1941.38727	1
1320	H	81.28100	67.60480	71.40290	-737.82683	1519.08542	2654.47119	1
1321	C	83.14400	69.72080	73.44490	-395.42291	812.29268	123.58130	1
1322	O	83.43900	70.90080	73.25090	539.79206	559.36134	-139.16412	1
1323	N	83.00700	69.24380	74.69190	-34.22935	573.50717	-618.53873	1
1324	H	82.62000	68.33680	74.84090	2966.83186	973.23497	385.93867	1
1325	C	83.27700	70.00580	75.90190	873.70478	24.39264	259.79983	1
1326	H	82.61000	70.85480	75.90990	-2612.51722	-285.31065	1729.61782	1
1327	C	83.12800	69.09680	77.13590	-189.12856	-631.34043	630.15130	1
1328	H	83.48300	69.52780	78.09690	-429.88148	1737.22478	2587.56221	1
1329	H	83.61800	68.12180	76.92790	552.37381	-3048.72003	-546.27430	1
1330	C	81.58900	68.79880	77.42290	506.34032	746.12677	-135.51871	1
1331	O	80.75700	69.59680	76.91990	634.58558	468.81093	33.83312	1
1332	O	81.33500	67.81580	78.15690	-681.02272	-129.27330	-378.31692	1
1333	C	84.71100	70.58080	75.95190	717.95488	52.30739	559.69253	1
1334	O	84.86800	71.75680	76.30490	-392.94383	-427.35786	535.33880	1
1335	N	85.74100	69.79480	75.67590	-415.04889	265.39372	-685.54568	1
1336	H	85.60700	68.83480	75.43990	2137.04559	-2200.43123	699.54610	1
1337	C	87.13300	70.09780	75.63590	-188.65217	-889.33474	-70.32133	1
1338	H	87.32400	70.52680	76.60790	1091.87028	-2116.68285	2055.65056	1
1339	C	87.91400	68.77880	75.41390	489.60820	-592.84580	490.17207	1
1340	H	87.59900	68.21680	74.50790	700.09827	2650.52625	1543.63184	1
1341	H	87.63200	68.11480	76.25890	-2482.03662	1382.94635	1350.99216	1
1342	C	89.44000	68.82480	75.48290	692.80416	570.40126	-161.60383	1
1343	H	89.72900	69.58180	74.72290	298.18466	-1746.60285	2599.74818	1
1344	C	89.94100	69.29480	76.88690	181.95516	681.49958	577.84223	1
1345	H	89.75800	68.53080	77.67190	2543.27422	1849.91670	-88.26466	1
1346	H	91.05200	69.32680	76.88190	1546.58761	710.38340	2646.06281	1
1347	H	89.44900	70.26980	77.09490	2913.61036	807.48848	870.09380	1
1348	C	89.95100	67.43480	75.03090	-434.95320	-440.02011	669.81267	1
1349	H	89.65900	67.25180	73.97490	-2229.65148	-1205.77526	1863.59505	1
1350	H	91.05800	67.51580	75.08490	-2346.62516	2037.49304	-490.10068	1
1351	H	89.58900	66.62280	75.69590	2317.98498	2115.13878	226.62696	1
1352	C	87.46200	71.14180	74.60090	243.29597	-515.30183	711.84416	1
1353	O	88.19800	72.07180	74.83790	242.16191	-373.73155	652.15762	1
1354	N	86.84400	71.04980	73.39090	-206.19084	-790.70397	212.00203	1
1355	H	86.17000	70.32580	73.26190	-2329.37301	-1645.87292	1327.91187	1
1356	C	87.01800	71.85880	72.20590	-797.26164	-385.05976	-218.06846	1
1357	H	88.03400	71.65880	71.90090	-1368.50983	-1180.41086	-2575.27421	1
1358	C	86.05600	71.26180	71.07990	-544.54715	-641.45881	351.35453	1

1359	H	85.03600	71.30180	71.51890	1898.93754	-2218.42496	1170.83439	1
1360	H	86.42000	70.23180	70.88090	-1156.17871	-2079.34627	2058.59080	1
1361	C	86.06000	71.96180	69.68690	-557.49996	616.60391	-374.75914	1
1362	H	85.52600	72.93580	69.71790	1897.10684	-331.51851	2487.83186	1
1363	C	87.48200	72.28980	69.17990	222.43514	-630.28591	-620.25259	1
1364	H	88.21400	71.45680	69.22790	757.91180	3044.92607	228.51948	1
1365	H	87.92000	73.10780	69.79090	-673.91154	2373.74099	-1951.77436	1
1366	H	87.44600	72.71180	68.15290	1938.39703	1427.72827	2025.44691	1
1367	C	85.20100	71.16880	68.59090	73.40772	-590.80600	690.65952	1
1368	H	85.60800	70.14180	68.47390	358.89761	-2861.34974	1257.81414	1
1369	H	84.15200	71.20580	68.95590	-2358.21230	2029.33669	-467.81789	1
1370	H	85.20300	71.73380	67.63390	1743.93046	-27.50855	-2618.43007	1
1371	C	86.64900	73.30080	72.42790	172.18240	-757.68989	477.18996	1
1372	O	87.45100	74.21280	72.17190	122.55922	-369.80880	-686.91187	1
1373	N	85.50800	73.52580	73.11090	162.34887	-288.33841	-776.64412	1
1374	H	84.97100	72.71180	73.31890	2621.72506	-1513.35586	-857.05191	1
1375	C	85.11500	74.80280	73.59690	627.09744	-477.05513	458.93159	1
1376	H	85.32400	75.60080	72.90090	1530.70822	1534.00608	-2280.78581	1
1377	C	83.55300	74.85180	73.84290	675.88439	204.91434	576.75073	1
1378	H	83.38800	74.05380	74.59790	-1785.28981	-1117.81202	2336.97728	1
1379	H	83.04800	74.70080	72.86490	-1449.53844	-2337.75312	1527.08051	1
1380	C	83.06600	76.20680	74.31390	-316.55822	790.68701	325.66234	1
1381	C	83.49400	77.39480	73.61290	-683.51343	354.64960	488.34830	1
1382	H	84.09300	77.25680	72.72490	-727.13514	2292.88436	-2027.85158	1
1383	C	83.02700	78.64780	74.04590	593.16071	-653.76433	-228.48102	1
1384	H	83.34500	79.53480	73.51790	2491.16766	408.28340	1877.66200	1
1385	C	82.11700	78.73280	75.12690	-66.97421	795.26514	-441.04288	1
1386	H	81.80600	79.73380	75.39090	-2023.60898	283.96525	2392.19495	1
1387	C	82.25700	76.31380	75.36790	516.22629	691.61670	-294.32595	1
1388	H	81.88900	75.42480	75.85690	-283.41445	3128.62409	-172.08652	1
1389	C	81.80600	77.52180	75.83390	161.00809	-648.26628	-620.70785	1
1390	H	81.02300	77.59480	76.57490	1616.68512	1950.46833	1865.53712	1
1391	C	85.85600	75.28680	74.89890	558.42224	-319.32804	646.25476	1
1392	O	86.21200	76.46780	74.94090	-617.03132	-329.65839	366.36720	1
1393	N	86.17100	74.39980	75.83690	365.84895	181.75465	738.77743	1
1394	H	86.02200	73.41680	75.76590	-963.78762	622.65670	2929.44334	1
1395	C	86.82000	74.75980	77.14490	92.88478	-707.91608	567.16686	1
1396	H	86.15300	75.48880	77.57990	-2690.93431	370.99464	1587.28125	1
1397	C	86.94000	73.58780	78.11590	410.88764	701.60620	-412.76033	1
1398	H	87.14500	72.68280	77.50590	2428.38666	1806.31783	859.29061	1
1399	C	88.11000	73.73880	79.17790	432.87521	-784.56392	-168.90679	1
1400	H	89.11200	73.50380	78.75790	-2802.28668	8.86839	-1430.15277	1
1401	H	87.89000	73.00680	79.98390	1689.26299	-2020.98145	1720.53793	1
1402	H	88.01200	74.79180	79.51590	-2365.18424	1456.71194	-1477.20008	1
1403	C	85.60400	73.41880	78.88190	489.21410	391.20761	662.62898	1
1404	H	85.67200	72.50580	79.51190	2305.33576	1919.54368	-948.15892	1
1405	H	85.36200	74.27280	79.54890	1150.20989	-2924.23098	-155.29525	1
1406	H	84.74200	73.40480	78.18090	848.83691	-2268.82709	2007.51732	1
1407	C	88.17300	75.40380	76.92690	269.85313	-698.95484	-519.70416	1
1408	O	88.54300	76.32780	77.61390	222.86699	-474.16548	-590.86769	1
1409	N	88.89700	74.85580	75.91890	-237.45874	-514.82712	-625.49074	1
1410	H	88.53000	74.08180	75.40890	-401.06002	2256.45471	2155.40930	1
1411	C	90.29200	75.32580	75.66290	-228.46060	-244.74551	848.14880	1
1412	H	90.89600	75.29980	76.55790	2246.14420	1860.68591	-1179.36865	1
1413	C	90.95300	74.41080	74.56690	341.32691	764.75637	360.68634	1
1414	H	90.23300	74.14880	73.76190	2554.11733	1652.47885	802.51140	1
1415	C	92.24400	75.00980	73.95790	-637.87628	639.76897	123.53346	1
1416	H	92.97600	75.11480	74.78690	-1452.19126	1638.97488	2259.01043	1
1417	H	92.67300	74.27880	73.23890	1802.54928	-2168.26235	1395.59331	1
1418	H	91.99400	75.90680	73.35290	2254.70122	-2192.03053	-97.72796	1
1419	C	91.30800	73.01580	75.20290	580.51474	-213.05230	-670.12115	1
1420	H	90.39500	72.66380	75.72790	-1253.55495	2442.55631	1536.47157	1

1421	H	92.16300	73.06880	75.90890	-2566.35490	-1170.15823	-1393.83589	1
1422	C	91.58000	71.93880	74.11790	-544.80879	723.46474	105.98658	1
1423	H	92.58900	72.13780	73.69690	-1849.55825	1926.39631	1663.23713	1
1424	H	90.83500	71.82580	73.30090	3081.44701	557.50540	303.47698	1
1425	H	91.68900	70.94580	74.60390	1172.41242	2849.92965	-633.70050	1
1426	C	90.27000	76.76580	75.16090	43.99705	529.99175	-740.69157	1
1427	O	91.26100	77.50980	75.35290	-669.29467	-418.02486	-30.44806	1
1428	N	89.15800	77.21180	74.50990	-185.76579	-545.19233	-617.19420	1
1429	H	88.43600	76.60280	74.19090	1200.96570	1543.34285	2464.54873	1
1430	C	89.12800	78.59280	74.10490	384.61821	503.00683	656.12801	1
1431	H	90.03400	78.84180	73.57190	1476.59375	-1263.13412	-2474.34624	1
1432	C	87.93400	78.86780	73.12990	-21.66292	-737.14628	536.28078	1
1433	H	88.03500	79.86580	72.65290	882.49886	-2368.00120	-1874.03103	1
1434	O	86.60800	78.75480	73.78290	501.75101	-525.68570	309.07555	1
1435	H	86.49900	77.90180	74.21090	3140.14368	27.99916	192.19760	1
1436	C	87.97000	77.75680	72.01390	-713.52948	-542.73673	-166.62390	1
1437	H	87.68400	76.74380	72.36890	1938.00761	2469.06701	-214.61793	1
1438	H	87.16200	78.06680	71.31790	1565.64258	-1314.16470	-2391.64393	1
1439	H	88.96600	77.83780	71.52890	202.51630	-1564.01020	2722.33089	1
1440	C	88.96700	79.58880	75.24390	-546.08792	-598.26994	-418.70284	1
1441	O	89.33600	80.75080	75.13190	-473.21638	-515.99724	-365.29486	1
1442	N	88.46200	79.15180	76.40990	-43.52075	-816.92906	-208.33901	1
1443	H	88.27300	78.17780	76.50590	-1752.13224	-1467.47552	-2162.12267	1
1444	C	88.07500	80.00680	77.54090	-22.34412	188.91236	891.77568	1
1445	H	87.30100	80.66680	77.17790	2302.06814	330.51885	-2118.83595	1
1446	C	87.30500	79.28680	78.65090	-594.77166	183.24338	-666.42294	1
1447	H	87.05400	79.85480	79.57290	-1998.90857	1716.74723	-1719.11887	1
1448	H	87.98500	78.45680	78.93890	48.26060	-2588.39189	1787.77084	1
1449	C	85.94700	78.73980	78.20890	-391.05240	313.85106	761.59473	1
1450	H	86.02600	78.13580	77.27990	-2803.23397	1413.33989	-206.33925	1
1451	C	85.44800	77.83980	79.37790	-895.95207	-10.76464	-169.13015	1
1452	H	86.11200	76.94880	79.37190	227.33190	-2794.30265	-1427.73216	1
1453	H	85.48900	78.35180	80.36290	-2610.76036	1750.12024	-138.69293	1
1454	H	84.39600	77.56880	79.14390	-3046.09747	-127.33998	776.72450	1
1455	C	84.96300	79.87180	77.92290	-896.33437	84.57238	144.51028	1
1456	H	85.05400	80.27480	76.89190	2459.16703	1961.86027	42.75521	1
1457	H	85.04300	80.76780	78.57490	-1997.82917	-1897.36799	-1518.84809	1
1458	H	83.95600	79.43980	78.10290	832.03319	-1456.25588	-2661.81626	1
1459	C	89.17800	80.94580	78.08890	-711.38404	491.58397	289.35955	1
1460	O	88.80600	82.04980	78.42590	650.20613	447.96805	13.55916	1
1461	N	90.47200	80.68380	78.13390	-569.16004	-19.26878	623.18364	1
1462	C	90.96500	79.30680	78.36890	-409.24103	-448.61170	-680.23550	1
1463	H	91.18800	78.92780	77.34790	-1619.60431	1655.05126	2129.76839	1
1464	H	90.26700	78.62680	78.90290	-1439.77459	-1857.19598	-2091.91263	1
1465	C	91.54100	81.64680	78.45690	-29.16890	-449.96339	-792.54850	1
1466	H	91.23900	81.98780	79.43590	1756.31519	-1808.82317	-1881.95163	1
1467	C	92.73700	80.82480	78.49790	-842.40104	144.23372	-317.81774	1
1468	H	93.63600	81.30280	78.94390	415.84241	-1809.51773	2539.87143	1
1469	H	93.12400	80.48380	77.51490	16.29837	-2368.52761	-2070.75773	1
1470	C	92.24000	79.53580	79.14890	-347.10386	-211.95636	816.11544	1
1471	H	92.99800	78.74380	78.96890	-2027.24786	2403.32760	-111.84286	1
1472	H	92.10900	79.69280	80.24090	1908.09932	919.17948	-2326.47637	1
1473	C	91.62700	82.88080	77.58990	248.42227	689.14329	-542.97228	1
1474	O	92.02600	83.95080	78.05690	149.28934	-171.04220	756.36267	1
1475	N	91.29900	82.78080	76.30590	-331.25744	596.28516	-497.37794	1
1476	H	91.10600	81.91780	75.84690	1445.82965	2792.18114	-107.36550	1
1477	C	91.14300	83.99380	75.47590	612.29400	-318.80955	-595.74116	1
1478	H	92.02900	84.60980	75.52090	341.74386	2835.43554	1319.75097	1
1479	C	90.89300	83.53080	73.98690	517.51697	-499.03601	-560.88346	1
1480	H	89.88900	83.05780	73.93690	2128.87328	1637.00740	1639.00321	1
1481	H	90.85600	84.47980	73.41090	-1256.47112	2228.18795	-1831.57992	1
1482	C	92.01000	82.69580	73.39690	-547.41416	493.30768	537.06264	1

1483	C	93.29400	83.19280	73.34590	786.37913	-200.80348	415.61620	1
1484	H	93.55400	84.19180	73.66590	2082.03614	1130.29365	-2070.21448	1
1485	C	94.39900	82.58680	72.68290	-618.47257	-290.02323	604.01093	1
1486	H	95.32400	83.13780	72.59590	655.95752	2022.12489	2319.25783	1
1487	C	94.10100	81.35380	72.07090	600.09640	408.89255	551.49089	1
1488	H	94.80900	80.81280	71.46190	2045.02833	-1258.14154	-2033.01875	1
1489	C	91.83500	81.41480	72.88390	-370.64793	-315.48317	-771.06516	1
1490	H	90.85900	80.95880	72.95990	2820.84396	1337.61107	-389.69505	1
1491	C	92.82900	80.73080	72.21990	278.11087	868.36814	-6.49039	1
1492	H	92.53500	79.82280	71.71490	666.69203	-2802.82065	1264.09824	1
1493	C	90.05300	84.85580	75.95490	652.77190	565.18946	-293.08825	1
1494	O	90.11200	86.05780	76.01790	493.61018	200.67176	582.84394	1
1495	N	88.89800	84.23980	76.38290	-68.55996	-686.47804	486.53851	1
1496	H	88.83200	83.24980	76.48090	1531.30311	541.27594	-2694.50503	1
1497	C	87.77100	84.95680	77.05290	-791.18086	69.28925	447.97639	1
1498	H	87.44200	85.79080	76.45090	-3066.76104	158.53757	684.15553	1
1499	C	86.55800	84.09580	77.20590	170.10671	496.42605	745.70496	1
1500	H	85.74200	84.75480	77.57290	-13.09365	1988.53377	2437.98856	1
1501	H	86.63600	83.28580	77.96190	-1439.65630	-2248.20643	1664.68730	1
1502	C	85.94200	83.48480	75.94290	-435.11005	-533.77840	-597.67121	1
1503	C	86.43200	82.68380	74.93490	-338.30142	779.26114	331.29328	1
1504	H	87.49000	82.51880	74.79890	2684.63309	-1076.73425	1237.58425	1
1505	N	85.42800	82.11980	74.20990	-285.59101	719.79103	336.17099	1
1506	H	85.59200	81.26780	73.76190	-655.80785	1782.74557	-2507.97937	1
1507	C	84.25200	82.63580	74.59690	748.67870	-449.43296	-262.56661	1
1508	C	84.51500	83.48880	75.69290	567.91079	473.39531	533.69019	1
1509	C	83.41000	84.02980	76.41090	-681.13713	147.45827	588.01299	1
1510	H	83.66700	84.57280	77.30890	-3135.43706	-243.59415	-89.00881	1
1511	C	82.13800	83.76480	75.96090	-655.08090	-465.58235	430.75873	1
1512	H	81.32000	84.18880	76.52390	2399.43516	-859.68149	1844.41993	1
1513	C	82.96000	82.40980	74.11690	-616.67597	-657.02197	139.58467	1
1514	H	82.82800	81.82880	73.21690	3104.40561	-417.61983	294.08451	1
1515	C	81.86200	82.98280	74.83290	-43.05539	653.94095	634.00195	1
1516	H	80.85600	82.74780	74.51690	1531.88442	-1265.78041	2439.13024	1
1517	C	88.12000	85.62380	78.36990	603.66975	-274.54961	625.82454	1
1518	O	87.76800	86.75980	78.66290	-446.35243	452.83276	-468.33667	1
1519	N	88.88700	84.89880	79.22090	-38.26233	140.60432	-831.52794	1
1520	H	89.17100	83.95280	79.08290	-2208.21740	-2231.00887	-211.19081	1
1521	C	89.39800	85.43280	80.43590	-184.12626	-726.89566	-518.81713	1
1522	H	88.57400	85.71980	81.07390	-1063.25225	2892.21071	-634.69530	1
1523	C	90.14400	84.27080	81.25390	380.34768	-503.85067	657.96744	1
1524	H	90.98300	83.74980	80.74590	2224.12780	1539.57874	-1606.60483	1
1525	H	89.46800	83.42280	81.49390	-1277.95220	882.25521	-2736.18167	1
1526	H	90.53800	84.71780	82.19190	-2540.64013	-1854.78556	-56.07572	1
1527	C	90.32000	86.64080	80.29190	-256.45285	659.79444	574.76450	1
1528	O	90.28400	87.59680	81.05490	-277.60373	739.16779	-13.94214	1
1529	N	91.18600	86.59780	79.21590	-513.28625	-467.09751	480.65520	1
1530	H	91.21500	85.75680	78.68190	-1275.27019	-972.57294	-2706.66105	1
1531	C	92.03900	87.71780	78.84690	447.74693	-335.55497	-719.98372	1
1532	H	92.47800	88.11080	79.75190	-2280.63503	1611.23119	1449.43581	1
1533	C	93.09200	87.28280	77.81590	774.51532	413.88680	245.50914	1
1534	H	92.62700	86.69580	76.99490	283.29337	3129.35837	158.38964	1
1535	C	93.79800	88.48080	77.20790	312.95632	443.58971	732.62372	1
1536	H	93.17800	89.12580	76.54890	-2713.01015	-503.80515	-1511.28505	1
1537	H	94.33500	89.07080	77.98190	2433.23099	1773.46808	912.37281	1
1538	H	94.65300	88.14580	76.58190	-758.90342	-580.18726	2997.61148	1
1539	C	94.13000	86.37180	78.49990	-40.57310	-208.98661	886.63940	1
1540	H	93.76300	85.48380	79.05690	2041.48776	-2018.16465	-1287.46472	1
1541	H	94.75700	86.90380	79.24790	-1069.84244	-2094.53980	2089.63308	1
1542	H	94.82300	85.90380	77.76890	1503.58468	17.68956	-2763.53875	1
1543	C	91.19400	88.88280	78.29690	-641.96273	-120.53241	-636.24429	1
1544	O	91.40600	90.01480	78.74490	-690.55796	-156.12769	349.83007	1

1545	N	90.23800	88.61480	77.37490	522.97310	634.92853	-189.83464	1
1546	H	90.14000	87.69080	77.01490	-2101.23102	-1078.31343	2078.53183	1
1547	C	89.28100	89.55280	76.77890	-618.82353	633.63615	-216.82635	1
1548	H	89.65800	90.38580	76.20390	-2109.39842	-1040.72630	-2089.39065	1
1549	C	88.31300	88.83980	75.79790	811.21825	374.52539	-181.95242	1
1550	H	88.85500	88.57180	74.86590	-1532.75225	-600.88605	2681.01338	1
1551	H	87.95900	87.89680	76.26790	-1177.72058	-2642.69199	1235.87196	1
1552	C	87.02600	89.57680	75.41090	51.91506	669.11502	-617.28512	1
1553	O	85.94100	89.06480	75.80290	565.61447	-288.51242	-469.54030	1
1554	O	87.12200	90.61380	74.76290	-697.40220	276.53110	246.55213	1
1555	C	88.51600	90.34080	77.86990	602.79954	292.72911	618.37965	1
1556	O	88.38700	91.51780	77.79990	-475.72218	61.08101	627.36333	1
1557	N	87.97500	89.63880	78.90190	-32.45126	-697.86445	-473.92448	1
1558	H	87.91400	88.64380	78.89390	2385.90573	-529.90168	1981.13207	1
1559	C	87.32900	90.35580	79.95990	-46.22999	874.98991	-252.40136	1
1560	H	86.53500	90.98280	79.58190	-2342.25663	639.64327	2000.72902	1
1561	C	86.68900	89.27980	80.87890	554.24159	674.93424	262.16605	1
1562	H	86.32000	89.69880	81.83990	-2030.06461	2209.71873	945.62520	1
1563	H	85.92900	88.71280	80.29990	-1649.45627	-1923.09796	1865.26525	1
1564	H	87.46500	88.49980	81.02890	-1986.22614	2365.64006	-597.39352	1
1565	C	88.19100	91.24280	80.82790	-439.92803	350.92025	717.47426	1
1566	O	87.79600	92.35880	81.18590	189.18815	539.38710	544.88222	1
1567	N	89.41800	90.87680	81.17190	-295.67887	730.81473	-301.92074	1
1568	H	89.69500	90.00980	80.76690	996.02180	1658.27780	2481.18551	1
1569	C	90.31000	91.79280	81.85490	259.60763	-731.97787	477.76906	1
1570	H	89.66800	92.28280	82.57190	2754.59908	-393.08571	1468.29621	1
1571	C	91.35400	91.17480	82.74790	-600.40064	-319.27841	-607.47953	1
1572	H	91.83200	91.97280	83.35490	-1436.03615	86.86322	-2797.94231	1
1573	C	90.69300	90.17980	83.69590	27.03317	-470.45225	-780.63749	1
1574	H	90.30300	89.29180	83.15490	-1366.98457	-2425.55716	1465.00918	1
1575	H	91.32400	89.80580	84.53090	2351.52614	-565.90061	2012.04064	1
1576	H	89.88500	90.68580	84.26490	1740.42123	1842.53102	1863.93123	1
1577	C	92.42900	90.52180	81.87390	391.02510	817.64146	100.06411	1
1578	H	92.04900	89.60080	81.38190	-1387.23036	-2392.38410	-1500.10549	1
1579	H	93.26300	90.10480	82.47690	373.15114	-1974.48924	-2420.82149	1
1580	H	92.82000	91.17680	81.06590	-801.75862	2126.27475	-2175.85961	1
1581	C	90.91900	92.99080	81.01890	-814.87564	-183.85307	-365.54993	1
1582	O	90.99500	94.04580	81.54690	-457.48252	-34.65367	-642.75664	1
1583	N	91.15100	92.74780	79.74390	-701.94588	308.97002	-352.81978	1
1584	H	91.02700	91.88880	79.25190	1822.20195	-2394.51070	-918.76263	1
1585	C	91.85900	93.82380	79.05390	-788.84457	228.03694	-396.45226	1
1586	H	91.80400	94.77680	79.55790	498.03487	3034.33451	-665.58361	1
1587	C	93.39600	93.42580	78.94790	822.56167	-140.91458	367.40494	1
1588	H	93.90700	93.27780	79.92290	-2731.13987	904.23351	-1273.36680	1
1589	H	93.34400	92.43980	78.43890	-1566.36053	2045.77663	-1805.41931	1
1590	H	94.03400	94.09880	78.33590	8.97752	-2757.85898	-1514.05399	1
1591	C	91.27100	94.10080	77.74790	729.12815	-494.44307	235.26410	1
1592	O	90.48200	95.01880	77.56790	500.74512	448.47967	414.42434	1
1593	N	91.60900	93.31480	76.69490	-357.14581	594.39578	-481.46943	1
1594	H	92.04900	92.43080	76.82990	271.86231	2381.12983	2038.26835	1
1595	C	91.30100	93.63780	75.29790	-415.20874	-595.33978	-551.92685	1
1596	H	90.34000	94.12380	75.37790	2831.60346	-1034.15834	-900.42468	1
1597	C	92.45000	94.53980	74.73790	-210.78168	-373.03538	-804.90166	1
1598	H	92.87900	95.13680	75.57090	2113.80486	-2233.69190	-663.83410	1
1599	H	93.29900	93.91580	74.38490	2628.45076	1098.92793	-1334.85214	1
1600	C	91.91400	95.54480	73.69590	432.91686	-419.46955	684.16320	1
1601	O	90.72900	95.59580	73.31890	92.18250	773.23643	131.28229	1
1602	N	92.86300	96.38480	73.12990	487.48499	295.29831	622.75965	1
1603	H	93.75000	96.60380	73.53690	-1869.21174	2527.99467	-116.26123	1
1604	H	92.51900	97.13680	72.56690	793.73848	-971.56295	-2885.18126	1
1605	C	91.08500	92.36180	74.55590	-340.00757	263.35053	-804.04748	1
1606	O	91.49600	91.28780	75.01690	412.36475	-660.96414	129.26312	1

1607	N	90.47900	92.38580	73.30490	-289.74671	-755.36442	241.13011	1
1608	H	89.97500	93.16380	72.93890	-1539.89936	2671.13697	626.06986	1
1609	C	90.64100	91.40580	72.30890	613.82568	501.44085	-450.80606	1
1610	H	90.74400	90.46680	72.83190	-2676.43745	-1423.76136	841.31587	1
1611	C	89.32300	91.23280	71.44490	713.43628	-149.66606	547.77710	1
1612	H	89.07000	92.22380	71.01090	513.40423	3006.12734	773.20161	1
1613	H	88.52900	90.98680	72.18190	-872.40087	2274.92978	1990.43650	1
1614	C	89.38100	90.19680	70.40690	-469.14235	365.14896	691.39185	1
1615	C	89.74800	90.26480	69.06090	-385.34685	347.09750	-749.98809	1
1616	H	90.08100	91.14980	68.53990	370.11855	-2959.06702	1002.57710	1
1617	N	89.81500	88.98480	68.55090	-780.96216	101.13283	-304.20805	1
1618	H	90.11800	88.73780	67.65690	662.58035	-1620.87833	-2613.80316	1
1619	C	89.35300	88.07380	69.50790	516.30052	509.33277	552.68879	1
1620	C	89.11000	88.79080	70.71990	-141.81440	-289.33260	853.01015	1
1621	C	88.66200	88.15080	71.86190	-626.90096	-289.66317	595.43382	1
1622	H	88.49800	88.59680	72.83190	-1493.98515	1681.96637	2199.36894	1
1623	C	88.41400	86.76380	71.73090	-468.72694	-173.98367	762.54557	1
1624	H	87.96700	86.19980	72.53590	-258.37376	-2273.45448	2159.36888	1
1625	C	89.23900	86.75180	69.40690	-125.63511	607.35422	668.42178	1
1626	H	89.56200	86.18980	68.54290	-961.10438	-2665.98358	1366.39532	1
1627	C	88.77200	86.08480	70.56790	678.50777	185.08496	-580.36348	1
1628	H	88.56400	85.02480	70.57790	1.58678	2992.48738	-971.20696	1
1629	C	91.94300	91.50380	71.52590	-868.67486	228.03305	157.65761	1
1630	O	92.06000	92.10180	70.44590	-168.27713	519.15118	-570.78200	1
1631	N	93.05400	90.91580	71.97490	588.35131	392.32893	461.07812	1
1632	H	92.96300	90.50880	72.87990	-2404.20306	1210.10912	-1629.00884	1
1633	C	94.35000	91.01880	71.30690	545.12654	-590.91712	-430.23833	1
1634	H	94.47500	91.98280	70.83690	-2723.83713	-449.96922	-1508.79595	1
1635	C	95.50600	90.81680	72.28090	617.17126	-577.27152	342.50289	1
1636	H	95.55500	89.80280	72.73090	221.04467	1342.63407	2836.67045	1
1637	H	96.44800	90.93180	71.70190	-1599.70713	-1372.43338	-2335.72043	1
1638	C	95.46300	91.76080	73.45790	525.73175	-149.83966	-729.79806	1
1639	C	96.08900	93.01480	73.41290	384.49096	784.11995	-262.24724	1
1640	H	96.54300	93.29080	72.47290	1991.75046	-238.97278	2423.64361	1
1641	C	96.24700	93.82380	74.54290	-444.31468	-467.96422	-644.23983	1
1642	H	96.74600	94.77980	74.47690	2397.29218	-1792.67610	-968.26073	1
1643	C	95.75200	93.37480	75.75090	-150.25994	544.14336	716.08726	1
1644	O	96.06400	94.08980	76.87990	-441.91258	-416.02229	-505.23851	1
1645	H	96.57500	94.84180	76.57290	105.42141	1991.33354	-2433.45501	1
1646	C	94.92900	91.30880	74.66790	-445.63643	-750.22929	264.60383	1
1647	H	94.57600	90.30380	74.84490	-482.99075	2457.88244	1903.61763	1
1648	C	95.07900	92.13080	75.81590	-248.75756	-46.06779	876.04134	1
1649	H	94.85900	91.71280	76.78790	1377.59260	1996.08186	-2004.02646	1
1650	C	94.51700	89.93980	70.24890	-500.29606	-628.06374	432.07730	1
1651	O	95.62700	89.71980	69.69590	730.99425	-259.77389	-147.62166	1
1652	N	93.42300	89.21580	69.88690	390.18621	194.34238	-722.95093	1
1653	H	92.54200	89.40880	70.31290	155.94001	-2428.14804	1994.49393	1
1654	C	93.58900	87.89880	69.19190	-558.27918	-395.74158	602.63087	1
1655	H	94.64700	87.68580	69.22990	2318.13742	-137.23707	2122.64720	1
1656	C	92.80600	86.81180	69.94090	350.19943	-783.35971	-308.47842	1
1657	H	93.03100	85.85080	69.42990	2790.97018	-979.42046	-1072.12278	1
1658	H	91.69800	86.86980	69.99190	-2388.59614	-491.06147	-1987.88665	1
1659	C	93.35000	86.83680	71.38690	-267.21160	-210.66064	-845.97344	1
1660	C	94.61200	86.34080	71.69290	655.75804	-564.39688	287.90375	1
1661	H	95.21600	85.79680	70.98190	334.43709	2494.07345	1888.37911	1
1662	C	95.06100	86.33180	73.02790	-375.00209	-754.50196	348.64199	1
1663	H	96.04700	85.93680	73.22090	-1727.33280	2352.20041	1175.45771	1
1664	C	94.24500	86.86180	74.05990	168.57779	-896.03843	-12.15211	1
1665	H	94.57100	86.73680	75.08290	-2216.01216	-981.64263	-2005.96463	1
1666	C	92.50300	87.41580	72.35390	397.42365	-533.22258	-623.84223	1
1667	H	91.51600	87.77480	72.10090	2533.82735	-1251.84279	-1382.32949	1
1668	C	93.01600	87.49180	73.71890	-799.10395	438.28107	28.17074	1

1669	H	92.45100	87.95780	74.51290	634.38809	1427.74225	-2730.81124	1
1670	C	93.18900	87.98680	67.65690	593.73866	152.84604	-674.95444	1
1671	O	93.08700	86.93280	67.02390	-215.50784	247.26186	-718.36284	1
1672	N	92.91300	89.17280	67.02790	521.85640	-461.99547	-476.33850	1
1673	H	93.05700	89.98680	67.58590	1535.59398	-2699.90410	500.69471	1
1674	C	92.57700	89.31980	65.60190	-667.94178	-579.26211	-223.06993	1
1675	H	93.47200	89.05380	65.05890	1384.10713	1933.02197	-2060.55812	1
1676	H	92.39200	90.37080	65.43790	-2265.35263	1005.89386	-1937.67418	1
1677	C	91.36200	88.56880	65.10290	-338.21148	576.74889	-620.01993	1
1678	O	90.58400	87.97180	65.85990	-527.56455	24.33275	-587.12077	1
1679	N	91.06900	88.61280	63.80390	258.72197	-802.41539	43.18302	1
1680	H	91.77400	88.96380	63.19190	2299.62585	-2030.67816	697.34740	1
1681	C	89.85900	88.04180	63.16090	400.90491	-656.62855	-489.45398	1
1682	H	89.00500	88.27780	63.77890	-2324.58395	-46.91799	2119.51277	1
1683	C	89.62900	88.63080	61.72090	884.72750	220.52244	8.83770	1
1684	H	88.99200	88.06880	61.00490	529.44609	-3092.97243	-226.79196	1
1685	H	90.64100	88.63280	61.26090	-1376.09791	-1176.59094	2572.97775	1
1686	C	89.06000	90.03980	61.75990	413.35551	777.20766	237.77403	1
1687	O	87.82900	90.27780	61.76490	635.71870	316.31167	345.59497	1
1688	N	89.92900	91.06780	61.75290	-685.32709	-34.16076	-491.76428	1
1689	H	90.90900	90.90380	61.63490	2225.71538	-34.57058	2223.33581	1
1690	H	89.47900	91.95780	61.81790	1952.47180	-2290.18832	-917.12462	1
1691	C	90.02800	86.49080	62.98590	-341.16812	-616.42940	578.85241	1
1692	O	89.09900	85.71380	63.09990	-327.55418	-475.33699	-538.87868	1
1693	N	91.27900	85.92980	62.74790	610.27266	-283.93615	509.52903	1
1694	H	92.02100	86.55680	62.52290	-2084.90234	-114.35491	-2353.36598	1
1695	C	91.51800	84.51480	62.52590	-303.85369	327.99406	-794.69732	1
1696	H	90.87200	84.13680	61.74790	653.10532	1475.78820	-2700.69044	1
1697	C	92.98800	84.28580	62.01190	-238.70131	369.43906	798.74118	1
1698	H	93.08100	84.82880	61.04690	1085.24458	-2922.78161	-421.68479	1
1699	H	93.75600	84.78580	62.63890	1128.55225	-2204.32737	1940.49914	1
1700	C	93.37900	82.83780	61.76390	608.72225	-553.81916	-392.67362	1
1701	C	93.09300	82.24380	60.53090	-468.98586	-656.18359	-425.35439	1
1702	H	92.55800	82.73080	59.72890	-1607.52473	-1776.61513	-2039.05104	1
1703	C	93.42400	80.89180	60.32490	-625.83448	-653.59781	112.21452	1
1704	H	93.07600	80.44380	59.40590	-1045.66976	1143.19553	2738.23026	1
1705	C	94.15700	80.14080	61.27890	579.68301	666.09819	-227.44627	1
1706	H	94.35300	79.09980	61.07090	1124.86553	-373.46759	2914.34825	1
1707	C	94.09900	82.07280	62.66490	462.54836	-777.13699	-116.43932	1
1708	H	94.24300	82.65980	63.55990	-85.87457	-3127.46285	331.40295	1
1709	C	94.50800	80.76380	62.47290	675.66046	106.19139	-603.04007	1
1710	H	94.97700	80.15980	63.23490	1560.44302	-1618.92325	-2200.52978	1
1711	C	91.15900	83.68080	63.73290	-511.73531	21.65640	754.39312	1
1712	O	90.49700	82.62580	63.60990	165.21243	358.61325	-683.90688	1
1713	N	91.54500	84.08880	64.97890	410.80864	-705.33174	215.44300	1
1714	H	92.25500	84.78180	65.07190	2449.11558	-1691.15549	1019.82949	1
1715	C	91.05900	83.46380	66.12890	-632.30974	219.01402	-619.40960	1
1716	H	90.97300	82.39880	65.96990	-1278.42454	-1123.25045	-2646.16049	1
1717	C	91.97900	83.68480	67.32190	679.12662	291.88879	533.89041	1
1718	H	92.00800	84.76880	67.56390	105.77246	2278.40069	2167.00916	1
1719	H	91.54900	83.17080	68.20790	2791.06047	1226.09723	-777.74883	1
1720	C	93.41300	83.09980	67.07090	463.97143	782.73025	59.28629	1
1721	H	93.86800	83.56380	66.16990	36.40771	2133.23610	2312.18607	1
1722	C	94.41000	83.62580	68.14990	-600.67703	-670.61488	-144.61603	1
1723	H	94.13600	83.23380	69.15290	1342.01646	-1105.45353	-2622.05846	1
1724	H	94.50000	84.72780	68.25790	-2084.70444	2346.69202	-212.76793	1
1725	H	95.41400	83.22980	67.88390	-2814.07102	-49.33852	-1405.98586	1
1726	C	93.41700	81.60480	66.91190	-587.30337	-417.38709	558.85040	1
1727	H	92.78300	81.17580	66.10690	69.58549	-2208.91414	2239.21469	1
1728	H	93.12900	81.18280	67.89790	-687.56433	1506.23164	-2675.20985	1
1729	H	94.45700	81.21880	66.84390	-1156.29635	-2827.12469	754.03643	1
1730	C	89.61400	83.83780	66.42890	-551.54040	-574.51235	-444.06052	1

1731	O	88.85000	83.03980	67.01290	275.76398	-630.50100	387.36281	1
1732	N	89.10300	85.05680	66.07090	488.92904	-684.66165	69.70732	1
1733	H	89.71700	85.58580	65.48890	-1386.15151	-2051.54263	-1941.12933	1
1734	C	87.69700	85.43480	66.28090	-506.32382	758.05385	-21.01315	1
1735	H	87.57200	85.41580	67.35390	1421.22074	-1757.90799	-2188.17671	1
1736	C	87.43000	86.86580	65.78490	-218.19577	-838.49218	284.20497	1
1737	H	87.71700	86.90780	64.71290	-2996.20863	-394.11366	-875.00544	1
1738	H	88.11300	87.55180	66.32990	753.61372	-239.34513	3045.16116	1
1739	S	85.78600	87.54880	66.04890	-103.88828	300.77893	458.20287	1
1740	C	86.67300	84.54580	65.53490	468.55176	-778.06349	-80.79270	1
1741	O	85.70400	84.06480	66.09490	-54.92999	-671.22255	412.39570	1
1742	N	86.85900	84.23180	64.25690	66.16328	-769.66710	340.45157	1
1743	H	87.68800	84.53680	63.79390	-135.63952	1068.33728	-2956.09263	1
1744	C	86.09400	83.32380	63.49490	130.49446	-830.37783	-353.40467	1
1745	H	85.03600	83.53880	63.49790	2368.38846	-1149.97036	-1722.36190	1
1746	C	86.54900	83.31080	62.03090	112.81255	636.57212	-643.03987	1
1747	H	86.13700	82.48080	61.41790	-304.47146	-3122.02448	-241.83976	1
1748	H	87.65600	83.22380	61.99490	2937.06650	-918.11379	654.93028	1
1749	C	86.19500	84.62180	61.36690	-497.36283	-287.74757	-708.01311	1
1750	H	86.37200	85.54180	61.96390	-1057.79252	-2332.86291	-1826.75994	1
1751	H	85.09100	84.55380	61.26190	-2298.96645	-1784.27605	1195.54945	1
1752	C	86.79500	84.65480	59.96290	660.26666	303.50348	-550.80358	1
1753	H	86.34400	83.82380	59.38090	2426.74497	-1992.59634	-196.71027	1
1754	H	87.86800	84.41480	60.12190	-1387.40064	-1541.07747	-2366.09931	1
1755	C	86.67400	85.97180	59.23590	-875.10080	-255.52354	18.90260	1
1756	H	87.01900	85.79080	58.19590	-1860.42353	-756.59909	-2421.69534	1
1757	H	87.30400	86.70080	59.78990	-1257.14476	201.69799	2877.00038	1
1758	N	85.24300	86.40480	59.13390	550.15190	-433.54662	471.21385	1
1759	H	85.25300	87.34180	58.68190	-1392.02402	-1412.62335	-2442.33303	1
1760	H	84.90600	86.51780	60.11190	1359.56767	2827.91179	229.60156	1
1761	H	84.65300	85.74180	58.59290	-2156.55298	-656.20582	-2194.74358	1
1762	C	86.02200	81.92880	64.05690	-25.20875	-730.95805	544.53269	1
1763	O	84.99900	81.30480	64.09590	-669.60571	-145.24746	392.63036	1
1764	N	87.20100	81.39480	64.42590	664.46358	323.69454	-407.89985	1
1765	H	88.05400	81.83980	64.16690	1874.68390	1570.92865	-1978.88092	1
1766	C	87.36500	80.09380	65.00890	-806.66962	406.06459	-125.88355	1
1767	H	86.88200	79.29380	64.46790	-840.29316	742.92660	-2939.42064	1
1768	C	88.86800	79.76980	65.00690	384.14217	412.45196	716.77694	1
1769	H	89.28500	79.59280	63.99190	242.40516	2840.98077	-1329.77225	1
1770	H	88.98400	78.87080	65.64790	-2622.91723	1509.52797	860.14927	1
1771	H	89.43500	80.62280	65.43790	-671.05250	313.67905	-3057.69852	1
1772	C	86.72700	79.92780	66.35090	447.81818	-666.23100	432.48831	1
1773	O	85.95200	79.01880	66.54290	18.07445	-533.90771	581.58671	1
1774	N	86.90000	80.80780	67.33590	52.24553	-1.42966	-842.57976	1
1775	H	87.40500	81.66380	67.25290	-635.55545	3074.58441	-203.04230	1
1776	C	86.19000	80.52680	68.62890	-45.17959	-746.01266	522.37431	1
1777	H	86.32400	79.48480	68.87990	2489.32848	-1413.08181	-1305.63002	1
1778	C	86.84000	81.26180	69.83390	897.64650	-110.01010	-116.53127	1
1779	H	86.44200	80.90480	70.80790	1408.17935	2475.00587	1337.76048	1
1780	C	88.33400	81.07680	69.72290	-582.43885	632.82097	-302.90858	1
1781	H	88.48300	79.98080	69.82890	-1210.19525	2649.47509	1189.09016	1
1782	H	88.82500	81.27280	68.74590	-2159.66932	-2208.90610	595.64124	1
1783	H	88.77100	81.69980	70.53290	-2075.46351	-2104.57188	1077.70805	1
1784	C	86.58200	82.78080	69.82590	-583.50057	-481.36666	509.17996	1
1785	H	86.96400	83.25980	70.75290	2213.50099	-179.52086	-2228.54478	1
1786	H	85.55100	83.08380	69.54390	624.68477	2755.71629	1383.48217	1
1787	H	87.13100	83.11580	68.91990	-244.60913	3125.03068	-269.39903	1
1788	C	84.70900	80.73080	68.63990	-624.07646	-121.06114	653.70006	1
1789	O	84.02200	80.17280	69.49290	-238.44104	571.68688	489.84406	1
1790	N	84.24600	81.55880	67.65790	-151.63758	-810.04598	183.04056	1
1791	H	84.91200	81.97480	67.04290	1977.50723	1873.26611	1574.34604	1
1792	C	82.80800	81.69580	67.40890	499.75622	-247.95496	721.25797	1

1793	H	82.37200	81.78180	68.39290	-348.33637	-218.96637	-3119.12515	1
1794	C	82.41500	82.92780	66.52990	742.69846	-31.02271	528.09810	1
1795	H	81.41600	82.87480	66.04590	896.14559	-2284.10859	-1969.26312	1
1796	H	83.13300	83.04280	65.69090	-1146.78510	1807.43618	2305.70697	1
1797	N	83.20600	85.28880	67.26290	505.69156	-647.14511	-195.32419	1
1798	H	83.95700	85.33180	66.60390	2316.47881	-476.55800	2074.86015	1
1799	C	82.39900	84.15480	67.43290	902.00239	-124.80661	-47.60248	1
1800	C	82.85600	86.07780	68.29290	-638.91953	-645.04109	84.58620	1
1801	H	83.50900	86.90180	68.58290	-2641.87769	495.78009	1634.90386	1
1802	N	81.91100	85.62880	69.10190	-349.74007	525.41036	560.62298	1
1803	C	81.65600	84.41580	68.51590	145.69151	-483.20267	-759.43411	1
1804	H	80.87200	83.84280	68.99590	-3021.51565	347.01583	-805.13936	1
1805	C	82.16700	80.46780	66.77990	725.62175	110.67695	-540.99418	1
1806	O	81.09700	80.01880	67.19390	479.04239	-454.87964	432.70097	1
1807	N	82.89000	79.89280	65.78590	188.12333	734.94736	-370.31646	1
1808	H	83.69400	80.36680	65.43590	1914.81718	-549.16846	2435.18283	1
1809	C	82.59700	78.59880	65.20790	54.12027	769.66613	-485.93832	1
1810	H	81.57800	78.58580	64.84890	-1049.03304	2426.50211	1705.82632	1
1811	C	83.57500	78.33080	64.01290	596.97102	-687.01777	55.52647	1
1812	H	84.59400	78.72480	64.21390	-496.89337	2038.51344	-2344.30931	1
1813	C	83.59900	76.78780	63.77490	232.22169	-880.38005	-49.54850	1
1814	H	84.31500	76.28780	64.46290	246.70180	201.97220	-3129.94755	1
1815	H	83.98300	76.51480	62.76890	-2337.88053	281.78683	2086.41728	1
1816	H	82.64600	76.27180	64.01990	-2667.66253	262.47740	-1647.09090	1
1817	C	83.00400	79.04680	62.75690	-678.67608	258.77949	551.25580	1
1818	H	81.91100	78.88580	62.63890	3119.82534	-308.84410	-263.68804	1
1819	H	83.47200	78.73680	61.79890	-191.64151	3022.17448	-853.20641	1
1820	H	83.14800	80.14080	62.88390	1772.08540	-2410.22431	-974.04228	1
1821	C	82.54300	77.54080	66.30590	-631.12913	145.22344	641.90122	1
1822	O	81.51500	76.91780	66.54690	-130.07486	580.52320	519.32704	1
1823	N	83.59100	77.46180	67.16990	126.88737	-117.38196	826.31311	1
1824	H	84.39600	78.01380	66.96890	1956.94730	-1116.92560	-2195.69140	1
1825	C	83.61000	76.47880	68.21290	172.84335	-885.22278	-134.00303	1
1826	H	83.48300	75.48980	67.79590	2001.37120	-2191.18902	-1044.71538	1
1827	C	85.03500	76.38780	68.80890	-548.43571	-706.59961	-177.16170	1
1828	H	85.44800	77.41780	68.87090	-1703.84352	1680.71119	2042.14431	1
1829	C	85.07400	75.72080	70.18590	-539.66435	-539.81379	498.81306	1
1830	H	86.10000	75.62280	70.60190	-2611.82489	1740.15603	-220.12259	1
1831	H	84.55100	76.30080	70.97590	-496.85295	-1171.17159	2877.45034	1
1832	H	84.66100	74.69080	70.12890	2368.40023	-2056.67944	242.85024	1
1833	C	85.97700	75.72480	67.76590	-89.73891	-245.42260	873.59354	1
1834	H	85.69100	74.65480	67.67490	-1508.14052	2268.84120	-1573.56220	1
1835	H	85.74100	76.16480	66.77290	1471.34731	1867.64784	2060.40163	1
1836	C	87.47200	75.97180	67.95890	398.49030	399.48319	716.28881	1
1837	H	88.05300	75.45780	67.16290	1584.70168	-2599.63602	-792.99393	1
1838	H	87.73000	75.66880	68.99590	1408.83570	-3.37167	2813.07605	1
1839	H	87.69600	77.04780	67.79490	1761.32265	-1730.37664	-1949.81164	1
1840	C	82.51700	76.61280	69.28290	-612.13101	80.81315	-670.98127	1
1841	O	81.96700	75.61980	69.76790	-700.48536	235.55583	278.31806	1
1842	N	82.13600	77.82380	69.67790	-397.17551	-497.81979	554.16546	1
1843	H	82.59400	78.62980	69.31090	651.88955	2517.34254	1770.94686	1
1844	C	81.05000	78.07380	70.56590	654.19916	-590.42628	-234.24616	1
1845	H	81.27600	77.50580	71.45590	-377.49390	-3116.51217	-207.54877	1
1846	C	81.05200	79.58980	71.00790	-114.37893	862.88896	271.64518	1
1847	H	80.98000	80.15680	70.05590	943.25906	-572.63602	-2946.28182	1
1848	H	82.02300	79.80180	71.50490	-1748.26127	656.72251	-2531.90132	1
1849	C	79.92200	80.03280	71.97990	452.51212	528.19214	589.65825	1
1850	C	79.38500	79.12780	72.88490	754.59482	199.91169	-471.24620	1
1851	H	79.82100	78.13980	72.84190	2344.68839	-2090.15074	178.69654	1
1852	C	78.46300	79.55580	73.85390	-193.29632	798.69741	-395.18348	1
1853	H	78.13700	78.88380	74.63390	509.82928	2843.38580	1246.37776	1
1854	C	77.98700	80.85580	73.88990	709.78619	190.32186	-539.84457	1

1855	O	76.96700	81.12580	74.81990	334.16104	-638.41461	-323.09504	1
1856	H	77.08100	82.02380	75.14090	1606.67949	-1710.99670	2095.06505	1
1857	C	79.47200	81.38480	72.01490	-504.04825	738.87999	177.32097	1
1858	H	79.94600	82.09480	71.35290	2005.67626	-799.99938	2288.11931	1
1859	C	78.48900	81.79280	72.93090	691.47901	405.71107	-434.40339	1
1860	H	78.06400	82.77980	73.03490	51.16103	757.40718	-3053.18574	1
1861	C	79.67300	77.54080	70.07190	-591.54483	-271.63962	-638.54337	1
1862	O	78.96500	76.79380	70.76590	480.63820	-472.80926	-411.17582	1
1863	N	79.39400	77.68380	68.75890	-742.13666	-402.33044	5.97397	1
1864	H	79.95300	78.19680	68.11190	-1152.78188	-985.56835	2756.44249	1
1865	C	78.20500	77.02080	68.19390	61.86485	795.84696	440.73955	1
1866	H	77.43900	76.92980	68.94890	2957.23336	311.72141	1027.53435	1
1867	C	77.48800	77.80880	67.07390	365.22154	-641.60525	-535.17000	1
1868	H	76.97700	77.12180	66.36490	1489.23193	-2376.00632	1426.53721	1
1869	O	78.48200	78.54080	66.33890	-429.72842	-403.07271	-525.82612	1
1870	H	77.96600	79.06380	65.71990	-574.08783	2164.89805	2209.49448	1
1871	C	76.51200	78.84980	67.67590	697.50266	558.61072	181.37007	1
1872	H	76.14500	79.53180	66.87990	2249.53106	-1717.20658	-1374.42272	1
1873	H	77.06600	79.47580	68.40790	2634.55936	-1601.01892	627.74326	1
1874	H	75.64300	78.39980	68.20290	-713.51949	1849.88532	2442.75264	1
1875	C	78.36700	75.56380	67.75190	-7.02825	-797.23219	442.51829	1
1876	O	77.49200	74.70580	67.73790	240.06474	726.04181	-197.12798	1
1877	N	79.64800	75.13880	67.41590	-408.58583	723.26836	150.37549	1
1878	H	80.37000	75.81880	67.31490	490.41974	-2731.32403	-1482.42496	1
1879	C	79.99100	73.68980	67.21490	96.94854	903.87318	-71.17058	1
1880	H	79.38000	73.32380	66.40290	1636.03180	79.93332	2686.11929	1
1881	C	81.38900	73.44280	66.61790	753.31258	-143.30555	493.39100	1
1882	H	82.10200	74.18380	67.03690	1.26167	-3129.15480	326.51929	1
1883	C	81.96200	72.04380	66.97190	590.03942	163.45730	675.71162	1
1884	H	82.88300	71.83080	66.38890	1734.49980	-1908.04658	-1802.52460	1
1885	H	81.18600	71.31880	66.64490	2503.40734	-883.74296	-1688.24652	1
1886	H	82.34400	71.99180	68.01390	424.99352	-1858.61728	-2502.62833	1
1887	C	81.32400	73.80080	65.10990	471.76441	434.85651	647.91139	1
1888	H	80.97800	74.84980	64.98990	2747.00389	-1517.00860	-225.56764	1
1889	H	82.37400	73.66580	64.77390	-1751.98534	1436.13269	-2183.18495	1
1890	H	80.63300	73.08980	64.60990	682.85022	-2983.27233	729.40251	1
1891	C	79.75400	72.79980	68.47990	-611.60228	619.69360	-270.87543	1
1892	O	79.20000	71.70380	68.33390	539.82664	389.62199	424.74596	1
1893	N	80.08100	73.22380	69.70090	180.51449	-501.80127	654.43280	1
1894	H	80.50800	74.12280	69.76890	-623.22305	-2689.20612	-1509.30106	1
1895	C	79.61600	72.58280	70.91190	-758.21121	77.84343	-500.50691	1
1896	H	79.83700	71.53080	70.80090	-2388.70021	-667.93170	1935.51150	1
1897	C	80.32000	73.15880	72.15090	173.62257	886.27264	125.80548	1
1898	H	80.52000	74.24680	72.04990	-487.35254	2917.52556	-1071.80145	1
1899	H	81.33400	72.70680	72.18690	-1942.63109	-1104.31059	-2214.70287	1
1900	C	79.57500	73.06880	73.50490	0.53602	-710.39638	571.65348	1
1901	O	78.59100	73.73680	73.79790	503.15830	-70.38296	-604.57025	1
1902	N	80.05400	72.13480	74.36090	397.13462	-702.76268	247.14571	1
1903	H	80.91400	71.64380	74.22290	2443.43042	1919.69813	-492.57803	1
1904	H	79.62900	72.06180	75.26290	-1603.97196	-1825.56446	1998.20284	1
1905	C	78.06400	72.62880	71.06090	-123.19949	902.26504	-46.80486	1
1906	O	77.44500	71.63380	71.38190	-387.17212	282.86592	627.46462	1
1907	N	77.42000	73.74480	70.75490	-507.13097	-667.59190	-99.05314	1
1908	H	77.98600	74.52280	70.49790	-2034.56775	-2307.93209	657.42663	1
1909	C	76.00300	73.97580	70.88590	-846.11252	99.95548	-324.88999	1
1910	H	75.75900	73.92180	71.93690	1782.92205	-2460.45939	815.81541	1
1911	C	75.56400	75.38480	70.54190	-253.18701	-871.19825	91.43828	1
1912	H	75.41200	75.53680	69.45190	2147.36810	1424.51941	1804.93239	1
1913	H	76.35700	76.10880	70.82590	2127.62731	-2289.29574	-361.32158	1
1914	C	74.25900	75.91580	71.28290	-525.10873	544.33656	509.32263	1
1915	H	73.50300	75.10180	71.26190	-1666.29387	-2300.37864	1352.75610	1
1916	C	74.54200	76.24980	72.74990	-617.90918	-485.30478	462.72943	1

1917	H	74.82100	75.38380	73.38690	-351.36839	2865.56617	-1250.31876	1
1918	H	73.69400	76.78080	73.23390	-1920.77585	2242.40229	1086.49821	1
1919	H	75.40100	76.95280	72.71390	-589.63127	-2948.43239	925.90908	1
1920	C	73.71700	77.15380	70.58690	-87.72335	480.98790	769.67932	1
1921	H	72.74800	77.35680	71.09090	-1276.29460	2225.82568	1820.71370	1
1922	H	73.66100	76.90080	69.50690	-2203.76964	934.25333	2041.76304	1
1923	H	74.31300	78.05480	70.84590	-1234.75030	-2563.91468	1341.62567	1
1924	C	75.09600	73.04480	70.08690	-823.19531	386.69312	-65.33692	1
1925	O	74.19500	72.43780	70.57690	526.45364	454.78628	-373.68869	1
1926	N	75.58000	72.79280	68.84390	443.93448	-712.83705	-86.35858	1
1927	H	76.37800	73.29880	68.52390	601.87010	1445.94777	-2728.59188	1
1928	C	75.03800	71.79380	67.92590	40.82754	-550.16236	-726.02031	1
1929	H	73.97500	71.68380	68.08490	-943.64116	2265.16292	1968.96027	1
1930	C	75.21300	72.27780	66.44590	0.42648	-911.21787	-33.65742	1
1931	H	74.68000	71.57580	65.76990	-390.88671	2219.09751	2195.68669	1
1932	H	76.30400	72.25780	66.23490	1252.60414	1664.08903	-2357.96879	1
1933	C	74.58800	73.64280	66.30190	26.48589	860.96915	299.13478	1
1934	C	73.40500	74.05580	66.90090	-621.48891	167.06086	-645.98236	1
1935	H	72.87400	73.31580	67.48090	2145.74123	2086.75121	-969.27303	1
1936	C	72.89700	75.36980	66.79290	-857.74780	244.13350	-190.04880	1
1937	H	72.03100	75.61380	67.39190	1603.14685	2173.95579	1613.09101	1
1938	C	73.59500	76.30480	66.07290	-539.21799	452.23959	-579.80541	1
1939	O	73.11000	77.58880	66.04690	460.31102	-255.30135	588.69535	1
1940	H	73.77800	78.08480	65.56790	2107.07791	-2267.33556	563.59415	1
1941	C	75.25300	74.59480	65.48390	-684.91077	80.98427	-596.48118	1
1942	H	76.17700	74.26580	65.03190	52.89202	-2929.72220	1145.49398	1
1943	C	74.76400	75.91180	65.39090	335.61882	465.96907	708.29643	1
1944	H	75.26000	76.67480	64.80990	2047.39318	-735.56354	-2272.74144	1
1945	C	75.55000	70.36280	68.08790	-730.70072	225.96520	-496.45462	1
1946	O	74.98700	69.48580	67.47890	492.52319	-467.35595	-403.26983	1
1947	N	76.64500	70.10980	68.85690	332.02813	-574.83824	-521.52719	1
1948	H	77.20900	70.81580	69.27890	-332.30311	-1613.18258	2680.56763	1
1949	C	77.21400	68.74780	68.93090	-683.50515	-67.23577	-599.79252	1
1950	H	76.76200	68.11280	68.18290	-2599.98571	1610.27686	738.45040	1
1951	C	78.76800	68.59680	68.72990	603.28981	448.25783	516.29190	1
1952	H	78.91700	68.76980	67.64290	2145.86021	-2299.79467	66.74314	1
1953	H	79.12100	67.55780	68.90390	-2639.78228	-698.79261	1562.51867	1
1954	O	79.43400	69.45380	69.61290	760.86385	211.04121	13.23026	1
1955	H	79.36600	70.29480	69.15390	-3047.61140	-664.88082	410.15176	1
1956	C	76.83600	68.12980	70.21990	505.51926	593.75309	-472.60824	1
1957	O	76.31600	67.01880	70.22490	-305.41886	529.60808	-499.86181	1
1958	N	76.90800	68.88580	71.39690	82.91860	470.09816	-696.27905	1
1959	H	77.09200	69.86380	71.34290	-1866.32202	2134.50234	1363.43982	1
1960	C	76.65900	68.29280	72.72790	499.97309	463.04944	-605.85735	1
1961	H	77.37300	67.49480	72.86990	-351.75708	-47.79780	-3126.05319	1
1962	C	76.99100	69.27280	73.89690	725.69444	72.90043	-547.26969	1
1963	H	78.08900	69.43780	73.90890	367.04990	3123.02768	-100.98865	1
1964	H	76.72300	68.86880	74.89590	2930.09636	78.26983	1143.08153	1
1965	O	76.37400	70.60180	73.75590	279.79270	520.02189	-524.32862	1
1966	H	76.99100	71.20580	73.33690	534.48385	2596.34613	-1694.56189	1
1967	C	75.22200	67.71180	72.98090	202.29665	-549.82311	698.72857	1
1968	O	75.04700	66.54180	73.22690	544.77936	-309.00250	-480.99910	1
1969	N	74.23400	68.54880	72.77190	-752.15878	-381.67568	-35.39965	1
1970	H	74.49300	69.49780	72.60890	1268.04132	2607.15182	1221.90704	1
1971	C	72.81700	68.20780	72.84690	710.04538	-428.18661	-379.39792	1
1972	H	72.69700	67.79180	73.83690	-686.59231	-1500.55204	-2678.64907	1
1973	C	71.92400	69.42580	72.75590	209.06955	-36.19039	886.80955	1
1974	H	72.28100	70.22380	73.44090	-2085.32984	2284.08993	576.67919	1
1975	C	71.88500	70.06880	71.32090	499.76581	-492.78721	-582.10471	1
1976	H	72.95400	70.30580	71.12690	2779.33005	739.84867	1275.21553	1
1977	H	71.46800	69.35080	70.58190	1524.64378	-1888.52651	-2001.78800	1
1978	H	71.31100	71.01980	71.33190	2637.64247	-1630.49978	-531.54386	1

1979	C	70.59100	69.04780	73.37790	-372.81460	-735.77503	388.70989	1
1980	H	69.91400	69.92780	73.42990	1625.06971	2261.93045	1463.23112	1
1981	H	70.01500	68.20180	72.94690	-864.21140	-2007.22371	2263.27592	1
1982	H	70.85600	68.68180	74.39290	-469.47901	2020.33590	2365.59898	1
1983	C	72.36900	67.11980	71.85690	629.43342	358.41755	-553.89659	1
1984	O	71.52900	66.26080	72.13090	-589.69875	363.08965	-379.53724	1
1985	N	72.91100	67.09180	70.61690	-449.40910	168.04409	-694.59696	1
1986	H	73.50900	67.85780	70.39290	1964.75811	-654.85447	-2368.35754	1
1987	C	72.45400	66.06380	69.71790	468.66728	-462.33048	630.91402	1
1988	H	71.39000	65.90280	69.80790	2191.61940	1245.69789	-1882.35688	1
1989	C	72.66000	66.54280	68.23090	-170.29364	-613.54213	652.69988	1
1990	H	72.52100	65.61380	67.63890	-2061.86786	-957.50340	2174.88261	1
1991	H	73.68700	66.96680	68.24990	2005.53283	408.55536	-2389.38210	1
1992	C	71.72500	67.59780	67.72090	128.59630	-727.81848	534.03582	1
1993	C	71.74100	68.95780	67.92090	894.52228	-29.63960	174.36279	1
1994	H	72.58600	69.44280	68.38690	2030.21511	2058.12856	1241.19285	1
1995	N	70.70500	69.55680	67.31790	727.30233	420.89478	-80.93944	1
1996	H	70.35400	70.42880	67.57890	-1973.75192	-1651.95424	1809.30284	1
1997	C	69.94900	68.58180	66.73890	243.32934	-63.35365	-876.48625	1
1998	C	70.55000	67.30580	66.99790	-190.94289	172.77976	874.72223	1
1999	C	69.90800	66.17080	66.61990	-93.85484	-660.48461	621.61271	1
2000	H	70.39900	65.26380	66.93990	2048.96375	-2016.74493	1277.77684	1
2001	C	68.76100	66.27480	65.85090	-377.12460	-617.76491	554.61208	1
2002	H	68.26800	65.37480	65.51390	1730.73166	-2328.72526	1216.48379	1
2003	C	68.83000	68.69180	65.97190	730.54797	-304.43379	-452.84736	1
2004	H	68.33200	69.62280	65.74690	-2320.43694	1339.02085	1649.49137	1
2005	C	68.20200	67.49880	65.54590	-244.50619	-641.80439	599.79567	1
2006	H	67.29300	67.52580	64.96390	-1265.65520	2117.35612	-1952.72789	1
2007	C	73.19300	64.74780	69.88990	-482.85355	-411.10843	-655.20478	1
2008	O	72.67800	63.69780	69.58190	-227.20677	516.73750	-552.25598	1
2009	N	74.40600	64.73880	70.51790	306.62036	443.17883	-649.80671	1
2010	H	74.96100	65.55880	70.63090	541.35490	-2263.20012	-2117.33000	1
2011	C	74.94700	63.53980	71.09390	211.47599	668.35783	583.11810	1
2012	H	75.05800	62.74180	70.37490	1193.44186	-1526.63374	2478.57059	1
2013	C	76.44200	63.74480	71.56290	-164.41428	-877.45988	-185.69629	1
2014	H	76.37000	64.76080	72.00790	-1630.38460	2144.49160	1625.18554	1
2015	C	76.85300	62.73380	72.62490	-608.62513	-648.12263	202.39444	1
2016	H	77.96400	62.74180	72.63890	2696.28003	-1620.77259	-37.36905	1
2017	H	76.59800	61.68380	72.36590	1179.64944	2730.85172	1024.25695	1
2018	H	76.41300	62.97180	73.61690	-1478.26273	1604.74732	-2266.66089	1
2019	C	77.39100	63.63880	70.36590	8.20750	265.60563	872.25987	1
2020	H	76.79400	64.06380	69.53090	462.68468	-2934.50414	-1035.77727	1
2021	H	77.58600	62.57880	70.09590	-1516.21961	1468.85257	2332.76155	1
2022	C	78.55700	64.57680	70.48490	839.58786	-355.09175	-21.28559	1
2023	H	79.21500	64.35480	71.35190	-436.62506	-2985.91408	-889.88870	1
2024	H	78.21700	65.63480	70.49190	2176.02064	-1949.66633	1167.03110	1
2025	H	79.23400	64.48180	69.60890	-331.58476	2196.46751	2227.96055	1
2026	C	74.09700	62.96180	72.24090	649.57505	638.24844	46.28366	1
2027	O	73.82900	61.77480	72.30290	-138.42758	177.31496	-756.98378	1
2028	N	73.51000	63.84680	73.06590	356.39596	-536.86647	545.37015	1
2029	H	73.79600	64.80180	73.04790	604.44629	2816.39918	1265.21403	1
2030	C	72.53000	63.56280	74.09690	-367.57465	819.53089	157.19097	1
2031	H	72.92800	62.80480	74.75590	-2230.80755	-2203.91626	-253.92325	1
2032	C	72.31300	64.68880	75.09590	-713.56169	533.97940	-192.73483	1
2033	H	71.43000	64.41080	75.70990	737.94673	-1447.00282	2694.40971	1
2034	H	71.98400	65.56780	74.50090	988.30864	-2623.77034	1427.34070	1
2035	C	73.46500	64.97780	76.06990	315.59796	810.29507	-274.35532	1
2036	H	74.37300	65.14780	75.45290	-1407.76648	-148.86095	2809.67261	1
2037	C	73.19900	66.08480	77.11390	-686.19111	-497.15689	-336.79043	1
2038	H	74.07700	66.31080	77.75590	175.12160	-2544.02273	-1842.69015	1
2039	H	72.87400	67.00380	76.57990	-2609.81228	-1501.90045	911.81200	1
2040	H	72.38300	65.70780	77.76590	1615.89084	-2455.22836	-1122.04132	1

2041	C	73.79100	63.67480	76.88490	651.44052	173.93095	-613.86015	1
2042	H	74.66400	63.90280	77.53190	1930.19295	-2010.98147	1458.94995	1
2043	H	72.87900	63.35080	77.43090	-537.77902	2884.37451	1135.51911	1
2044	H	74.16100	62.87780	76.20390	843.70987	-2804.94804	-1148.32328	1
2045	C	71.22700	62.91880	73.51690	187.75238	-389.88903	-802.61235	1
2046	O	70.71800	61.98380	74.14690	577.28224	-43.37584	537.11357	1
2047	N	70.70300	63.40180	72.34790	128.20291	632.22047	544.54896	1
2048	H	71.10300	64.26580	72.05290	186.89101	98.28880	-3139.05038	1
2049	C	69.73400	62.58180	71.58590	654.06218	-578.57456	-262.49789	1
2050	H	68.87900	62.38480	72.21590	1298.20440	-2813.05665	-547.36078	1
2051	C	69.26800	63.38280	70.33890	-409.82423	454.41187	676.02141	1
2052	H	68.28800	62.96680	70.02090	2106.20782	-2278.35270	520.79157	1
2053	H	69.96100	63.29480	69.47590	-2163.36909	25.16517	-2284.16881	1
2054	H	69.03900	64.45180	70.53990	1007.43167	948.51124	-2825.53253	1
2055	C	70.21000	61.21680	71.12590	491.19168	598.24155	-481.96346	1
2056	O	69.50700	60.27980	71.39790	-532.73410	-403.46037	-420.76280	1
2057	N	71.39700	61.10080	70.48690	-225.28400	-777.07639	240.98069	1
2058	H	71.96500	61.91780	70.43290	2166.94562	691.93797	-2173.42926	1
2059	C	71.91600	59.80780	70.10590	-126.00536	575.75589	695.75772	1
2060	H	71.21400	59.26580	69.48990	-690.27769	-1789.79050	-2493.67057	1
2061	C	73.26300	60.01580	69.27590	224.21008	184.41705	-864.39065	1
2062	H	73.86400	59.08180	69.30890	-1619.40231	-2123.66932	-1663.06675	1
2063	H	73.85400	60.81780	69.76790	1913.52656	-1741.36255	-1790.05552	1
2064	C	73.07700	60.37180	67.86290	-622.17021	-263.70164	612.22274	1
2065	C	71.99300	61.12680	67.38390	-153.95335	-692.81968	-572.49477	1
2066	H	71.19200	61.52980	67.98490	-1051.61428	-1867.79130	2302.97401	1
2067	C	71.80300	61.37380	66.02090	-108.51949	-460.74910	-779.34895	1
2068	H	70.93800	61.91180	65.66190	-2696.83752	568.12273	-1517.40904	1
2069	C	72.70500	60.88880	65.10690	558.68542	-586.75041	418.38447	1
2070	H	72.48900	61.01780	64.05590	-1393.58512	1798.98202	-2172.51247	1
2071	C	73.97600	59.87980	66.90290	-668.38031	-292.36310	-547.03070	1
2072	H	74.74700	59.17780	67.18090	-519.74511	-1949.36202	-2414.14145	1
2073	C	73.75000	60.08480	65.52790	345.24016	-765.15780	356.08113	1
2074	H	74.35200	59.44180	64.90390	1616.51876	-2429.04107	1176.79770	1
2075	C	72.12500	58.72180	71.18490	-303.75585	855.95742	-80.74823	1
2076	O	71.74000	57.56280	70.96290	-445.51117	517.35292	-396.85386	1
2077	N	72.61100	59.07480	72.37390	624.43315	-41.74067	566.58030	1
2078	H	72.89000	60.02280	72.50490	-2034.23856	-302.64010	-2380.86301	1
2079	C	72.68100	58.14080	73.49390	713.61045	-433.99477	365.86837	1
2080	H	73.09600	57.19180	73.18990	-1633.72734	654.31360	-2607.87939	1
2081	C	73.64600	58.74880	74.51190	260.21211	-18.29780	873.73100	1
2082	H	74.62300	58.87080	73.99490	-2067.64718	-1943.85280	-1358.12284	1
2083	C	73.16700	60.07580	75.15390	440.04924	-542.59235	-586.00444	1
2084	H	72.36900	59.90880	75.90790	-1735.24072	-1838.97854	-1872.25100	1
2085	H	72.74200	60.71680	74.35090	2076.29169	1145.42748	-2067.66413	1
2086	H	73.98700	60.55380	75.73090	61.29541	-2003.23385	-2425.18520	1
2087	C	74.00800	57.66680	75.58290	-407.78799	564.90514	-588.25347	1
2088	H	74.22300	56.72280	75.03790	-1794.03469	1567.45159	-2054.93583	1
2089	H	73.10600	57.48480	76.20490	-1525.73716	1839.86572	-2045.78750	1
2090	C	75.17000	58.18180	76.40990	765.16157	229.69992	-439.56423	1
2091	H	76.07100	58.47080	75.82890	2386.89484	-203.53102	2039.49366	1
2092	H	74.83000	59.07680	76.97390	-1837.93490	2218.18707	-1264.85874	1
2093	H	75.49500	57.43180	77.16290	2558.80596	729.98521	1678.64822	1
2094	C	71.27200	57.86480	74.12990	-473.64884	546.29694	-555.57847	1
2095	O	71.00500	56.75880	74.66690	-269.51525	338.64344	660.53719	1
2096	N	70.33700	58.79980	73.99790	646.29447	534.45494	96.61090	1
2097	H	70.55600	59.61580	73.46790	781.07339	-2098.00231	-2210.55127	1
2098	C	68.93700	58.59380	74.35490	593.35796	568.41995	-395.31771	1
2099	H	68.88800	58.26980	75.38390	207.37911	2077.34144	-2353.69341	1
2100	C	68.03700	59.88580	74.21290	-217.45794	-817.13132	341.26157	1
2101	H	66.94500	59.71580	74.32590	-659.08708	-2535.99944	1741.41819	1
2102	H	68.26200	60.32580	73.21790	-1033.35935	-2156.23168	-2044.76396	1

2103	O	68.38100	60.83480	75.21390	-253.99409	745.99177	51.09315	1
2104	H	69.14200	61.29780	74.85590	803.33209	3021.09575	-354.77355	1
2105	C	68.26600	57.55280	73.49690	-30.08678	-625.98435	-662.33630	1
2106	O	67.62400	56.66180	74.00890	-147.26451	764.27598	-133.50141	1
2107	N	68.41900	57.71580	72.14690	-287.87827	-29.02419	-793.06745	1
2108	H	68.91000	58.48880	71.75390	1145.58148	-2423.08517	1647.58234	1
2109	C	68.00800	56.73880	71.10290	159.68382	-403.84943	-801.78409	1
2110	H	66.93000	56.69380	71.05990	-2629.37076	1715.92865	-200.56050	1
2111	C	68.42200	57.32980	69.74790	-560.24413	-688.18695	-209.70514	1
2112	H	68.40100	56.60980	68.90190	705.45967	2170.66254	-2165.35841	1
2113	H	69.46400	57.71380	69.75790	-2176.69301	979.14654	2049.75751	1
2114	C	67.53700	58.48480	69.21390	-503.21823	77.51028	756.44866	1
2115	H	67.35400	59.16180	70.07590	1502.90016	-2763.10212	69.16678	1
2116	C	68.30300	59.44180	68.21290	-889.39703	87.46079	-181.03738	1
2117	H	67.50000	60.12880	67.86990	-467.28716	2715.87637	-1517.85523	1
2118	H	68.58400	58.83980	67.32290	3139.17701	-199.59344	-62.89984	1
2119	H	69.13000	60.00380	68.69590	-2149.99199	625.97437	-2209.95854	1
2120	C	66.27600	58.00980	68.50990	-855.61590	268.32927	-165.44437	1
2121	H	66.46300	57.26280	67.70990	-2981.96851	-570.26593	825.15865	1
2122	H	65.65900	58.82780	68.07890	802.82144	-1280.83377	-2759.19713	1
2123	H	65.59800	57.65380	69.31590	1210.31431	2486.21506	-1500.69990	1
2124	C	68.65300	55.42080	71.41890	391.22034	-381.16090	-730.14657	1
2125	O	67.96100	54.39280	71.36790	455.71177	545.16498	-344.59999	1
2126	N	69.99700	55.34680	71.65690	351.48327	563.15960	521.51995	1
2127	H	70.50300	56.19780	71.54090	-1979.51661	-2341.54775	704.90735	1
2128	C	70.66600	54.11680	71.95390	435.66842	173.61348	-781.98618	1
2129	H	70.37400	53.43580	71.16790	863.62376	2358.74427	-1894.38795	1
2130	C	72.21100	54.42880	71.99990	391.20592	677.24236	-468.77683	1
2131	H	72.41300	55.16980	72.80390	351.82945	-486.90668	-3088.26232	1
2132	H	72.52700	54.79380	70.99990	-2874.21529	-490.39723	-1181.78815	1
2133	C	72.99600	53.16680	72.28990	-158.05239	897.39430	33.96919	1
2134	O	73.09800	52.74080	73.45190	-319.86522	-36.92665	721.07551	1
2135	O	73.42800	52.48280	71.30890	21.67933	-572.38710	543.62693	1
2136	C	70.16900	53.41580	73.19190	746.88087	11.67975	522.95655	1
2137	O	70.09800	52.19680	73.28190	-322.11435	-301.26398	655.06457	1
2138	N	69.80300	54.19280	74.24790	-534.60853	-443.75660	479.52694	1
2139	H	69.85400	55.18780	74.23790	-98.47031	2179.77530	2266.51924	1
2140	C	69.17300	53.66180	75.45390	489.20023	634.45007	435.43913	1
2141	H	69.73600	52.83980	75.86990	-2529.30393	-1780.19729	-575.97347	1
2142	C	69.09800	54.71380	76.61790	-508.57795	603.74851	-456.38494	1
2143	H	69.19700	55.75280	76.23590	-2706.36543	520.13211	-1517.65444	1
2144	H	68.12200	54.60580	77.13890	1669.27123	1344.82401	-2302.86955	1
2145	C	70.26100	54.47080	77.66490	628.80261	-236.01511	616.72940	1
2146	H	70.11000	55.20080	78.48890	-1946.14455	1913.91686	1564.50308	1
2147	H	70.18700	53.40880	77.98390	-1769.25170	-2205.48983	1379.77870	1
2148	C	71.68300	54.73580	77.10590	323.18171	728.31266	443.35680	1
2149	H	72.30700	54.92680	78.00490	1725.79829	1879.44631	1840.52385	1
2150	H	71.52300	55.67780	76.53890	1230.80889	-706.21838	2807.95144	1
2151	N	72.29500	53.58780	76.26790	-646.18371	-481.90583	250.77015	1
2152	H	72.33300	53.71780	75.27790	-2297.33232	1210.76458	-1776.10235	1
2153	C	72.51900	52.36480	76.67390	661.82706	237.93006	580.36647	1
2154	N	72.45100	51.90980	77.92390	523.04594	587.03562	307.38317	1
2155	H	72.43900	52.51280	78.72190	-1787.39077	2469.37472	778.23451	1
2156	H	72.53400	50.92280	78.06190	619.34052	36.08832	3084.37047	1
2157	N	72.86300	51.48580	75.77490	-499.76751	365.50436	573.85650	1
2158	H	72.93300	51.87680	74.85690	428.56464	-2759.31526	-1449.39224	1
2159	H	73.24600	50.61580	76.08390	2888.30830	25.41442	-1247.09883	1
2160	C	67.78400	53.02580	75.23090	419.40290	-701.88434	403.62183	1
2161	O	67.57600	51.90080	75.66890	739.58384	-7.74335	-276.73636	1
2162	N	66.94800	53.66880	74.42790	272.18759	-526.80115	-600.88830	1
2163	H	67.26800	54.51680	74.01190	-114.68577	570.29813	3091.89803	1
2164	C	65.70600	53.17180	73.94890	802.44318	-342.17193	-265.43233	1

2165	H	65.24000	52.91680	74.88890	-773.61628	2935.24407	827.09510	1
2166	C	65.01600	54.39180	73.21590	-514.19369	-573.38898	-488.14028	1
2167	H	65.75700	55.08780	72.76690	586.04189	-1171.70827	-2860.39872	1
2168	H	64.48300	54.96280	74.00590	-1918.41273	-1950.05892	-1554.08784	1
2169	C	63.96000	54.00580	72.20890	589.46538	-651.03714	-245.21870	1
2170	C	62.81500	53.27380	72.56890	82.15858	-902.01760	105.19132	1
2171	H	62.64500	52.99980	73.59990	-1367.78945	-1996.15587	2010.65660	1
2172	C	61.86200	53.00680	71.55590	-399.62295	295.36783	764.53276	1
2173	H	60.98800	52.51080	71.95090	-292.73603	-3089.36869	-518.00862	1
2174	C	62.07000	53.38380	70.23690	-273.52043	79.29525	866.22736	1
2175	O	61.17200	53.02380	69.23190	495.62397	-74.81991	-610.23446	1
2176	H	61.57000	53.06280	68.35890	851.61547	-2247.43352	2030.27581	1
2177	C	64.22300	54.25280	70.86090	650.27815	-305.94784	-561.23547	1
2178	H	65.19200	54.70680	70.71490	1349.63683	2773.39621	-620.46766	1
2179	C	63.28000	53.95980	69.85490	-277.81554	535.08939	684.06789	1
2180	H	63.50300	54.29180	68.85190	1275.25847	-1228.78225	-2600.39156	1
2181	C	65.83400	51.91380	73.11590	574.02176	142.30897	-694.04480	1
2182	O	65.14200	50.94680	73.39390	552.31917	520.35186	-218.64288	1
2183	N	66.72600	51.85580	72.13990	422.02364	574.53356	-452.19411	1
2184	H	67.18100	52.70080	71.86790	1203.14880	-1030.59614	2718.18520	1
2185	C	67.06100	50.73780	71.34590	790.22595	424.03887	-164.87872	1
2186	H	66.18800	50.37980	70.82090	-2262.06129	-451.42444	-2139.51418	1
2187	C	68.18900	50.95680	70.27890	613.00707	645.78500	196.55807	1
2188	H	68.49600	49.97580	69.85790	1447.96023	1574.31117	2307.20215	1
2189	H	69.07300	51.42780	70.75990	-522.29934	3100.87838	99.91442	1
2190	C	67.74500	51.90280	69.18490	-391.16536	-815.71745	114.21783	1
2191	H	67.22000	52.78380	69.61290	-1776.43918	1361.34034	2211.16316	1
2192	C	68.90400	52.46280	68.26490	510.25515	640.32723	-401.33741	1
2193	H	69.21300	51.65180	67.57190	-814.81842	2419.76861	1838.21028	1
2194	H	69.81900	52.69180	68.85290	2307.23219	-1576.31507	-1445.73049	1
2195	H	68.67000	53.44480	67.79890	-512.84722	2259.63912	2128.20229	1
2196	C	66.79800	51.18780	68.16290	113.62520	245.58611	-870.76276	1
2197	H	67.28100	50.33580	67.63890	-1961.02823	-2100.52277	-1280.78047	1
2198	H	66.50300	51.92080	67.38290	-1866.41494	477.41028	-2487.32807	1
2199	H	65.90400	50.68680	68.59190	-1249.88407	1244.38661	-2605.28655	1
2200	C	67.57100	49.59980	72.22890	-510.18512	-755.64773	12.59556	1
2201	O	67.16500	48.45580	72.05690	170.02894	-395.46220	-662.06271	1
2202	N	68.39700	49.92080	73.24090	644.36919	409.26202	-360.50692	1
2203	H	68.72700	50.85680	73.34190	1479.30347	-47.64056	2776.25969	1
2204	C	69.08400	48.91580	74.02090	-270.91730	-767.29334	411.47996	1
2205	H	69.46000	48.13080	73.38090	1797.65204	435.01954	2545.07983	1
2206	C	70.26000	49.50580	74.88190	468.22097	-770.57178	135.79122	1
2207	H	69.96200	50.21280	75.68490	2054.26700	1367.04935	1951.76572	1
2208	H	70.89000	50.10780	74.19090	-2146.73375	1282.63419	-1909.08616	1
2209	H	70.83600	48.64580	75.28590	1459.47504	2739.95025	-510.71662	1
2210	C	68.12500	48.26380	75.04290	756.15586	506.05180	-59.92406	1
2211	O	68.45400	47.23480	75.64590	296.21782	-703.34129	202.96123	1
2212	N	66.89700	48.82080	75.37790	97.57007	399.55034	737.23259	1
2213	H	66.81100	49.74780	75.01990	-1511.28522	28.39929	-2759.24568	1
2214	C	65.93700	48.35880	76.39690	-624.55313	501.03365	-436.29082	1
2215	H	66.38800	47.45080	76.76890	-1511.13383	-1840.62939	2055.91445	1
2216	C	65.75500	49.42180	77.42890	-341.69308	-696.41013	479.28047	1
2217	H	65.76800	50.45180	77.01090	-1462.77981	1153.28881	2535.43416	1
2218	C	64.37800	49.29580	78.19190	-248.81438	762.72529	-433.35037	1
2219	H	64.35700	50.15180	78.89890	1472.39796	2763.45699	305.90179	1
2220	H	63.54600	49.42280	77.46690	1387.58266	-2563.18625	-1184.44790	1
2221	H	64.34900	48.32980	78.73890	2105.62272	-2040.34506	1140.86423	1
2222	C	66.94300	49.36980	78.37390	601.89979	-537.61864	424.42177	1
2223	H	67.87300	49.13980	77.81290	1558.10070	2341.21922	-1410.40454	1
2224	H	66.93800	48.50780	79.07490	1414.57683	694.44056	-2723.04075	1
2225	C	67.20200	50.71380	79.14890	-595.51929	367.18638	584.79222	1
2226	H	68.24400	50.65780	79.52990	-1747.67030	852.83322	-2473.16604	1

2227	H	66.39500	50.70680	79.91290	1661.18725	-1989.41852	1783.50697	1
2228	H	67.23000	51.56080	78.43090	2692.93388	-1447.99748	741.37483	1
2229	C	64.68400	47.94480	75.66090	12.54828	-908.34415	78.76834	1
2230	O	64.12400	46.89680	75.93190	-369.21429	-539.63082	-442.83926	1
2231	N	64.12500	48.67480	74.69190	88.43404	127.31748	829.84454	1
2232	H	64.58500	49.51780	74.42290	1222.07498	2313.77896	-1746.76440	1
2233	C	62.87300	48.23880	73.93890	700.69683	574.78948	-100.45899	1
2234	H	62.32800	47.76380	74.74190	1626.40524	-736.02938	2590.61633	1
2235	C	62.19700	49.49980	73.38790	-825.74470	64.46257	381.36763	1
2236	H	62.95800	50.04680	72.79190	30.59940	2226.53833	2222.56990	1
2237	C	61.03600	49.08980	72.50190	-498.83728	-243.21960	-723.50301	1
2238	H	61.35600	48.76480	71.48890	-2526.11441	1854.13627	-281.33770	1
2239	H	60.40500	48.31080	72.98290	-2242.58347	-1795.54235	1282.60410	1
2240	H	60.31000	49.90180	72.28490	2313.48785	-1447.36120	-1565.61354	1
2241	C	61.82500	50.37880	74.60090	-591.38656	-661.95142	208.64624	1
2242	H	61.06500	51.09380	74.21890	1955.52936	-432.03524	2426.41231	1
2243	H	62.72800	50.86480	75.02890	1190.10654	-2493.82458	1504.23124	1
2244	H	61.21500	49.71080	75.24590	-2259.28048	2110.24103	-583.74717	1
2245	C	63.20100	47.23580	72.87290	417.80222	307.40444	749.92988	1
2246	O	62.38700	46.38080	72.49590	-492.71843	595.46477	-162.10330	1
2247	N	64.47400	47.13380	72.43890	-193.69306	672.65699	-471.89815	1
2248	H	65.23300	47.65180	72.82590	470.99995	-1159.54275	-2886.49370	1
2249	C	64.77200	46.31680	71.22390	-609.91446	214.90419	-642.86199	1
2250	H	64.08400	45.51580	70.99690	-2480.15667	1231.58407	-1493.40210	1
2251	C	64.96500	47.11680	69.95990	-646.88090	640.06767	57.52811	1
2252	H	65.19000	46.42980	69.11690	790.08686	-2387.03599	-1891.04420	1
2253	H	65.80000	47.84180	70.06290	-1996.62865	-1793.95742	-1641.16332	1
2254	N	62.80000	47.30780	68.67190	248.17708	-160.52799	-790.76620	1
2255	H	62.85700	46.39880	68.25890	-1772.11809	2275.94912	1256.13665	1
2256	C	63.74700	47.92880	69.43990	-677.71136	604.87165	79.30073	1
2257	C	61.90700	48.23880	68.29190	398.74466	-522.32628	632.16213	1
2258	H	61.02100	47.93880	67.73390	-685.14795	487.19339	-3031.73896	1
2259	N	62.23400	49.43580	68.75890	414.44244	-668.32608	-307.00163	1
2260	C	63.35500	49.21480	69.53490	-529.59590	698.22968	-251.90175	1
2261	H	63.91700	50.02480	69.98390	-1320.23936	1001.53031	2674.34689	1
2262	C	66.09300	45.60480	71.41390	748.32666	-202.42896	-480.08408	1
2263	O	67.00800	45.60980	70.60490	549.98168	-566.01703	27.78668	1
2264	N	66.26200	44.96680	72.58690	-401.93304	-341.53202	659.14945	1
2265	H	65.54000	44.88280	73.26990	-1650.61831	1008.01634	2481.44887	1
2266	C	67.55100	44.53680	72.97490	-444.39073	536.63254	-588.21204	1
2267	H	68.36100	45.24380	72.87890	2748.24951	-1450.17862	492.27311	1
2268	C	67.54100	44.11380	74.52790	684.43262	130.49388	-588.19583	1
2269	H	67.20500	45.01580	75.08290	1852.05488	-1067.55999	-2308.34023	1
2270	H	66.79700	43.31280	74.72290	2410.20495	595.60692	-1932.45718	1
2271	H	68.52800	43.74880	74.88590	-1383.08883	-911.40774	-2674.81353	1
2272	C	68.08100	43.25480	72.25790	-398.17893	100.57878	814.11821	1
2273	O	69.24900	42.90780	72.37290	636.46954	-463.33057	-62.11712	1
2274	N	67.23100	42.50780	71.53190	4.30664	598.47252	595.38591	1
2275	H	66.32800	42.91980	71.44090	2912.59593	-475.07240	1090.55829	1
2276	C	67.54800	41.26580	70.93090	-335.31234	258.58779	807.55742	1
2277	H	68.32300	40.86780	71.56890	-2010.33196	1752.49858	-1668.99382	1
2278	C	66.43900	40.21380	70.95290	658.31779	513.60753	-366.43690	1
2279	H	66.01200	40.24680	71.97790	-1852.94001	1355.80876	-2150.95843	1
2280	O	66.96200	38.92080	70.87490	550.85539	82.34729	559.82541	1
2281	H	67.72100	38.72880	71.43090	-1576.56453	-1211.14979	2438.39839	1
2282	C	65.34400	40.37980	69.88590	749.87638	-35.58720	-517.56156	1
2283	H	64.40400	39.92280	70.26290	1715.98814	2070.02727	-1633.58441	1
2284	H	65.72800	39.97280	68.92590	-218.60340	-3067.59484	663.55156	1
2285	H	65.10900	41.45680	69.74290	1934.06509	1985.81936	-1487.99863	1
2286	C	68.04700	41.39180	69.50990	-678.69371	-598.30908	113.36708	1
2287	O	68.49600	40.41480	68.88190	293.00025	-344.02636	-647.62948	1
2288	N	67.97800	42.58880	68.90590	-98.72521	-227.23125	807.02638	1

2289	H	67.40400	43.31080	69.28390	1231.01158	1517.88517	2465.53469	1
2290	C	68.25700	42.84080	67.50690	-681.96376	472.33319	378.52053	1
2291	H	69.24300	42.47480	67.26390	1563.84161	-1931.99102	-1928.73957	1
2292	C	67.21300	42.10680	66.52190	757.31941	496.00431	109.07811	1
2293	H	67.50300	42.52180	65.53290	-2122.92264	366.82424	2292.78557	1
2294	H	67.39400	41.01280	66.44490	1704.69488	-133.87949	-2640.89339	1
2295	C	65.73100	42.38580	66.82990	-606.63431	-671.11848	-114.21820	1
2296	O	65.28300	43.17080	67.69590	700.57820	200.82518	304.11620	1
2297	N	64.85100	41.84280	65.95390	-470.70949	144.07806	685.81803	1
2298	H	65.23300	41.18080	65.30890	1897.93127	-1554.74088	-1969.48317	1
2299	H	63.87600	42.02380	66.07990	-976.37974	-1779.46187	-2403.83533	1
2300	C	68.28700	44.37280	67.28890	603.54252	251.75734	635.45705	1
2301	O	67.32600	45.05080	66.84790	-283.11668	71.34098	-733.74562	1
2302	N	69.42800	45.01480	67.51390	-509.83989	439.26624	509.68691	1
2303	H	70.29900	44.54280	67.62790	3073.41697	96.42858	665.60942	1
2304	C	69.59800	46.39680	67.30590	-250.56010	-750.92999	-452.52049	1
2305	H	69.34300	46.64780	66.28690	2380.22491	527.76585	1988.52176	1
2306	C	68.81800	47.28080	68.35890	-751.25610	368.83109	-361.97915	1
2307	H	67.74200	47.08880	68.15690	-1135.32986	1162.85284	2693.88671	1
2308	H	68.95200	48.36380	68.15390	2621.79742	1598.95014	683.93200	1
2309	O	69.09100	46.87480	69.72790	82.97477	577.35857	-532.35279	1
2310	H	68.34100	46.30280	69.90690	-994.29190	-1709.16046	2447.11674	1
2311	C	71.05900	46.81080	67.33990	-598.58095	-246.29948	-642.25262	1
2312	O	71.31200	47.99080	67.04890	-119.88413	-416.63787	660.05144	1
2313	N	72.08300	46.00080	67.59690	-235.47629	186.73699	-788.89321	1
2314	H	71.88000	45.04780	67.80590	-1941.52766	367.00668	2448.26523	1
2315	C	73.48600	46.44780	67.59790	-117.31300	808.07841	405.82995	1
2316	H	73.52400	47.26880	68.29890	-94.15309	555.56409	-3095.27219	1
2317	C	74.37500	45.29980	68.15590	349.24143	-694.52830	476.56255	1
2318	H	74.02300	44.33880	67.72490	2187.56157	1734.49200	-1450.63369	1
2319	H	74.17000	45.24680	69.24690	-462.21592	-675.52413	3037.80345	1
2320	C	75.92100	45.26480	67.94090	-688.34064	-188.53166	-567.53325	1
2321	H	76.30900	44.56380	68.70990	900.64859	2483.23659	1708.97465	1
2322	H	76.31100	46.28280	68.15790	2722.79775	917.21387	1281.91941	1
2323	C	76.47700	44.90180	66.52690	-694.39980	62.00798	587.72011	1
2324	O	77.48800	45.40880	66.06490	-583.38469	-402.96791	-347.71597	1
2325	N	75.84000	43.91380	65.89590	677.82138	-414.44226	-285.42615	1
2326	H	75.05300	43.46880	66.32490	1601.33989	2239.89573	1522.10510	1
2327	H	76.20200	43.57880	65.02690	1908.02434	-180.88731	-2494.98479	1
2328	C	74.06300	47.03080	66.32090	522.08630	-575.61216	-477.01944	1
2329	O	74.69700	48.06380	66.27790	244.51640	-347.06706	665.87042	1
2330	N	73.75600	46.55480	65.10790	-757.58830	144.48831	-343.30071	1
2331	H	73.25200	45.70380	64.98290	-484.25524	488.11033	3070.09306	1
2332	C	74.08400	47.23980	63.86290	-161.53046	-750.43013	492.15193	1
2333	H	75.12800	47.51180	63.92690	-1065.13115	-2932.33163	406.39032	1
2334	C	74.06800	46.20880	62.72890	-731.28525	-469.71222	275.75953	1
2335	H	73.13500	45.60880	62.79690	-2009.06986	-1599.06496	1817.92623	1
2336	H	74.85700	45.42680	62.72790	-416.58161	-528.78603	3073.28347	1
2337	C	74.06200	46.76480	61.27790	-776.95958	-436.42055	193.18882	1
2338	H	73.11700	47.30680	61.06290	1417.32230	2737.90974	-627.11560	1
2339	H	74.90400	47.46680	61.10090	-1647.08289	868.00982	-2536.11970	1
2340	C	74.25100	45.71380	60.15490	787.69201	-432.25438	-155.39769	1
2341	H	75.13100	45.04580	60.27290	-2340.97760	1034.54472	1829.69051	1
2342	H	73.41700	44.99080	60.02890	-276.37492	2903.44781	1179.76013	1
2343	N	74.37500	46.45680	58.85890	-541.96141	-484.39141	429.31933	1
2344	H	73.83000	47.27780	58.68890	439.68406	2676.96414	1593.35092	1
2345	C	74.66200	45.80580	57.73890	412.49453	602.72693	-545.91163	1
2346	N	75.21300	44.60980	57.67290	343.28745	-484.01684	600.46125	1
2347	H	75.14000	43.94180	58.41390	1066.64886	1702.06179	-2421.46073	1
2348	H	75.29600	44.15880	56.78390	-2741.62249	591.53017	-1425.42078	1
2349	N	74.43800	46.41980	56.59390	-652.77470	441.51959	-302.68453	1
2350	H	74.35200	47.41580	56.55990	-366.14760	-834.01819	-3011.40761	1

2351	H	74.81700	46.00380	55.76690	-2089.51111	-2352.02812	-11.54432	1
2352	C	73.45900	48.66280	63.65890	367.37472	-648.97084	524.71294	1
2353	O	74.22500	49.62080	63.25590	591.72685	-305.57477	-424.39443	1
2354	N	72.19600	48.93680	63.88290	-569.87937	557.90511	-276.86041	1
2355	C	71.15200	47.91380	63.64390	554.89815	314.54020	651.61607	1
2356	H	71.01200	47.26380	64.53490	-408.21656	-2507.78575	1855.42343	1
2357	H	71.30300	47.24080	62.77290	2314.20547	-2085.90791	437.79846	1
2358	C	71.58800	50.28980	63.86990	223.43296	-572.17464	673.90274	1
2359	H	71.84300	50.86080	62.98890	2443.94981	-1878.97436	628.32388	1
2360	C	70.07700	50.06480	63.96190	-439.81422	-571.98101	557.54119	1
2361	H	69.46100	50.84980	63.47390	-2705.05160	792.16700	1397.63854	1
2362	H	69.73700	49.93580	65.01190	-1616.19085	-411.24491	-2667.77641	1
2363	C	69.87000	48.68880	63.34890	-607.08387	-680.02370	21.63219	1
2364	H	69.82900	48.81780	62.24590	2001.62042	2191.28034	-1044.04615	1
2365	H	68.94600	48.19980	63.72390	-1180.94778	-2507.16573	1489.19729	1
2366	C	72.06400	51.10980	65.08690	418.51034	-615.39546	-526.86671	1
2367	O	72.36800	52.25980	64.91690	-310.85032	-687.91968	231.87457	1
2368	N	72.14200	50.58980	66.34490	-289.32400	-596.50411	522.63444	1
2369	H	71.85400	49.64680	66.48990	1363.66697	2593.04601	-1146.62592	1
2370	C	72.81900	51.31980	67.35990	357.30677	628.45541	555.72176	1
2371	H	72.31400	52.25080	67.56990	2502.65950	1397.91440	1296.44011	1
2372	C	72.89600	50.49980	68.67390	-257.51074	-482.49481	-729.61495	1
2373	H	73.60400	51.00680	69.36290	-2483.46327	1672.50487	966.10759	1
2374	H	73.30500	49.50780	68.38590	-1677.63239	2346.91290	1255.29902	1
2375	C	71.62900	50.31280	69.43890	-163.66395	-590.59331	-675.17750	1
2376	H	70.76200	49.92680	68.86190	-554.84535	2989.57813	-807.95758	1
2377	H	71.29200	51.26680	69.89990	481.09859	-1476.23941	-2736.32739	1
2378	C	71.72500	49.24180	70.58390	446.76018	-774.28284	-179.84001	1
2379	H	70.75000	48.93880	71.02290	1486.63614	-1571.06313	2284.71002	1
2380	H	72.23500	48.32680	70.21490	-1807.91618	1953.25876	1677.63092	1
2381	N	72.53600	49.96180	71.58390	-293.05361	786.60279	-89.71019	1
2382	H	72.73100	50.93480	71.46790	-1194.06061	2648.21785	-1208.05119	1
2383	C	73.24800	49.36280	72.44790	810.67973	-416.96001	19.84276	1
2384	N	73.02000	48.12780	72.87290	-787.41695	-159.99390	258.93781	1
2385	H	72.19900	47.67380	72.52690	-2513.64235	-426.69839	1843.30052	1
2386	H	73.73800	47.68480	73.40890	1844.99598	1762.05733	1841.02417	1
2387	N	74.05500	50.13280	73.16390	-11.35797	841.95718	60.42671	1
2388	H	74.03900	51.12880	73.07790	-990.59967	-2636.73108	1401.63752	1
2389	H	74.58500	49.72780	73.90890	-1576.76848	1001.33361	2531.67106	1
2390	C	74.26400	51.75680	67.03390	490.81175	-88.58160	-763.35321	1
2391	O	74.70400	52.87880	67.34290	-97.63868	-781.84572	53.02065	1
2392	N	74.99000	50.84080	66.43790	391.45388	-416.25300	-621.42545	1
2393	H	74.53700	50.00780	66.12990	-2434.88356	1263.10961	-1540.81873	1
2394	C	76.32900	51.05180	65.91890	755.75258	424.99039	282.26265	1
2395	H	76.92000	51.30980	66.78590	2383.14925	975.35757	1807.62371	1
2396	C	76.94900	49.70280	65.47390	-127.10057	449.84396	-782.90284	1
2397	H	76.30500	49.24080	64.69590	-1462.01769	-776.97564	2675.26435	1
2398	H	76.96900	49.10280	66.40990	2351.35848	2038.64845	-461.79218	1
2399	C	78.38400	49.85180	64.90690	507.13821	429.47325	624.35131	1
2400	H	78.99800	50.42380	65.63490	1539.25316	2178.00992	-1668.89147	1
2401	H	78.48000	50.46080	63.98190	497.81871	1585.92457	-2671.18813	1
2402	C	79.08600	48.50880	64.76090	-465.49210	-579.50324	-528.15158	1
2403	H	80.13800	48.65880	64.43590	-1798.56283	2098.41842	-1503.34231	1
2404	H	79.13800	48.00180	65.74790	-1712.44281	2016.17196	1703.17835	1
2405	C	78.42400	47.54480	63.73590	-276.83746	-461.54264	736.06414	1
2406	H	77.43900	47.19580	64.11290	2062.78229	-900.72626	2198.14641	1
2407	H	78.43800	48.07180	62.75690	-581.77017	-1296.54614	2806.90894	1
2408	N	79.19100	46.31480	63.58490	668.80042	-48.88060	512.82451	1
2409	H	79.15700	45.54480	64.28290	-1455.35871	2733.96206	-552.81890	1
2410	H	78.84600	45.88880	62.70090	2802.27857	696.03767	-1249.39690	1
2411	H	80.20700	46.41180	63.38790	-1395.14776	167.54165	-2814.91008	1
2412	C	76.45600	52.09780	64.76190	-340.64362	379.01610	-756.14795	1

2413	O	77.33400	53.00380	64.73790	480.83886	274.14261	-563.26464	1
2414	N	75.49900	52.07180	63.80890	474.66355	163.46394	-678.70932	1
2415	H	74.82500	51.33980	63.87890	-1343.72188	-1828.90196	-2178.93446	1
2416	C	75.37200	53.05880	62.72290	505.86493	-644.58825	-400.07208	1
2417	H	76.24900	53.07880	62.09390	1996.30797	-1795.19527	1640.19958	1
2418	C	74.08200	52.69580	61.93290	467.02505	-635.74028	-457.35423	1
2419	H	73.19500	52.54980	62.58490	2992.05203	-698.08008	677.15216	1
2420	H	74.18000	51.73280	61.38690	-2643.66720	-1378.09349	1005.04144	1
2421	C	73.59900	53.60380	60.75090	746.41321	-148.09729	502.37985	1
2422	H	73.51200	54.61580	61.20090	-2259.59392	2000.75123	888.51342	1
2423	C	74.75200	53.70080	59.70190	392.86651	818.16838	-87.79179	1
2424	H	75.73100	53.99880	60.13390	973.97142	-2231.00409	-1993.04456	1
2425	H	74.40100	54.35980	58.87990	-2807.57231	-610.77700	-1281.68460	1
2426	H	74.77600	52.72380	59.17190	461.01885	-2966.66190	940.53442	1
2427	C	72.26900	52.99980	60.24790	145.82257	-611.60754	-660.39609	1
2428	H	72.31900	51.91280	60.01990	-2677.86183	717.21180	-1487.57839	1
2429	H	71.53100	53.17380	61.05890	2811.05797	716.38731	-1217.77196	1
2430	H	71.90400	53.53280	59.34390	-582.05890	1814.68262	-2503.26999	1
2431	C	75.26700	54.48680	63.29190	864.36087	-210.32899	-200.23236	1
2432	O	75.99400	55.39780	62.81990	-722.97101	-65.10869	-310.96785	1
2433	N	74.42500	54.77980	64.32690	56.26413	662.10682	-520.69299	1
2434	H	73.71000	54.13580	64.58490	1481.70092	2723.79880	-532.64312	1
2435	C	74.40000	55.99780	65.09690	135.32019	888.85078	151.93334	1
2436	H	74.15100	56.75380	64.36690	1816.38195	-1659.32307	1961.02774	1
2437	C	73.31000	55.86980	66.17990	147.39433	803.00974	-406.08038	1
2438	H	73.30000	56.73880	66.87090	-1879.52770	558.27214	2460.47436	1
2439	H	73.61800	54.94780	66.71790	-124.36038	1122.47502	2936.46225	1
2440	C	71.87600	55.65080	65.62390	-292.57289	-459.05976	-731.51640	1
2441	H	71.83700	54.60480	65.25090	853.61981	-51.96252	-3027.68217	1
2442	C	70.97400	55.48080	66.86590	-262.24589	276.38742	-828.42506	1
2443	H	71.23100	54.55980	67.43290	-35.86831	1339.43061	-2846.55324	1
2444	H	71.08600	56.36480	67.52890	690.15356	-2302.03786	2030.40291	1
2445	H	69.94100	55.32880	66.48690	789.05455	-2499.06386	1740.77540	1
2446	C	71.25800	56.61480	64.56090	507.07240	560.70252	-509.84435	1
2447	H	70.17700	56.37880	64.46190	-1746.50458	-1860.64461	1840.09500	1
2448	H	71.83700	56.72880	63.61990	1435.80627	2799.35657	17.01108	1
2449	H	71.32500	57.64680	64.96790	-602.34540	-2187.68669	-2179.31943	1
2450	C	75.73500	56.27280	65.77590	449.23342	690.57438	-390.82908	1
2451	O	76.34600	57.33580	65.63190	98.01944	-737.45968	-264.90119	1
2452	N	76.31200	55.24680	66.49890	474.00165	695.72037	62.99122	1
2453	H	75.88100	54.35180	66.58390	-2128.34693	2169.62168	813.08508	1
2454	C	77.48200	55.40080	67.33590	-188.92237	684.46151	-572.07673	1
2455	H	77.32600	56.29280	67.92390	-2248.40509	1524.77759	-1586.80624	1
2456	C	77.62100	54.17580	68.29490	656.69761	-251.44449	580.49541	1
2457	H	78.49700	54.34580	68.95590	-1355.25345	2557.13823	1233.91994	1
2458	H	76.75900	54.12480	68.99390	-186.38175	-699.89618	-3061.63901	1
2459	H	77.70900	53.20180	67.76690	763.93062	-1527.50127	2642.22938	1
2460	C	78.78300	55.65680	66.64290	-504.56942	517.63806	555.79811	1
2461	O	79.62000	56.37780	67.15490	-520.37260	-556.13294	208.70012	1
2462	N	78.96700	55.15180	65.41590	-170.22067	783.12437	-265.35529	1
2463	H	78.26300	54.58880	64.98890	-2830.38522	295.52187	-1341.57092	1
2464	C	80.24300	55.01480	64.81890	-742.71501	-319.79120	-421.37752	1
2465	H	80.93500	55.54480	65.45490	-1284.08264	1406.65318	2504.13355	1
2466	C	80.74100	53.60680	64.68090	369.62887	-790.28411	-265.09721	1
2467	H	81.54200	53.50280	63.91790	1367.07050	2829.87709	-145.39652	1
2468	H	79.93900	52.99380	64.21490	-1230.72456	-447.92394	-2860.57817	1
2469	C	81.19200	53.07180	66.00590	-439.81834	431.09233	672.43604	1
2470	H	80.21400	52.97080	66.52290	822.31980	-2077.29909	2215.13992	1
2471	H	81.98500	53.67880	66.49090	2425.71536	1965.56947	-388.15957	1
2472	C	81.80000	51.67080	65.81990	-194.87544	641.85926	-617.64978	1
2473	O	82.54700	51.38680	64.86090	490.51294	511.21769	348.82770	1
2474	O	81.46400	50.77080	66.62690	586.86452	97.56209	519.32543	1

2475	C	80.24800	55.64180	63.46990	-393.60719	-299.78151	765.93435	1
2476	O	81.28400	56.18180	63.05390	185.46925	-763.79646	-76.44188	1
2477	N	79.10300	55.73680	62.73990	1.18328	620.27752	-572.64884	1
2478	H	78.21300	55.39680	63.03490	-2991.28572	-323.39887	919.70058	1
2479	C	79.08500	56.37380	61.44790	456.82388	-551.93061	564.03506	1
2480	H	80.07800	56.57180	61.07090	2080.94848	-158.14349	2354.33011	1
2481	C	78.41800	55.43180	60.43790	595.38611	-262.83251	-638.65911	1
2482	H	77.80000	55.86380	59.62190	-1201.22448	1916.78934	-2186.59658	1
2483	H	77.61800	54.90880	61.00490	-2339.72894	2080.30056	-310.23263	1
2484	C	79.39200	54.30580	59.96390	523.91545	550.26969	-504.14965	1
2485	H	80.20100	54.78780	59.37390	1632.38826	612.06032	2618.95341	1
2486	H	79.81400	53.79280	60.85490	3082.36072	-630.18896	-11.85261	1
2487	C	78.69400	53.25980	59.05890	535.32051	-553.97053	-487.85204	1
2488	H	78.18300	53.69880	58.17490	-2896.45892	-1228.09288	-23.23467	1
2489	H	77.89200	52.86580	59.71890	574.79550	-3068.48749	-390.15494	1
2490	C	79.52300	52.08780	58.64990	119.91645	-217.39813	-877.38766	1
2491	H	78.88900	51.18480	58.52290	1550.97321	-136.94496	2733.85340	1
2492	H	80.17100	51.87080	59.52690	-1835.80481	76.09568	-2553.87086	1
2493	N	80.41500	52.29680	57.45590	-340.75312	-238.62309	734.58738	1
2494	H	81.01600	53.14280	57.39090	2077.51361	1710.64734	1629.67761	1
2495	H	80.99800	51.45480	57.27390	2036.95678	-1679.36001	-1711.36882	1
2496	H	79.79000	52.30380	56.62490	-136.84474	-2232.74320	2212.31949	1
2497	C	78.36900	57.66680	61.44790	-436.04995	495.04796	-629.47515	1
2498	O	78.89200	58.71780	61.08490	-87.52700	-612.14327	491.16888	1
2499	N	77.09500	57.58980	61.86190	607.50853	527.28763	-256.07310	1
2500	H	76.77100	56.72180	62.22990	1458.51518	-1997.19696	-1944.77865	1
2501	C	76.09900	58.66480	61.66090	133.28248	-784.46330	445.31350	1
2502	H	76.35500	59.15680	60.73390	-2975.33665	-993.06191	243.77466	1
2503	C	74.63500	58.10880	61.42090	-235.67123	686.81576	-551.53802	1
2504	H	74.40700	57.32080	62.17090	-2592.77985	286.31803	-1758.90331	1
2505	C	73.63900	59.25180	61.53490	412.54753	67.66444	810.35613	1
2506	H	73.66300	59.64980	62.57190	1124.66712	1030.89139	-2751.47470	1
2507	H	72.61900	58.85480	61.34290	-2442.61912	-1685.69764	1044.15588	1
2508	H	73.85800	60.07080	60.81690	1055.85425	-1531.17459	2537.49924	1
2509	C	74.54200	57.54180	59.97590	-322.67470	385.89947	760.53510	1
2510	H	75.40900	56.88280	59.75790	1220.58053	-2103.52528	1995.89348	1
2511	H	73.71200	56.81880	59.81990	2015.11253	1366.60431	1992.47093	1
2512	H	74.61300	58.32480	59.19190	301.43086	-2515.68369	1865.12768	1
2513	C	76.21100	59.84480	62.65990	-12.43828	6.78298	-911.72928	1
2514	O	75.93300	60.98580	62.30390	576.43795	213.03201	-495.94745	1
2515	N	76.85000	59.71980	63.88290	-395.10264	459.78809	-587.50414	1
2516	H	76.85700	58.81880	64.30890	-1745.59768	-2615.25319	-107.54412	1
2517	C	77.20900	60.88380	64.76190	682.57926	-366.07454	481.17147	1
2518	H	76.28000	61.42980	64.83790	-1968.94770	1636.93714	1828.08861	1
2519	C	77.73400	60.39280	66.08790	-528.03511	-107.94521	-735.51190	1
2520	H	77.00500	59.71580	66.58190	2074.08785	1543.57762	1792.69461	1
2521	C	79.03700	59.53180	65.95890	-159.07311	-559.93267	-701.87047	1
2522	H	79.91700	60.21080	65.96790	3081.88190	-14.18254	632.47849	1
2523	H	79.30200	58.94780	65.05190	-1119.62649	-2552.41944	-1459.38951	1
2524	H	79.18400	58.75480	66.73890	-2398.91850	585.98352	-1949.36902	1
2525	C	77.96200	61.63780	66.98490	237.71013	-728.35172	494.41751	1
2526	H	78.82900	62.29580	66.75890	2530.62891	1755.47006	-642.23704	1
2527	H	78.00300	61.31880	68.04790	-1566.25258	1835.16075	2019.22364	1
2528	H	77.05900	62.28480	66.98290	-1195.10023	2422.04621	-1613.58416	1
2529	C	78.17500	61.78680	63.99590	591.43949	297.00416	-627.24705	1
2530	O	78.09900	62.98780	64.12390	-680.00288	401.52001	-2.23548	1
2531	N	79.04000	61.27880	63.15690	461.53381	222.71467	-670.86288	1
2532	H	79.21600	60.30180	63.07090	-351.47570	1952.59601	2441.73297	1
2533	C	79.83300	62.16880	62.23990	-743.29342	-451.56983	273.95362	1
2534	H	80.38500	62.91080	62.79690	-567.46054	2257.40796	2116.67760	1
2535	C	80.87800	61.35180	61.53590	247.62975	876.88086	-34.79164	1
2536	H	81.46900	62.00780	60.86190	1668.15668	-2662.34459	165.53182	1

2537	H	80.48200	60.49880	60.94490	3032.26998	320.36756	775.19650	1
2538	C	81.78800	60.76180	62.55890	-542.31176	452.41814	-576.77273	1
2539	C	81.47900	59.48980	63.13990	610.43304	80.23188	-672.59598	1
2540	H	80.54500	58.99280	62.92390	2094.09441	-2307.64190	-433.34013	1
2541	C	82.33100	58.99680	64.14690	-627.84855	-285.72860	596.33579	1
2542	H	82.11600	58.00880	64.52490	1288.86116	-2499.37535	-1410.73952	1
2543	C	83.50600	59.67180	64.52090	597.32487	558.50971	-403.38680	1
2544	O	84.34300	59.10380	65.48790	784.82525	-16.16578	-86.11168	1
2545	H	85.16400	59.59980	65.50190	1989.31837	2340.00078	-682.08136	1
2546	C	82.96400	61.42180	62.94590	-743.72146	-227.65914	-475.92091	1
2547	H	83.22800	62.37680	62.51590	-1601.44261	-1953.72382	-1875.25225	1
2548	C	83.79600	60.81880	63.85490	-646.60004	642.81176	-12.34635	1
2549	H	84.68400	61.36680	64.13590	-1077.47896	1761.32941	2373.81213	1
2550	C	79.07200	63.01480	61.18490	755.97992	-504.10201	76.33172	1
2551	O	79.35300	64.19780	61.05590	305.27495	532.93805	496.39850	1
2552	N	78.11400	62.42880	60.51990	-330.48286	752.95759	-191.07130	1
2553	H	77.89300	61.46280	60.63090	-1800.74236	-2418.28065	-898.59439	1
2554	C	77.45200	63.00280	59.37490	-171.02718	887.28241	122.19095	1
2555	H	77.88600	63.93180	59.03590	1745.28610	-293.13041	-2601.20688	1
2556	C	77.51400	62.02580	58.15990	496.29923	423.73091	-636.85963	1
2557	H	78.58700	61.74980	58.07590	-1987.58359	1594.16214	1845.63940	1
2558	C	76.64800	60.74380	58.20490	-838.08345	59.05954	354.37142	1
2559	H	76.89000	60.04880	57.37290	1950.03968	-933.72632	-2285.54733	1
2560	H	75.57900	61.03780	58.26890	-1395.33314	2687.81368	852.60148	1
2561	H	76.88300	60.24480	59.16990	-855.71685	683.96007	2949.26661	1
2562	C	77.07000	62.83080	56.90790	-570.77126	-609.60883	366.12599	1
2563	H	77.53500	63.83980	56.88090	476.65632	-683.53386	3033.77759	1
2564	H	77.24600	62.12980	56.06390	-2189.15145	-1811.11047	1351.19245	1
2565	H	75.98500	63.07180	56.90790	-1330.65511	-1417.88160	2473.29638	1
2566	C	75.96700	63.43180	59.71690	-272.22670	-592.10152	-637.77693	1
2567	O	75.23100	63.95280	58.88690	-83.50511	410.59184	-669.37917	1
2568	N	75.55600	63.14580	60.96990	-150.57332	825.49864	92.47680	1
2569	H	76.07500	62.48980	61.51290	504.16011	2415.79102	1951.41040	1
2570	C	74.24300	63.52480	61.53090	-523.91201	361.70244	-652.79288	1
2571	H	73.64800	62.66780	61.80990	-1282.59050	2670.70883	1058.53775	1
2572	H	73.74100	64.17580	60.82990	-2164.17609	-669.96139	-2183.05287	1
2573	C	74.39400	64.47380	62.76890	667.40836	-593.81190	-182.76899	1
2574	O	73.38900	65.08080	63.16490	213.44088	492.89450	578.90002	1
2575	N	75.62000	64.65580	63.34290	407.76159	-528.08353	517.23356	1
2576	H	76.40600	64.05980	63.19790	-1565.45391	-724.90537	2630.98698	1
2577	C	75.80700	65.65780	64.37690	248.54503	560.24445	675.13149	1
2578	H	74.96800	66.32780	64.49790	-134.98160	2855.56669	-1313.67617	1
2579	C	76.01200	64.93380	65.67590	278.61279	-370.56758	785.17870	1
2580	H	76.89500	64.26080	65.65490	2093.60022	-2303.69237	-456.14232	1
2581	C	76.30800	65.94080	66.83790	659.81054	-153.30146	-610.40947	1
2582	H	77.32300	66.35880	66.66890	2604.30123	1417.98064	-1051.27172	1
2583	H	76.23100	65.35680	67.77990	1842.88595	1275.58512	2207.91308	1
2584	H	75.48500	66.68680	66.80890	2557.02413	-1828.61020	-126.64340	1
2585	C	74.73100	64.15080	66.04990	-260.84914	590.19267	-644.26807	1
2586	H	73.85200	64.82480	66.13390	-1559.89301	-2590.09786	-869.68563	1
2587	H	74.86500	63.63880	67.02690	-1583.21081	890.33354	-2568.84720	1
2588	H	74.49800	63.28680	65.39090	-1477.86579	-1563.69327	-2295.43074	1
2589	C	76.98200	66.54980	64.00090	-311.36156	-663.92101	541.95376	1
2590	O	76.81300	67.75280	63.82890	493.09283	-568.06205	240.40009	1
2591	N	78.17500	65.95380	63.88490	669.45657	322.63646	-400.50705	1
2592	H	78.34800	64.98480	64.04090	-1952.26483	-1901.95370	1571.45169	1
2593	C	79.38000	66.79380	63.80390	275.33721	269.64065	-826.39842	1
2594	H	79.33300	67.52180	64.60090	435.59070	-1565.41234	-2694.06221	1
2595	C	80.72500	65.95580	63.88190	783.96094	-408.45164	-223.65934	1
2596	H	81.57500	66.47980	63.39390	952.56650	2545.70453	1584.37108	1
2597	H	80.62700	65.05980	63.23190	-935.60924	-1361.43225	-2677.56677	1
2598	C	81.07600	65.46380	65.23690	756.59391	-502.07413	-83.29604	1

2599	C	81.17800	64.13780	65.68490	-792.75719	-351.50764	-281.83227	1
2600	H	81.15400	63.23580	65.09090	409.44274	1620.97532	-2665.14950	1
2601	N	81.54500	64.11680	67.03990	-628.07833	249.30732	-505.99977	1
2602	H	81.89000	63.41080	67.61890	-799.53679	1852.52640	-2413.94140	1
2603	C	81.67300	65.44380	67.41590	799.83290	-399.14944	-179.99461	1
2604	C	81.36600	66.28480	66.35090	-261.53011	-603.09923	631.92114	1
2605	C	81.43800	67.69780	66.49390	449.92375	-625.12954	-488.09085	1
2606	H	81.35400	68.36680	65.64990	2137.35506	1826.49301	1412.04209	1
2607	C	81.95200	68.19480	67.67890	795.64160	-402.47773	190.83272	1
2608	H	82.20600	69.23880	67.78590	-1100.00132	2894.86718	554.94806	1
2609	C	81.95100	65.96580	68.65390	-476.80441	764.53960	139.95628	1
2610	H	82.12500	65.34080	69.51690	2152.14988	774.02491	2160.40796	1
2611	C	82.16800	67.36880	68.71590	112.25910	-691.74216	-583.38811	1
2612	H	82.68500	67.67280	69.61390	-1251.40173	-1419.70961	2513.29357	1
2613	C	79.54100	67.60780	62.56990	-662.04951	-398.77358	-483.86060	1
2614	O	79.68900	68.83180	62.62190	-72.69763	683.15442	389.41279	1
2615	N	79.43900	66.98780	61.39490	234.11088	-475.89358	-656.80263	1
2616	H	79.52900	65.99580	61.36090	-1658.50736	-143.70214	2669.63092	1
2617	C	79.40100	67.72880	60.09790	664.72391	-587.29714	211.36507	1
2618	H	80.27400	68.36380	60.06790	816.95783	600.97156	-2978.19397	1
2619	C	79.57800	66.71580	58.97690	-89.51908	129.76712	898.10792	1
2620	H	79.06400	65.76680	59.23990	1520.52353	1979.92785	1914.71150	1
2621	C	79.02300	67.18080	57.59490	-566.26586	586.52737	408.38661	1
2622	H	79.08700	66.33780	56.87390	-745.45430	-1568.61513	2623.35104	1
2623	H	77.97200	67.53780	57.64990	2928.32411	1084.36958	-383.77957	1
2624	H	79.57700	68.09680	57.29790	2043.77050	-2084.93708	-1172.29081	1
2625	C	81.08100	66.50980	58.92390	388.43729	695.20120	444.14273	1
2626	H	81.56100	66.51280	59.92590	2721.90919	-1233.68186	983.59831	1
2627	H	81.53800	67.31980	58.31590	1799.36522	2401.52655	945.08269	1
2628	C	81.48100	65.22680	58.17990	554.61258	-314.94345	-651.66442	1
2629	H	82.58100	65.23080	58.01990	-548.99997	-2333.92582	-2037.06051	1
2630	H	81.14600	64.38880	58.82690	-1062.72655	1845.77819	2315.58662	1
2631	H	81.07500	65.34680	57.15190	-2526.76737	-1845.25930	-329.68320	1
2632	C	78.20300	68.68480	59.97390	-169.06395	509.15556	737.31201	1
2633	O	78.39300	69.81780	59.50690	-730.96421	-163.19824	250.36949	1
2634	N	76.94300	68.38580	60.25590	382.34420	-450.46081	602.96788	1
2635	C	76.40600	67.04980	60.23790	101.55111	39.63848	-905.29949	1
2636	H	76.84500	66.50280	61.09990	-35.26389	-2364.76667	-2074.81596	1
2637	H	76.61900	66.55080	59.26890	-2215.49163	1831.81047	-1278.39488	1
2638	C	75.89100	69.36780	60.47890	-503.71622	-382.96712	-656.54944	1
2639	H	75.63800	69.83980	59.54090	2410.32531	1718.91546	-1064.84167	1
2640	C	74.79500	68.58480	61.07990	322.65296	-422.80851	740.66121	1
2641	H	74.84900	68.53780	62.18890	-1040.70574	-1901.65108	-2280.10547	1
2642	H	73.81200	69.09380	60.98690	2242.03676	-2148.05451	-507.30583	1
2643	C	74.91000	67.23780	60.38990	-325.40783	-656.23778	-543.05867	1
2644	H	74.48000	66.36180	60.92190	2405.11862	197.92356	2018.52840	1
2645	H	74.36300	67.34880	59.42990	-56.49788	846.00936	3029.73636	1
2646	C	76.27700	70.60180	61.32290	703.01954	-46.61631	-578.82766	1
2647	O	75.93900	71.65980	60.85690	-723.71387	-201.97021	-243.05039	1
2648	N	76.98300	70.49280	62.53090	441.73769	351.29978	627.79660	1
2649	H	77.22900	69.59880	62.89790	-998.57522	-2127.28062	2091.82956	1
2650	C	77.34300	71.60280	63.34590	51.77988	707.65465	-572.70825	1
2651	H	76.43300	72.10680	63.63490	2898.13603	-1172.21801	-353.46674	1
2652	C	78.07100	71.11780	64.56590	-253.11347	659.10138	-577.03548	1
2653	H	77.40400	70.42680	65.12390	-1411.15697	-2314.43961	-1596.94444	1
2654	H	78.32800	71.98480	65.21090	-2709.75096	367.84358	1555.68861	1
2655	H	79.06500	70.67980	64.33290	-3067.13397	137.45548	-687.03816	1
2656	C	78.26200	72.58380	62.57290	682.49780	447.18425	407.03071	1
2657	O	77.99600	73.79480	62.52490	-478.25785	550.39124	303.25920	1
2658	N	79.28600	72.04380	61.88190	-190.06427	-631.23312	-527.34487	1
2659	H	79.45000	71.06180	61.82190	1714.14310	1948.78440	-1778.25167	1
2660	C	80.16600	72.83480	60.97290	-481.45767	-367.76633	681.46712	1

2661	H	80.56600	73.62780	61.58790	1.92333	3141.55384	-169.88815	1
2662	C	81.26100	71.99780	60.26490	-642.24492	-600.79952	240.85763	1
2663	H	80.87300	71.21680	59.57690	1253.90065	-2877.67719	-211.97497	1
2664	H	81.86300	72.79880	59.78490	1351.93614	-2410.42112	-1503.45100	1
2665	C	82.21600	71.17680	61.14290	37.20441	698.82925	584.55497	1
2666	H	81.67600	70.33280	61.62390	-1335.69003	-1079.49409	-2636.06731	1
2667	C	83.30900	70.67280	60.22790	-647.67314	-293.02833	571.05596	1
2668	H	82.82200	70.02180	59.46990	-334.40520	1911.46601	2476.42829	1
2669	H	83.81700	71.51980	59.71990	-1094.50796	2151.03179	2018.25192	1
2670	H	84.03400	70.09680	60.84190	2169.42575	-2232.25064	-457.02871	1
2671	C	82.83200	72.00880	62.34890	-734.31262	-29.66428	-539.77404	1
2672	H	81.97800	72.18080	63.03890	1618.46271	2641.76034	547.63768	1
2673	H	83.61500	71.40980	62.85990	1034.92887	1218.91969	-2709.49871	1
2674	H	83.28400	72.93580	61.93590	904.06768	2719.56616	1298.01685	1
2675	C	79.39800	73.56380	59.85490	-412.89558	811.61597	-47.41066	1
2676	O	79.60700	74.74080	59.58190	-265.26780	686.81507	285.56135	1
2677	N	78.44400	72.86480	59.19490	630.45625	456.03448	-327.45955	1
2678	H	78.25100	71.91980	59.44990	-2228.30596	1238.06642	1843.92796	1
2679	C	77.51900	73.42580	58.26290	466.52900	-601.72352	501.72752	1
2680	H	78.15500	73.93980	57.55690	1337.24937	-2722.63665	-835.00899	1
2681	C	76.60000	72.37380	57.56490	309.95694	430.93829	-741.39725	1
2682	H	75.90000	72.97980	56.94990	342.40933	-2245.93785	2176.40650	1
2683	H	76.05600	71.96080	58.44090	1084.66154	928.89903	-2803.36979	1
2684	C	77.41200	71.39580	56.68990	866.46906	252.80207	129.51252	1
2685	H	78.23700	70.92380	57.26490	-1870.34412	-1592.98019	1965.31250	1
2686	C	76.51500	70.32580	56.03890	-579.50716	-525.10325	468.92328	1
2687	H	75.79800	70.79480	55.33190	1948.98959	-2450.34638	308.97967	1
2688	H	77.06300	69.52180	55.50390	935.83366	-2836.40874	988.54796	1
2689	H	76.02800	69.82180	56.90090	-2204.04567	997.94039	-2011.10017	1
2690	C	78.08700	72.20080	55.55590	-548.67517	-215.89980	695.55290	1
2691	H	78.93000	72.84180	55.89090	2446.53965	-890.45067	-1766.28638	1
2692	H	77.35600	72.90380	55.10290	-19.42709	-3080.31590	-639.92405	1
2693	H	78.47800	71.55980	54.73690	-1972.30071	-1450.31055	1976.07071	1
2694	C	76.65800	74.51080	58.81890	231.98561	562.33357	-679.27508	1
2695	O	76.44500	75.53780	58.13990	714.06837	-40.17815	-334.84222	1
2696	N	76.13800	74.39180	60.04090	617.36970	286.62132	-499.37476	1
2697	H	76.10800	73.55980	60.58990	2165.59712	-1853.48418	-1331.54487	1
2698	C	75.18900	75.41980	60.53390	701.13198	-525.05250	253.34724	1
2699	H	74.52600	75.63580	59.70990	942.78482	-2944.10920	584.46903	1
2700	C	74.32700	74.98880	61.72290	-449.78881	-343.47278	-714.95978	1
2701	H	73.68700	75.85480	61.99690	2635.01368	188.31622	1708.64454	1
2702	H	75.08200	74.73680	62.49790	-2836.22068	1121.91519	771.61179	1
2703	C	73.43400	73.79580	61.37990	-400.29774	366.91327	732.52125	1
2704	H	73.87200	73.05280	60.67990	-2481.98041	-1112.62012	1581.16285	1
2705	C	73.20600	72.96180	62.64590	524.56692	373.61649	-645.51628	1
2706	H	72.47500	72.15780	62.41390	-135.19921	1449.58460	-2789.02347	1
2707	H	72.89900	73.58880	63.51090	-219.67440	-1200.96979	2899.59324	1
2708	H	74.09900	72.35780	62.91390	1564.87649	1580.78756	-2224.97157	1
2709	C	72.04600	74.18280	60.80190	-273.69235	416.04256	763.84036	1
2710	H	71.38500	73.30880	60.62390	749.99034	-2806.24561	1208.60509	1
2711	H	71.56400	75.00680	61.36990	1626.87072	-1973.16836	-1832.51863	1
2712	H	72.15400	74.59180	59.77490	-2157.38483	-596.93883	-2210.78741	1
2713	C	75.85100	76.71480	60.91390	422.05272	-388.77636	-708.64338	1
2714	O	75.24100	77.76980	61.06290	-536.29828	147.64734	560.54585	1
2715	N	77.17700	76.61080	61.06990	435.26067	426.40441	-584.29420	1
2716	H	77.61500	75.74080	60.85690	3076.65370	-173.31295	634.34286	1
2717	C	78.06900	77.62580	61.56690	-385.31104	623.44216	-542.50003	1
2718	H	77.44900	78.34180	62.08490	1219.20639	2253.68843	1825.55484	1
2719	C	79.05700	77.17280	62.62790	-209.66098	-676.59296	574.20837	1
2720	H	79.78300	77.96780	62.90290	-2046.86423	791.12563	2254.48293	1
2721	O	79.81600	75.99880	62.30490	-537.29814	487.37630	-312.09339	1
2722	H	79.18000	75.28680	62.20490	1726.20155	-1706.24308	2001.79644	1

2723	C	78.13500	76.76780	63.83490	244.30263	-860.47520	177.05836	1
2724	H	77.36500	77.55080	64.00490	-1786.84574	-1433.28235	-2156.64328	1
2725	H	78.74600	76.71880	64.76190	-1218.63170	2026.93918	2074.77241	1
2726	H	77.51500	75.84680	63.79690	-466.71224	-692.76123	3033.23059	1
2727	C	78.80100	78.28280	60.43990	-665.85034	456.81807	-423.57004	1
2728	O	79.82000	78.91780	60.65690	-552.27533	557.56958	87.95085	1
2729	N	78.35900	78.17880	59.20190	-162.28026	-574.47720	596.91989	1
2730	H	77.57900	77.59780	58.98190	-367.52315	-1901.80390	-2479.17222	1
2731	C	78.86300	79.05080	58.16390	-14.04506	-447.73381	-794.22174	1
2732	H	79.93700	78.96980	58.24790	-1992.67779	-1609.82420	1826.45216	1
2733	C	78.55500	78.55580	56.73090	655.95336	-529.40855	-347.71078	1
2734	H	77.45400	78.54380	56.58590	-2215.42451	2227.87174	-163.42572	1
2735	C	79.23400	79.47680	55.69190	-159.48417	502.42681	744.03166	1
2736	H	79.23300	79.06580	54.66090	2879.15674	-1266.80384	62.37558	1
2737	H	78.67300	80.41380	55.48890	3132.71444	-55.29409	-285.07721	1
2738	H	80.26600	79.78080	55.97290	-366.21256	-1156.54205	-2902.84775	1
2739	C	79.06900	77.10780	56.54390	-394.22383	621.10379	-538.76587	1
2740	H	79.00500	76.45980	57.44390	-2499.35262	-1550.88304	1116.34425	1
2741	H	80.15200	77.14780	56.29690	700.62728	2262.72359	-2070.61093	1
2742	C	78.26600	76.33080	55.51690	-565.96897	-633.65471	-331.07678	1
2743	H	78.23500	76.94280	54.59090	-1800.90823	-2245.03912	-1270.73015	1
2744	H	77.16900	76.27180	55.68190	2418.72941	-1963.84501	437.36376	1
2745	H	78.74700	75.33680	55.39290	667.24415	-2148.85118	2198.96568	1
2746	C	78.55300	80.52180	58.35990	641.49862	-13.07469	-647.88856	1
2747	O	79.45400	81.34280	58.28290	429.95962	-391.11820	-534.59191	1
2748	N	77.30800	80.94280	58.79090	-701.89462	110.25088	455.91773	1
2749	C	76.06600	80.31780	58.47990	-458.25423	444.20150	-651.25962	1
2750	H	75.80500	79.49080	59.17390	1834.49021	2545.03429	235.94993	1
2751	H	76.09400	79.92480	57.44090	-2289.01874	1680.45934	1354.50206	1
2752	C	77.11200	82.34380	59.28390	685.39954	588.08551	125.83284	1
2753	H	77.25900	83.06080	58.48990	-2803.66106	-1131.60613	-870.16002	1
2754	C	75.62100	82.35380	59.68890	265.07419	809.50247	-325.41118	1
2755	H	75.54600	82.00980	60.74290	-1970.85200	2004.33411	-1413.01571	1
2756	H	75.08500	83.32580	59.65190	-1975.54576	246.85397	2436.08462	1
2757	C	75.00600	81.34580	58.64290	-729.52436	511.26967	-194.54699	1
2758	H	74.62200	81.75380	57.68290	27.38355	2677.86276	1651.21997	1
2759	H	74.09500	80.94680	59.13790	-1442.41782	-2487.04692	-1277.59722	1
2760	C	78.03700	82.78180	60.40490	-288.39612	-864.61200	-26.92155	1
2761	O	78.48700	83.90380	60.44290	71.24541	-687.37751	-382.18253	1
2762	N	78.30300	81.91980	61.40090	198.69635	742.53901	349.03850	1
2763	H	77.87300	81.02280	61.32790	-2899.48114	1090.08704	550.40495	1
2764	C	79.25100	82.16380	62.47790	-722.98745	417.40509	-366.76032	1
2765	H	78.89200	83.09180	62.89790	1628.09794	-2323.51493	-1359.70648	1
2766	C	79.28600	81.04580	63.50590	819.55453	342.94851	205.34772	1
2767	H	80.16800	81.03780	64.18090	-2671.41909	1114.04009	-1233.15082	1
2768	H	79.41000	80.13580	62.87990	-1620.82808	-1182.19392	2423.54288	1
2769	C	78.00000	80.97680	64.30490	482.25145	637.00377	-439.44368	1
2770	O	77.75200	81.96580	65.02190	-547.32903	563.75195	79.00572	1
2771	O	77.25500	79.98480	64.24790	471.88587	-373.17630	511.55685	1
2772	C	80.65900	82.48880	61.91190	-606.37378	-460.62791	501.58127	1
2773	O	81.35100	83.42380	62.34390	426.03667	-539.98626	387.98817	1
2774	N	81.09300	81.65880	60.95190	222.40387	228.73368	781.59434	1
2775	H	80.60900	80.81980	60.71590	878.16134	-204.40596	-3014.17934	1
2776	C	82.35100	81.84880	60.18090	-65.79329	-908.34534	45.06656	1
2777	H	83.14500	81.81080	60.91190	960.33334	-2233.31578	-1997.06954	1
2778	C	82.61200	80.57680	59.36790	656.24266	-411.00044	-481.53422	1
2779	H	81.68500	80.38480	58.78690	2137.83445	256.08662	-2293.97248	1
2780	H	82.65500	79.66680	60.00390	1811.37974	2258.80147	1230.83126	1
2781	C	83.86900	80.51280	58.43890	592.11703	-547.29352	-425.81478	1
2782	C	85.11900	81.10280	58.74990	458.80924	-635.21661	-466.30992	1
2783	H	85.29600	81.67880	59.64590	-1969.18704	-1703.49115	1765.96900	1
2784	C	86.16200	81.10780	57.83790	-577.35659	-705.72029	-8.32061	1

2785	H	87.06200	81.63480	58.11890	917.19045	2209.95698	-2042.81131	1
2786	C	85.98200	80.43580	56.65890	-883.29316	208.07235	89.16331	1
2787	H	86.69700	80.46980	55.84990	-1065.22346	-984.63313	-2791.77772	1
2788	C	83.79600	79.72480	57.31990	462.88303	622.13985	-479.72107	1
2789	H	82.86100	79.25980	57.04390	-888.21074	1701.64388	-2492.73264	1
2790	C	84.80600	79.76980	56.36290	531.78267	-487.63267	-557.55948	1
2791	H	84.81800	79.17080	55.46490	-2241.90357	-1139.90078	-1890.16423	1
2792	C	82.49700	83.11280	59.39990	-4.58079	-673.93494	-614.20006	1
2793	O	83.51000	83.80280	59.50090	289.26115	-607.22467	413.80360	1
2794	N	81.49500	83.40680	58.56490	-483.96202	-633.02836	-278.79768	1
2795	H	80.75700	82.74780	58.43890	-2093.70205	-2006.71631	1219.72440	1
2796	C	81.46900	84.64280	57.71890	451.47373	-784.39792	111.09623	1
2797	H	82.41100	84.77380	57.20590	-1818.09101	-1530.39103	-2061.71642	1
2798	C	80.38000	84.70980	56.67890	591.42356	-262.21945	-642.58084	1
2799	H	79.41800	84.79380	57.22890	-1933.84250	-1014.42248	-2264.82372	1
2800	C	80.53000	85.93080	55.79390	618.45462	137.25568	-655.83974	1
2801	H	80.49300	86.84980	56.41690	554.59581	-2818.18485	-1283.93297	1
2802	H	79.71100	86.14580	55.07490	-3032.68240	-702.46243	-455.64262	1
2803	H	81.47200	85.93480	55.20490	-1309.39751	-2768.80406	719.32501	1
2804	C	80.27800	83.41680	55.77490	71.22585	-730.26392	541.38017	1
2805	H	80.08400	82.53880	56.42690	1881.30631	2002.94117	-1532.03769	1
2806	H	81.26700	83.29280	55.28390	586.69067	2093.17112	2274.34715	1
2807	C	79.15000	83.46480	54.79990	521.37426	-376.54092	-646.40298	1
2808	H	79.31000	82.70080	54.00990	-857.53232	1957.92398	2308.54895	1
2809	H	79.14200	84.43280	54.25390	1805.22892	-574.56076	-2511.82299	1
2810	H	78.13300	83.27280	55.20590	1499.02114	-2753.28145	-265.71247	1
2811	C	81.41100	85.83880	58.66890	-22.11314	881.79637	-231.07828	1
2812	O	82.18600	86.82180	58.58390	-40.13828	-545.56839	-569.53602	1
2813	N	80.53200	85.84680	59.71390	-108.28283	598.29957	585.64899	1
2814	H	79.88600	85.10280	59.86190	-490.18561	1813.24831	-2523.90073	1
2815	C	80.16500	87.06180	60.37190	201.98906	803.36332	381.12833	1
2816	H	80.34800	87.87080	59.68090	307.28550	2987.22972	-938.22195	1
2817	C	78.64300	87.01580	60.60090	-337.77149	845.86108	43.36420	1
2818	H	78.38000	86.19280	61.29990	2195.63541	1670.97116	-1511.70988	1
2819	H	78.29200	87.97580	61.03690	-423.32751	-2976.39496	927.41202	1
2820	C	77.77100	86.93180	59.39390	626.34891	-212.63972	627.63237	1
2821	C	78.12500	87.67480	58.24290	-544.91853	274.25159	677.71739	1
2822	H	78.96000	88.35880	58.27390	-3021.94084	-375.05072	-790.84558	1
2823	C	77.42200	87.53780	57.00990	-521.86666	667.34667	-337.27528	1
2824	H	77.64100	88.11680	56.12490	2115.33760	671.91291	-2229.82199	1
2825	C	76.41600	86.58680	56.93190	234.37523	-722.18983	504.93673	1
2826	H	75.85400	86.46680	56.01690	2738.44443	1472.30966	-481.09519	1
2827	C	76.59700	86.08180	59.31690	-32.58226	661.55531	626.68490	1
2828	H	76.31800	85.54980	60.21490	-389.71503	-2937.94041	1055.86673	1
2829	C	75.96400	85.91380	58.06690	209.35086	-736.74909	494.79693	1
2830	H	75.05900	85.32780	58.01090	-416.41562	-2165.10162	-2244.36165	1
2831	C	80.91200	87.39680	61.64790	321.30218	-451.06033	-724.40354	1
2832	O	80.78100	88.53880	62.11090	-532.81926	-379.84184	442.09845	1
2833	N	81.80500	86.48280	62.13090	-351.57856	-473.71698	-603.86839	1
2834	H	81.96900	85.57680	61.74990	2790.44983	-742.03048	1249.40256	1
2835	C	82.69800	86.74580	63.25490	-438.29741	-714.93486	358.07058	1
2836	H	82.09300	87.21380	64.01690	-489.07405	2396.76294	-1978.52476	1
2837	C	83.23800	85.45980	63.76690	658.80438	-585.54875	233.58178	1
2838	H	84.03900	85.66880	64.50790	-368.25003	-1136.87784	2910.34825	1
2839	H	83.68000	84.87680	62.92990	-2797.18605	-1173.47946	834.81879	1
2840	H	82.44800	84.78880	64.16490	741.18275	1458.74523	-2687.18007	1
2841	C	83.73700	87.78180	62.83590	-413.31390	-740.42472	-335.25193	1
2842	O	84.45600	87.59580	61.85590	485.65687	41.53547	-621.32072	1
2843	N	83.86400	88.88680	63.57090	-322.39834	-608.69326	488.08208	1
2844	H	83.31900	89.01480	64.39590	-1680.88733	-993.57362	-2466.91214	1
2845	C	84.77900	89.94580	63.16290	287.78812	352.02637	-790.38373	1
2846	H	85.66600	89.46580	62.77490	-3000.03754	946.14999	52.92597	1

2847	C	84.18100	90.98080	62.22090	-805.08025	-314.70983	290.26630	1
2848	H	84.74200	91.93980	62.22490	-1113.91325	-1978.42255	2177.90443	1
2849	H	83.09900	91.16380	62.39090	1617.85215	-2288.73627	1429.14902	1
2850	C	84.17800	90.52180	60.75190	665.95017	620.17102	57.87291	1
2851	O	83.09200	90.41180	60.08290	27.71212	285.16049	735.89589	1
2852	N	85.34800	90.18380	60.19090	186.48306	627.81018	-532.68258	1
2853	H	86.20200	90.51280	60.59290	-772.01393	-2247.59439	-2061.68382	1
2854	H	85.25800	89.91080	59.23290	-582.73514	2028.88638	-2332.86648	1
2855	C	85.23100	90.69380	64.33790	274.98917	676.15741	-546.48249	1
2856	O	84.59300	90.65980	65.39590	242.85121	-457.05748	596.44696	1
2857	N	86.37700	91.43280	64.20790	419.96340	616.18023	395.75870	1
2858	H	86.95000	91.30080	63.40190	1654.40191	1819.70936	-1962.10050	1
2859	C	86.86800	92.36080	65.20990	676.64468	-611.03018	-15.65585	1
2860	H	86.53200	92.16380	66.21690	472.55277	2359.57149	-2026.65796	1
2861	C	88.36600	92.28680	65.35290	-565.49679	136.26667	702.20779	1
2862	H	88.87500	92.77380	64.49390	54.51447	320.02359	3129.35126	1
2863	C	88.65400	93.12380	66.62890	258.53672	583.47180	-651.28367	1
2864	H	88.41000	94.20280	66.52190	-2349.57603	1674.06237	-1255.08322	1
2865	H	89.76500	93.15280	66.60990	12.65731	-2222.23579	-2227.04605	1
2866	H	88.19800	92.61880	67.50690	2313.17537	1323.45364	1672.09941	1
2867	C	88.86200	90.87680	65.56690	-755.61416	-122.63340	495.43849	1
2868	H	89.95600	90.80780	65.75290	2123.15399	379.73135	2290.46883	1
2869	H	88.17000	90.38680	66.28490	-2558.03829	1082.27731	1477.61366	1
2870	H	88.73700	90.25580	64.65490	-869.78412	2992.64638	-431.00978	1
2871	C	86.36400	93.75580	64.95590	-582.56426	140.23023	687.31752	1
2872	O	86.57000	94.35280	63.90990	188.47169	766.53711	22.94595	1
2873	N	85.74100	94.43580	65.96190	-639.96451	521.39674	176.81391	1
2874	H	85.49000	93.95280	66.79690	-1287.19626	-1500.50621	-2447.41356	1
2875	C	85.18400	95.74580	65.88090	402.71475	-563.88605	592.70934	1
2876	H	85.61500	96.34380	65.09190	-537.95990	3008.54571	746.64453	1
2877	C	83.61000	95.62180	65.77890	-398.93092	-553.57395	-604.86445	1
2878	H	83.19100	95.28480	66.75090	-215.95775	-2283.30903	-2153.62215	1
2879	H	83.39900	94.88280	64.97690	-514.99583	-430.76300	-3073.67024	1
2880	O	82.98500	96.86580	65.50290	-594.75588	312.47630	-415.03161	1
2881	H	82.95600	97.01580	64.55490	299.13801	500.40859	-3091.65553	1
2882	C	85.57700	96.55380	67.08990	787.27227	-185.69108	420.91829	1
2883	O	86.26100	96.06980	68.02790	580.03053	-315.39623	433.26323	1
2884	N	85.25600	97.85280	67.18390	-465.07522	-244.03374	660.92727	1
2885	H	84.70800	98.30380	66.48390	-845.79053	605.30711	-2969.25376	1
2886	C	85.67300	98.70880	68.28390	606.31617	467.36301	-495.38220	1
2887	H	86.19400	98.12780	69.03090	2535.27816	-1850.49918	-215.04340	1
2888	C	86.49600	99.91680	67.84390	-643.70931	436.72904	475.76998	1
2889	H	86.63700	100.54580	68.74990	498.60485	-2323.32339	2061.98639	1
2890	H	85.85000	100.50980	67.16090	-1361.16545	1079.56152	-2622.97575	1
2891	C	87.91100	99.58580	67.26190	649.19315	-593.25615	-240.92820	1
2892	H	88.66000	99.34080	68.04490	-1734.90115	-1328.09038	-2263.74031	1
2893	H	87.89700	98.70980	66.57990	-1040.07678	256.89350	2958.11971	1
2894	C	88.42000	100.76080	66.40690	193.81339	-408.74259	-791.71767	1
2895	O	87.88100	101.03180	65.33990	540.03381	-337.40863	467.06116	1
2896	O	89.41200	101.32880	66.84290	51.06230	638.52047	-461.85656	1
2897	C	84.50400	99.21580	69.08090	-385.43449	-574.79018	-593.72343	1
2898	O	83.45000	99.56580	68.55090	-563.48700	-137.47884	535.91903	1
2899	N	84.62100	99.23780	70.38090	-91.28000	-359.27453	758.46032	1
2900	H	85.45200	98.89080	70.80990	-2074.68543	-20.13668	2365.05838	1
2901	C	83.55600	99.70680	71.26890	-684.62141	-75.53675	-597.52718	1
2902	H	83.07200	100.60080	70.90690	1055.54582	-2885.61182	676.23493	1
2903	C	82.37200	98.76980	71.48190	-499.36074	526.64628	-552.02676	1
2904	H	82.25700	98.28080	70.49090	-1612.27525	-1784.55763	2028.33647	1
2905	H	81.49700	99.32980	71.87490	-591.40789	-2227.72044	2141.43049	1
2906	H	82.67000	97.97380	72.19690	-1765.55613	-2074.94864	-1573.41218	1
2907	C	84.15600	100.14680	72.56590	-419.70123	750.06400	304.47639	1
2908	O	84.92400	99.46980	73.28390	515.89267	-288.61956	-523.62270	1

2909	N	83.77400	101.37680	72.94790	512.01979	-165.46656	-650.48355	1
2910	H	83.08300	101.96680	72.53790	-2211.47680	-2183.79836	488.48880	1
2911	C	84.36000	102.05880	74.14390	-904.30226	-73.71556	90.85400	1
2912	H	83.99800	103.07680	74.13290	1993.44733	-489.12971	-2384.35444	1
2913	C	83.80800	101.41580	75.44890	-543.77686	717.91892	-142.65398	1
2914	H	84.24200	100.39580	75.52690	-2010.18612	1852.74334	1557.15127	1
2915	H	84.17900	101.90080	76.37690	2007.58957	-1406.19641	1972.41527	1
2916	C	82.27300	101.26180	75.49290	674.75715	-452.31401	-414.20506	1
2917	O	81.45800	102.17180	75.16490	-100.26355	-550.12991	557.61235	1
2918	O	81.86900	100.23580	76.07190	306.27276	-210.75589	-696.71097	1
2919	C	85.89000	102.21780	74.21590	822.75771	-314.55955	-235.73935	1
2920	O	86.53100	102.11480	75.24190	-424.74015	523.73245	411.00772	1
2921	N	86.55900	102.52980	73.07790	168.04760	738.06344	-373.75748	1
2922	H	86.04700	102.83480	72.27890	-1721.58178	-253.01000	2621.13875	1
2923	C	87.99700	102.51980	72.95490	667.57129	-166.25899	598.46263	1
2924	H	88.23500	102.51880	71.90190	-2321.40485	1728.29933	-1233.81002	1
2925	C	88.75900	103.72080	73.51690	-571.07052	-686.61683	184.08365	1
2926	H	89.85200	103.60380	73.35790	-1613.82085	-1584.21234	-2187.25393	1
2927	H	88.47600	103.68380	74.59090	536.44052	-2543.41300	1772.43000	1
2928	C	88.35600	104.98980	72.86890	340.91790	-426.13415	730.50371	1
2929	O	87.69500	105.03980	71.80390	524.06502	-433.45520	401.37223	1
2930	O	88.94100	106.05480	73.24590	401.74842	408.16747	-543.71385	1
2931	C	88.72400	101.19780	73.36790	-37.75605	754.50114	-510.64030	1
2932	O	89.78300	101.20980	74.02190	-505.00163	-271.91426	542.82891	1
2933	N	88.10000	100.07680	72.97690	-308.59958	-643.08763	-451.52727	1
2934	H	87.17700	100.09780	72.59990	-1851.98901	-152.09036	-2538.74604	1
2935	C	88.68300	98.74680	73.11590	-724.72827	-521.44715	-185.23719	1
2936	H	89.74600	98.78880	72.93390	-1839.87262	567.74288	-2488.12439	1
2937	C	88.58400	98.08680	74.49490	-211.78605	-693.14120	553.31089	1
2938	H	89.18800	97.15680	74.56590	787.28146	-2212.53146	-2093.58990	1
2939	H	89.02300	98.76780	75.25490	-2141.04566	-2199.14361	691.31547	1
2940	C	87.17400	97.86380	75.03590	-755.69893	-505.60369	68.81167	1
2941	H	86.50200	97.57780	74.19790	-1469.64694	-1820.90266	2103.01632	1
2942	H	86.92800	98.81880	75.54790	661.85404	-2364.70311	1966.81332	1
2943	C	87.13200	96.63380	76.01790	-14.17894	461.03678	-786.57171	1
2944	H	86.14800	96.57680	76.52990	-1375.53556	145.95227	2825.74346	1
2945	H	87.98200	96.59980	76.73290	1249.11616	2326.76640	-1709.99801	1
2946	N	87.19400	95.40980	75.15390	-802.89733	41.45839	-257.50606	1
2947	H	87.22200	95.49380	74.15790	-2334.47975	1287.11482	1670.85786	1
2948	C	87.26500	94.17580	75.58590	-358.05376	-632.80350	550.28014	1
2949	N	87.33600	93.24680	74.65890	207.26513	-806.81170	-136.99759	1
2950	H	87.25200	93.50180	73.69590	2994.81805	714.48113	647.15362	1
2951	H	87.32800	92.28980	74.94890	-70.00799	-735.93913	-3058.05800	1
2952	N	87.44200	93.84480	76.85890	498.46296	-40.67939	-680.11187	1
2953	H	87.53200	94.52480	77.58690	-242.05718	3056.71768	-704.35190	1
2954	H	87.63500	92.91280	77.16790	516.43613	2944.83375	979.52751	1
2955	C	88.19000	97.86780	71.99190	-402.51475	-663.21030	479.15026	1
2956	O	87.21900	98.21680	71.34290	-237.77104	-70.63068	749.73560	1
2957	N	88.79500	96.66280	71.75890	225.62622	-474.49160	-660.77441	1
2958	H	89.46100	96.24680	72.37390	-2659.53420	34.48109	1680.45087	1
2959	C	88.29300	95.80580	70.62290	75.28646	899.45375	129.48324	1
2960	H	87.87200	96.42680	69.84690	-2118.79370	-2263.30218	535.16608	1
2961	C	89.45600	94.97780	70.03190	-737.26414	418.15517	336.21250	1
2962	H	89.25500	94.22680	69.23890	-1996.46048	-1898.49971	-1519.23356	1
2963	H	89.85800	94.43980	70.91690	-1042.91693	-2900.30144	631.50776	1
2964	C	90.57800	95.84980	69.51290	-280.13327	78.89038	864.14852	1
2965	C	90.38600	96.79480	68.46590	324.74263	282.81798	803.74574	1
2966	H	89.38500	97.05980	68.15890	-2307.06260	910.31012	-1935.72308	1
2967	C	91.44100	97.45780	67.86390	679.04405	-422.73602	-437.77213	1
2968	H	91.25100	98.22080	67.12390	542.45878	476.41770	3062.18727	1
2969	C	92.74000	97.16980	68.35590	-700.97525	284.77725	508.90727	1
2970	O	93.82400	97.96880	67.87890	-549.98019	-390.79587	410.39933	1

2971	H	93.60400	98.44180	67.07290	-2995.76702	-533.91066	799.09048	1
2972	C	91.87400	95.55280	69.85090	828.20006	-85.67220	371.74715	1
2973	H	92.09500	94.84980	70.63990	1659.86126	-2569.27003	736.16461	1
2974	C	92.95600	96.20280	69.27690	-489.12188	769.01537	28.74297	1
2975	H	93.97900	96.16280	69.62190	1634.06497	-146.71735	2684.49845	1
2976	C	87.25600	94.87680	71.10790	-630.90389	-651.86562	-92.10049	1
2977	O	87.33700	94.36680	72.23490	58.46103	701.21973	358.46957	1
2978	N	86.23100	94.55480	70.29690	-238.40270	701.31434	404.96251	1
2979	H	86.20700	95.03580	69.42390	685.69856	-1488.63374	2685.51919	1
2980	C	85.17700	93.65180	70.62590	-19.64658	324.13178	852.05845	1
2981	H	85.45300	93.05980	71.48690	2410.11278	-348.99175	1991.93057	1
2982	C	83.87600	94.46680	70.97290	577.21179	325.46301	-626.37958	1
2983	H	83.63900	95.29380	70.26990	1297.81579	-2422.15899	1532.00725	1
2984	C	82.66000	93.46080	70.91490	538.48962	-648.94068	346.92352	1
2985	H	82.57500	93.03880	69.89090	-1223.12363	-1210.94878	2633.59030	1
2986	H	82.81000	92.62380	71.62990	-2827.35189	-912.03981	-1035.61135	1
2987	H	81.75500	94.01380	71.24590	2637.92094	-1297.85890	1120.33995	1
2988	C	84.01700	95.17280	72.32390	423.54265	-647.41087	-482.61971	1
2989	H	83.05500	95.71680	72.43390	249.81908	-2659.00299	1662.98520	1
2990	H	84.80100	95.95980	72.31590	364.09177	1714.93999	2612.40201	1
2991	C	84.21000	94.24780	73.51690	-503.12905	-297.58898	-699.82352	1
2992	H	85.09500	93.57580	73.50090	1258.92648	-2858.69740	-375.73865	1
2993	H	84.29100	94.82880	74.45990	-2403.29007	-2026.52476	-124.98197	1
2994	H	83.30600	93.61280	73.63590	-1171.00539	-1446.94598	-2536.39901	1
2995	C	85.02700	92.67980	69.49890	-640.02508	640.22694	-109.21701	1
2996	O	84.79900	93.11880	68.34090	-271.55674	-612.85530	417.48358	1
2997	N	85.23800	91.33080	69.79390	-590.48661	531.53347	285.42953	1
2998	H	85.37600	91.05280	70.74090	1058.28672	1631.50870	2473.14270	1
2999	C	85.03900	90.23180	68.94490	-786.43527	15.20389	461.23682	1
3000	H	85.08300	90.57180	67.92090	-1033.59701	-2971.27095	-38.11061	1
3001	C	86.11700	89.17080	69.15890	153.23179	624.95943	646.06248	1
3002	H	87.06700	89.67880	68.88690	2013.69023	-1339.17496	2012.43344	1
3003	H	86.09100	88.84980	70.22190	671.20904	1089.35111	2874.19881	1
3004	S	85.97400	87.72980	68.04990	-287.75078	420.21714	-227.65688	1
3005	C	83.66300	89.69880	69.14990	-867.57642	238.19461	-148.40988	1
3006	O	83.34700	89.18880	70.25090	-587.38510	36.08698	-526.59634	1
3007	N	82.85200	89.65080	68.06590	-817.77750	-174.68192	115.75180	1
3008	H	83.17700	89.93180	67.16590	883.39297	-1538.95198	2597.97419	1
3009	C	81.48000	89.35180	68.14790	426.43426	727.32769	-347.27404	1
3010	H	81.37500	88.44780	68.72890	2575.44033	-1804.47448	-95.94358	1
3011	C	80.71100	90.50080	68.79390	-641.09561	-645.14971	65.03282	1
3012	H	80.95300	91.42480	68.22690	1864.87952	-2012.08074	1540.12393	1
3013	H	81.10100	90.68080	69.81890	-1965.90742	-2403.32418	-507.41218	1
3014	C	79.20500	90.34780	68.95290	-303.47521	-614.07391	-601.88624	1
3015	O	78.78900	89.17980	68.89090	-544.74802	-346.26729	454.94592	1
3016	O	78.48400	91.32780	69.18990	-570.45743	-503.96647	-210.29348	1
3017	C	81.13700	89.03280	66.71390	-733.20510	484.86676	-242.41597	1
3018	O	81.97700	89.21780	65.81990	-649.14730	434.18821	117.11369	1
3019	N	79.91200	88.54380	66.42590	251.66558	-325.46389	737.16347	1
3020	H	79.31000	88.57880	67.21990	-2088.10081	1506.41273	-1807.97730	1
3021	C	79.46700	88.44680	64.98590	684.85885	-600.85886	37.25568	1
3022	H	80.37200	88.40880	64.39790	-466.84998	-1733.14485	2583.88975	1
3023	C	78.58200	87.27080	64.70790	499.87848	540.39876	538.09079	1
3024	H	78.48200	87.25680	63.60190	2059.78309	1590.50628	-1767.99594	1
3025	H	77.52400	87.41480	65.01390	-1928.27331	-2441.07512	-470.25580	1
3026	C	79.07300	85.87680	65.16590	-461.09083	782.17797	-83.92781	1
3027	H	80.16900	85.86280	64.98390	1766.21931	-935.75464	2429.62113	1
3028	H	78.66300	85.16780	64.41490	-1840.27305	-1964.84831	1628.18685	1
3029	C	78.69100	85.47280	66.60290	-485.29762	158.94962	-755.42852	1
3030	H	79.40300	85.87580	67.35490	-1053.96920	1992.70376	-2194.65415	1
3031	H	77.62400	85.77780	66.65190	185.27286	-1324.56077	2847.70767	1
3032	N	78.71300	83.93980	66.64390	139.49274	632.25749	541.72366	1

3033	H	78.51800	83.39480	65.82790	1546.00063	1711.60222	-2139.74908	1
3034	C	78.40500	83.36480	67.75690	-660.28185	376.69649	-503.56592	1
3035	N	78.10900	83.97080	68.86490	784.59473	306.33082	-56.96336	1
3036	H	78.26600	84.95480	68.95690	-1717.42843	1638.68264	-2064.79661	1
3037	H	77.74400	83.35480	69.56290	-1352.92526	1935.42880	-2078.92637	1
3038	N	78.05200	82.10080	67.70790	-565.40399	528.41277	-337.29892	1
3039	H	78.04200	81.66580	66.80690	-1268.65259	2583.95523	1269.61498	1
3040	H	77.44800	81.87880	68.47390	-1851.91353	1823.05462	-1773.44702	1
3041	C	78.69900	89.69080	64.55990	-843.15971	-29.12928	345.95404	1
3042	O	77.90400	90.28080	65.27790	272.09443	701.03984	-241.11200	1
3043	N	79.15700	90.22880	63.43090	-352.55633	765.58652	47.47222	1
3044	H	79.90400	89.80280	62.92690	-803.47171	2043.56282	2253.11128	1
3045	C	78.50500	91.35780	62.83390	242.82816	618.09522	624.85501	1
3046	H	77.71600	91.78880	63.43190	1925.86543	-2164.72582	1226.06308	1
3047	C	79.48900	92.56080	62.61290	-27.65838	550.81425	-726.14715	1
3048	H	80.46300	92.22080	62.20290	-519.71816	3085.59790	327.42154	1
3049	H	79.14400	93.30680	61.86590	-145.28703	16.17621	-3142.74661	1
3050	C	79.69500	93.20580	63.92390	-61.10557	-654.99018	631.43089	1
3051	C	79.02700	94.38280	64.28490	60.70304	-699.15010	-582.19866	1
3052	H	78.26800	94.75180	63.61090	236.25091	76.61065	-3136.32628	1
3053	C	79.26900	95.01380	65.52590	545.31856	695.59345	224.11698	1
3054	H	78.77400	95.92680	65.82390	1811.96676	1610.83841	2005.04421	1
3055	C	80.26000	94.46780	66.39590	-572.49298	629.83999	327.11524	1
3056	H	80.57300	94.87980	67.34490	357.75004	2840.82360	-1303.82607	1
3057	C	80.61200	92.65780	64.82490	236.95107	224.70877	851.35842	1
3058	H	81.32300	91.87380	64.61090	1531.38001	1866.01400	2017.69503	1
3059	C	80.96000	93.37080	66.02290	537.20387	734.29828	60.57262	1
3060	H	81.73700	93.04080	66.69590	-2735.49444	1211.55025	-973.36652	1
3061	C	77.86200	90.88080	61.58490	385.07464	-678.68233	-471.76139	1
3062	O	78.49200	90.47880	60.60890	-270.97988	535.95406	-512.78687	1
3063	N	76.48600	90.78680	61.61790	-340.32058	55.87217	-770.54039	1
3064	H	75.93000	91.19480	62.33790	32.82856	2827.76922	1378.72032	1
3065	C	75.62900	90.22480	60.62490	151.55644	798.81900	412.75883	1
3066	H	76.17700	89.45380	60.10590	2439.90646	1977.10070	-190.14604	1
3067	C	74.34500	89.60080	61.32790	-169.32098	-874.02750	-197.12265	1
3068	H	73.62400	89.19780	60.58390	2732.14124	-231.21634	-1542.77979	1
3069	H	73.82200	90.42980	61.85090	2892.64287	-19.61786	1237.11705	1
3070	C	74.60400	88.61080	62.44390	674.55711	190.70004	-583.14424	1
3071	C	74.96300	87.27480	62.09390	-321.99734	-460.63195	-718.04381	1
3072	H	75.01100	86.94880	61.06590	-589.99434	1487.80925	-2708.60786	1
3073	C	75.20000	86.28380	63.09090	517.57782	-742.41817	-111.26308	1
3074	H	75.40900	85.26680	62.79190	-2782.89935	60.04875	1466.31906	1
3075	C	75.09600	86.55380	64.44390	-728.47527	-492.85847	-240.55210	1
3076	O	75.30600	85.58880	65.44290	-302.49231	508.65647	-522.87114	1
3077	H	75.54600	84.77580	64.99090	11.90255	-1173.96099	2918.88680	1
3078	C	74.61200	88.86580	63.80990	492.63088	-654.96857	399.72739	1
3079	H	74.48400	89.90780	64.06090	-1553.70120	-2014.95306	1850.46021	1
3080	C	74.82300	87.89080	64.77390	528.57158	683.15329	-292.17234	1
3081	H	74.71700	88.14880	65.81690	13.37643	-2248.27139	-2200.75511	1
3082	C	75.18000	91.27180	59.59490	142.12608	-693.07206	575.24108	1
3083	O	75.59300	92.42180	59.74490	-780.83749	-109.54778	-43.81017	1
3084	N	74.47800	90.91580	58.49590	422.18555	-496.42284	536.65260	1
3085	C	74.35000	89.53680	57.97590	-391.53141	796.59838	208.77066	1
3086	H	75.16500	88.86780	58.32590	-2845.78889	-1270.62410	430.37919	1
3087	H	73.39000	89.20380	58.42590	2134.92521	2205.91301	-688.67145	1
3088	C	74.17400	91.83280	57.47490	702.20476	-328.09598	480.32542	1
3089	H	75.07100	92.39780	57.26790	1401.23152	2279.62547	-1654.71573	1
3090	C	73.73600	90.99480	56.30490	-588.90108	577.39613	-388.92187	1
3091	H	72.63900	90.81680	56.29490	-2954.74876	-369.91321	-1015.30793	1
3092	H	74.13400	91.54580	55.42590	2155.31963	-1990.43715	-1136.21453	1
3093	C	74.37800	89.60580	56.44290	-484.51738	763.39278	-118.00586	1
3094	H	73.80700	88.78080	55.96690	-1114.65608	2230.86698	-1918.07210	1

3095	H	75.43300	89.67580	56.10090	2474.99905	-1941.77476	-46.00758	1
3096	C	73.10400	92.77380	57.95290	-342.59538	343.44875	-772.08961	1
3097	O	73.32900	93.95380	57.75190	457.59786	-628.16726	-140.13325	1
3098	N	72.00100	92.25380	58.61190	758.57737	-319.69526	187.15663	1
3099	H	71.79600	91.28380	58.71890	-67.62625	-3145.16236	-40.08276	1
3100	C	71.08000	93.20680	59.32690	-596.95364	681.56216	102.81231	1
3101	H	71.65900	93.93880	59.86890	-1500.04098	1782.52513	-2114.40475	1
3102	C	69.98600	93.89380	58.42590	466.83114	-593.93995	510.64178	1
3103	H	69.28100	94.58780	58.93290	2377.85569	-431.14751	-2014.48266	1
3104	H	70.54600	94.43880	57.63590	-2016.47580	2188.33390	-1021.39429	1
3105	C	69.03900	92.90780	57.71190	-740.15811	523.90286	-95.61783	1
3106	O	69.10200	91.68780	57.76390	416.80758	41.24232	669.47572	1
3107	N	68.20300	93.43180	56.81490	-532.82128	615.45082	-223.59352	1
3108	H	68.42100	94.35780	56.50490	2729.80507	-1364.44025	764.65241	1
3109	H	67.58900	92.77680	56.37490	2686.40596	-1088.54750	-1223.32072	1
3110	C	70.37700	92.46280	60.43890	-15.89909	911.27431	27.88117	1
3111	O	70.58000	91.23680	60.64390	-546.78021	-293.95568	488.10725	1
3112	N	69.60900	93.15080	61.24690	-99.80355	228.90303	806.42107	1
3113	H	69.68100	94.14380	61.21090	-450.54094	1745.32864	-2578.57849	1
3114	C	68.71500	92.61680	62.28090	831.03153	325.04932	187.56475	1
3115	H	69.37400	92.11780	62.97590	2733.89177	203.89619	1543.53114	1
3116	C	68.23300	93.82380	63.12490	674.30975	-591.68538	-163.29658	1
3117	H	68.04700	93.59780	64.19690	-1143.77336	2592.94403	1366.25400	1
3118	H	69.14400	94.45780	63.10790	-1680.35772	-2365.33888	1216.46870	1
3119	C	67.13600	94.70480	62.55690	681.10816	-359.30277	488.30748	1
3120	O	66.92500	94.68280	61.35890	215.54790	-660.26749	375.78341	1
3121	O	66.52900	95.47680	63.28490	393.67950	-569.55472	-379.80403	1
3122	C	67.62800	91.65580	61.83490	439.53685	-557.33589	-572.39415	1
3123	O	67.25000	90.68680	62.53590	-464.33978	-151.70442	-620.48495	1
3124	N	67.06100	91.77080	60.59990	499.63464	-679.79613	30.24459	1
3125	H	67.25800	92.59280	60.07190	-2252.46405	-2193.40372	-116.67078	1
3126	C	66.23300	90.73980	59.97490	674.79755	381.80870	479.91810	1
3127	H	65.41000	90.57180	60.65390	-2095.65086	1083.62019	2081.40361	1
3128	C	65.64800	91.13880	58.55590	367.89151	-807.74834	208.92454	1
3129	H	66.43100	90.99380	57.78090	2038.36274	2072.99438	1202.49651	1
3130	H	64.81300	90.42780	58.37690	-198.93491	-2966.98350	-1027.45317	1
3131	C	65.27600	92.63680	58.47390	-444.75254	-625.08469	-492.86440	1
3132	H	66.08700	93.32080	58.80390	2172.31399	2118.27683	831.97442	1
3133	C	64.90500	92.96480	57.01690	-12.10528	759.87713	-503.87619	1
3134	H	65.48000	92.49980	56.18890	-2938.68197	-1110.52064	-170.64122	1
3135	H	64.82900	94.05680	56.82690	-2518.58425	-677.62155	1759.48533	1
3136	H	63.87000	92.56180	56.98390	864.32135	-1684.85644	-2512.45570	1
3137	C	64.03300	92.95580	59.30590	-266.95772	869.94368	-58.15984	1
3138	H	63.21900	92.23980	59.06190	2210.49420	-1431.20975	-1721.50523	1
3139	H	64.31300	92.90380	60.37890	980.33656	-1939.53307	2274.94570	1
3140	H	63.70600	94.00980	59.17390	-1964.62785	-1986.36270	-1446.66060	1
3141	C	66.92300	89.38480	59.90390	45.97922	-634.99412	-652.77820	1
3142	O	66.35100	88.33280	60.30490	185.70058	-767.14650	25.07538	1
3143	N	68.24400	89.36280	59.47290	-643.66149	500.55803	-218.66373	1
3144	H	68.59100	90.13980	58.95390	2197.94600	-2196.75884	491.43688	1
3145	C	69.09100	88.19280	59.60490	-284.47269	600.31975	624.61388	1
3146	H	68.51300	87.34680	59.26390	-617.94389	1932.16636	-2404.80867	1
3147	C	70.34600	88.34380	58.71390	459.59627	-541.46360	571.87362	1
3148	H	71.15400	87.68080	59.08990	2287.30485	-2153.05635	-175.53086	1
3149	H	70.86400	89.30480	58.92090	-185.87604	-3127.14635	290.91582	1
3150	C	70.08300	88.11080	57.26090	-211.79256	319.15345	-827.48776	1
3151	C	70.04800	88.92680	56.19490	-840.67621	278.73129	216.84874	1
3152	H	70.08900	90.00580	56.17090	-694.43641	-2231.57637	-2106.19353	1
3153	N	69.83900	88.20280	55.04390	483.58999	64.00705	-688.99645	1
3154	H	69.47800	88.60480	54.23190	1359.74878	589.22914	-2775.26909	1
3155	C	69.80000	86.85980	55.35490	455.51993	608.32094	503.88316	1
3156	C	69.89600	86.77080	56.77790	647.53820	1.27654	-641.98415	1

3157	C	69.81100	85.53980	57.37690	-383.52825	544.66747	622.65113	1
3158	H	69.96700	85.35180	58.42890	-1761.85414	2128.42680	1504.62474	1
3159	C	69.68000	84.43180	56.55090	-249.17678	520.15760	706.25633	1
3160	H	69.73600	83.43380	56.95890	1509.78763	463.94103	2720.94217	1
3161	C	69.49400	85.77880	54.51890	699.48008	-584.42341	25.05801	1
3162	H	69.31500	85.82980	53.45490	-982.33038	-1310.33874	-2686.31079	1
3163	C	69.46400	84.55980	55.13790	-726.02323	-516.91701	192.71243	1
3164	H	69.43900	83.61780	54.60990	-1237.27372	2881.62697	252.20224	1
3165	C	69.43800	87.78780	61.03290	264.15943	-418.08809	-766.07647	1
3166	O	69.58400	86.57980	61.24590	-586.34986	-528.56853	20.88976	1
3167	N	69.56600	88.70080	61.99990	647.79913	-455.69419	-292.18381	1
3168	H	69.43100	89.65580	61.74390	2359.40135	1874.51857	904.22987	1
3169	C	69.80300	88.41280	63.38790	531.70700	-701.15702	-238.99268	1
3170	H	70.72600	87.85380	63.40290	-3120.36519	230.41472	329.32712	1
3171	C	70.02500	89.65980	64.23890	-517.48663	-537.14556	524.53144	1
3172	H	69.27200	90.43580	63.98390	-2524.39813	1796.58899	545.80978	1
3173	C	69.83500	89.46180	65.76090	-274.68066	650.80809	576.58509	1
3174	H	70.27100	88.52780	66.17490	1724.38717	1112.69244	2384.66573	1
3175	H	68.74300	89.43480	65.96790	-1368.67998	2465.99810	-1394.20039	1
3176	H	70.29900	90.30680	66.31390	1644.28268	1753.96113	-2029.33020	1
3177	C	71.39000	90.30480	64.03190	477.06655	1.51879	777.08185	1
3178	H	71.65900	90.31980	62.95390	-1838.26078	-1539.31166	-2037.04274	1
3179	H	71.40800	91.30480	64.51490	1623.31929	2157.68221	1614.76568	1
3180	H	72.13300	89.68480	64.57790	-388.30119	-3116.32795	-189.60096	1
3181	C	68.77200	87.43280	63.95090	-63.17081	-851.30184	320.53960	1
3182	O	69.14200	86.39680	64.55590	548.21991	568.39175	-3.60310	1
3183	N	67.48900	87.66980	63.69390	-498.68242	354.19484	-581.83688	1
3184	H	67.35500	88.51080	63.17490	-2340.02903	1294.84850	1657.06299	1
3185	C	66.36200	86.87580	64.02290	-171.78222	294.51301	-845.69732	1
3186	H	66.40700	86.86080	65.10190	169.62441	779.44429	3043.34033	1
3187	C	65.05000	87.59180	63.59990	-361.25187	-215.17681	-809.10261	1
3188	H	65.12200	87.90880	62.53790	-1072.30199	876.75754	-2824.83466	1
3189	C	63.81100	86.63280	63.66590	711.09214	-312.98229	477.32699	1
3190	H	63.96700	85.78780	62.96190	-2791.47791	-1443.97540	-144.26484	1
3191	H	63.73400	86.23480	64.70090	-511.74995	2088.90395	2296.26186	1
3192	H	62.98200	87.29380	63.33390	-2054.12404	-2381.02365	97.60650	1
3193	C	64.73800	88.86180	64.45590	579.91598	-408.42475	573.00757	1
3194	H	63.78500	89.26980	64.05690	1004.01090	1783.95418	-2389.07845	1
3195	H	64.76800	88.63780	65.54390	3108.25516	-87.85104	478.80925	1
3196	H	65.56400	89.56980	64.22990	1406.56642	2655.08738	932.90306	1
3197	C	66.48900	85.43980	63.50890	-668.52375	505.67599	-358.91335	1
3198	O	66.19800	84.42780	64.14390	-482.57715	592.64948	198.77909	1
3199	N	67.06000	85.29280	62.28690	297.37484	577.42394	-539.27922	1
3200	H	67.19500	86.04380	61.64590	1693.22093	-1907.84288	1841.56582	1
3201	C	67.17300	83.92780	61.67790	685.68798	321.67274	507.74959	1
3202	H	66.24200	83.39480	61.79890	1649.61620	2256.69318	1443.72038	1
3203	C	67.57000	83.97580	60.15290	605.11168	-412.29603	543.41774	1
3204	H	68.48300	84.59580	60.02690	2104.62655	2018.10975	-1181.52712	1
3205	C	67.61400	82.57980	59.52390	-543.91757	453.41528	574.47303	1
3206	H	66.79600	81.88480	59.80990	1862.33532	-1444.02710	-2084.39898	1
3207	H	68.52000	82.02080	59.84090	2864.49075	1300.75818	-30.77500	1
3208	H	67.66500	82.68580	58.41990	-2611.94440	-1738.28447	-233.10893	1
3209	C	66.50700	84.79580	59.46790	834.42392	349.32340	-114.72088	1
3210	H	66.63300	84.77480	58.36390	-2506.74778	-471.96867	-1841.65343	1
3211	H	66.49400	85.86380	59.77090	1852.12964	2492.27997	506.34235	1
3212	H	65.54000	84.29880	59.69790	-1698.05578	-2195.07427	-1482.05322	1
3213	C	68.20200	83.10680	62.39890	550.50155	589.32564	-425.55181	1
3214	O	68.02100	81.91380	62.76490	265.05037	-645.49038	-369.75357	1
3215	N	69.35700	83.66280	62.70190	611.51693	-452.93843	-365.46698	1
3216	H	69.64500	84.55180	62.35490	-1783.86180	-1016.25432	-2383.96528	1
3217	C	70.38900	83.01780	63.55090	-417.00848	393.99101	708.74961	1
3218	H	70.48900	81.98180	63.26390	-1071.58594	2667.34841	-1278.74246	1

3219	C	71.76000	83.63580	63.31290	-484.47360	707.47680	310.18206	1
3220	H	72.58800	82.97480	63.64590	-2638.63833	1671.58017	376.34261	1
3221	H	71.82400	84.63980	63.78390	-798.91887	3040.56766	122.07846	1
3222	C	72.03300	83.72280	61.79390	-215.29745	-521.99840	715.97184	1
3223	C	71.81600	82.59080	60.95990	279.85305	-717.87178	-487.64063	1
3224	H	71.47000	81.69580	61.45590	-2316.48263	1909.86806	940.49903	1
3225	C	72.08100	82.67680	59.54890	606.64568	99.14528	673.49999	1
3226	H	71.79200	81.91980	58.83390	-2128.87791	1667.81113	-1607.64148	1
3227	C	72.48800	83.89180	59.02390	195.93976	854.07363	-252.22381	1
3228	H	72.66000	83.92580	57.95890	-2538.06704	1495.79316	1104.10359	1
3229	C	72.42300	84.92880	61.19290	-50.29512	126.63266	-901.60167	1
3230	H	72.56400	85.79180	61.82690	-1253.69949	2365.48905	1652.55117	1
3231	C	72.64400	85.05180	59.81190	-690.54677	458.64801	-379.78700	1
3232	H	72.94700	85.99380	59.37990	3014.41700	675.46679	596.03774	1
3233	C	70.05300	82.90880	64.99590	-703.64877	567.76549	118.20222	1
3234	O	70.29400	81.84380	65.59190	582.21902	-257.82227	-467.09306	1
3235	N	69.42700	83.89580	65.60790	-669.99197	-228.23948	-460.09759	1
3236	H	69.17200	84.72080	65.10890	-2598.22064	1215.83658	1291.98188	1
3237	C	68.97800	83.85380	67.00790	-783.83523	-179.54670	429.90268	1
3238	H	69.89000	83.70380	67.56490	346.22594	-2277.71589	-2142.51351	1
3239	C	68.16600	85.14180	67.39690	499.54056	-746.63885	156.33509	1
3240	H	67.20300	85.21680	66.84790	1519.90309	-1363.03899	-2393.79313	1
3241	H	68.78600	85.92680	66.91090	-387.04246	2488.43321	-1885.76895	1
3242	C	67.99600	85.28580	68.92090	708.24611	-228.72943	526.80291	1
3243	H	67.37700	84.47980	69.36990	-251.79211	455.35365	-3102.81808	1
3244	H	67.44000	86.22080	69.14890	1246.12225	1387.32933	-2533.91454	1
3245	C	69.31100	85.50480	69.70890	-365.77845	-822.03664	-148.03005	1
3246	O	69.83300	86.60280	69.87390	-771.92348	-136.28462	95.85342	1
3247	N	70.01700	84.39780	70.10590	430.88271	-474.21138	-549.66895	1
3248	H	69.81800	83.47480	69.77790	1631.46249	1462.02418	-2258.10577	1
3249	H	70.95200	84.61280	70.38790	-1617.99244	-2635.09471	580.17461	1
3250	C	68.01400	82.64180	67.17590	-681.98160	-75.25730	-600.57343	1
3251	O	68.15500	81.79780	68.04290	503.60685	290.79634	534.27039	1
3252	N	67.09000	82.50080	66.23490	-542.00045	99.79091	-639.49165	1
3253	H	67.03700	83.21580	65.54290	-1827.24928	1527.47529	2055.77371	1
3254	C	66.19800	81.42780	66.04390	-649.22657	631.11082	107.95832	1
3255	H	65.61500	81.36480	66.95090	-749.82018	2991.41556	622.43786	1
3256	C	65.20800	81.57280	64.87290	376.31415	-425.96708	-713.01523	1
3257	H	64.70000	82.55680	64.95890	712.68056	-2278.81910	-2048.73038	1
3258	H	65.78400	81.60080	63.92390	-2781.34911	1454.07416	-219.07002	1
3259	C	64.14300	80.54880	64.85190	197.69820	-878.72599	142.15153	1
3260	C	64.10100	79.51580	63.85590	-289.94759	-542.79390	672.87159	1
3261	H	64.80100	79.56380	63.03490	2747.58171	331.57114	1496.35610	1
3262	C	63.15900	78.47080	63.93090	616.79588	321.75980	589.47814	1
3263	H	63.17600	77.65880	63.21990	2085.84444	1593.50673	-1734.42080	1
3264	C	62.29400	78.35380	65.04990	334.18835	-806.48764	263.33788	1
3265	H	61.65200	77.48780	65.10490	-1195.28903	-2707.66152	1066.80806	1
3266	C	63.23200	80.41480	65.92290	655.30633	-207.67647	599.07854	1
3267	H	63.26300	81.05080	66.79490	-1807.55544	938.41900	2397.98652	1
3268	C	62.34100	79.34080	66.02690	-637.91715	628.11748	-173.15066	1
3269	H	61.57100	79.40480	66.78190	-2428.13455	820.79013	1824.47044	1
3270	C	66.93500	80.04880	65.78090	195.05360	-792.53318	-406.56642	1
3271	O	66.63200	79.06580	66.49690	52.23850	680.28599	-397.62964	1
3272	N	67.94200	79.96780	64.95690	-147.37618	-825.15603	100.34977	1
3273	H	68.28900	80.79880	64.52890	641.78635	-2949.29133	887.70332	1
3274	C	68.76200	78.73780	64.76490	-283.59104	413.20314	761.76787	1
3275	H	68.18600	77.88280	64.44390	893.12959	-331.38519	-2998.45454	1
3276	C	69.92700	79.06480	63.73590	-20.02066	736.77696	-536.85183	1
3277	H	70.79800	79.64880	64.10390	720.16800	-286.26712	-3049.20242	1
3278	H	69.47600	79.59580	62.87090	-1766.34439	2477.45026	800.30865	1
3279	C	70.63800	77.74080	63.25190	-567.84164	-695.72988	-158.00889	1
3280	H	69.81100	77.09780	62.88090	1469.65111	2639.96115	-876.90192	1

3281	H	71.15600	77.18480	64.06190	1330.39681	2323.18840	1652.59379	1
3282	C	71.61500	77.98280	62.06390	-173.31241	676.02989	-586.85382	1
3283	O	71.30400	77.62580	60.88590	253.19284	748.00484	-3.06174	1
3284	N	72.76000	78.65180	62.30290	-756.73621	248.18430	280.04847	1
3285	H	73.02500	78.74080	63.26290	-76.03550	1762.26803	2605.15954	1
3286	H	73.53400	78.74680	61.67590	-1129.91214	2023.67923	-2127.49787	1
3287	C	69.42700	78.31480	66.03490	-551.28833	-311.69731	656.03123	1
3288	O	69.49300	77.10380	66.30090	607.35783	152.72270	481.06078	1
3289	N	69.91900	79.24580	66.90290	444.31337	-385.07350	-605.78570	1
3290	H	69.86900	80.20080	66.61990	2595.52861	35.76156	-1777.68910	1
3291	C	70.55000	78.86580	68.12590	-784.14317	-52.59372	462.38987	1
3292	H	71.32000	78.13480	67.92590	-462.13645	-2699.23387	1548.80362	1
3293	C	71.25000	80.09480	68.80590	197.12909	890.15955	14.39087	1
3294	H	71.58700	79.73080	69.79990	2746.32061	303.57606	-1504.58994	1
3295	H	70.61000	80.97980	69.01290	-3097.61543	-546.90067	-62.48631	1
3296	N	73.40700	81.20880	68.59690	-209.07347	622.14253	530.94185	1
3297	H	73.43300	81.28880	69.59390	-2040.68413	1011.31339	2170.50219	1
3298	C	72.35200	80.62980	68.01290	-248.12391	564.18458	-671.99799	1
3299	C	74.26900	81.55580	67.58590	-155.31937	-898.50238	-4.51232	1
3300	H	75.19500	82.08080	67.81790	973.62003	-220.44013	2983.57108	1
3301	N	73.76200	81.31280	66.40590	163.43278	-152.13122	814.13642	1
3302	C	72.56300	80.67780	66.66290	684.80954	300.46282	-521.73651	1
3303	H	72.02400	80.25780	65.82290	1199.36856	-2026.37391	-2086.51625	1
3304	C	69.64000	78.25780	69.17190	-747.16856	355.58843	383.07573	1
3305	O	70.02400	77.39280	69.98090	-534.25265	-579.67242	46.70353	1
3306	N	68.39300	78.68480	69.17490	45.48387	-842.94896	6.36779	1
3307	H	68.03400	79.38880	68.56790	-2083.58571	1357.88664	-1926.92519	1
3308	C	67.34400	78.10680	69.99190	-486.39842	359.06583	682.59747	1
3309	H	67.88300	77.80780	70.87890	1823.64178	-2248.54392	-1231.50603	1
3310	C	66.26800	79.14380	70.38190	354.39673	-755.01887	-368.51114	1
3311	H	65.65100	79.44880	69.50990	-1685.12818	2208.34413	1477.08682	1
3312	C	65.27500	78.49980	71.45990	818.16250	369.91638	158.81751	1
3313	H	65.85400	78.09680	72.31790	-704.60158	2358.52233	1959.37114	1
3314	H	64.71300	77.63880	71.03790	-1922.40656	1060.30325	-2253.51642	1
3315	H	64.49100	79.19980	71.82090	966.05373	2011.63690	2217.72032	1
3316	C	66.88300	80.46080	70.88990	578.45802	-638.70251	298.15505	1
3317	H	67.63100	80.93980	70.22190	1961.27994	-586.94183	-2388.95511	1
3318	H	67.49200	80.42380	71.81890	-2311.42056	1813.39268	1125.68567	1
3319	C	65.83800	81.51180	71.27090	-829.22184	-344.94732	-157.64989	1
3320	H	65.02200	81.53180	70.51890	1146.57994	789.58334	-2821.37180	1
3321	H	65.46700	81.24480	72.28390	429.82659	-2165.50649	-2241.44083	1
3322	H	66.38100	82.47880	71.20490	-2331.25248	-1872.54511	-978.29592	1
3323	C	66.76900	76.84280	69.45490	-340.18826	610.30084	-585.88040	1
3324	O	66.63400	75.81380	70.12590	101.89568	-622.84987	474.66044	1
3325	N	66.31500	76.98580	68.18590	158.99257	828.45462	32.50530	1
3326	H	66.41500	77.87280	67.74190	-2616.55087	-325.30913	-1716.40955	1
3327	C	65.74200	75.94280	67.37790	151.60799	-222.65958	-871.14220	1
3328	H	64.79300	75.72480	67.84490	332.72533	2444.91621	1951.89775	1
3329	C	65.55500	76.47180	65.99690	516.47904	744.65398	100.94974	1
3330	H	65.01800	77.43680	65.87590	-2309.33922	-1649.80974	1357.68420	1
3331	H	66.57200	76.68280	65.60290	-2378.86400	1325.20877	1575.77093	1
3332	C	64.89500	75.49180	64.95890	699.04891	-87.30804	578.92913	1
3333	H	65.50600	74.59380	64.72490	1876.96401	-2499.29325	358.83921	1
3334	H	64.58300	76.09980	64.08290	-1213.58057	2898.57565	153.97275	1
3335	S	63.30800	74.83580	65.62490	416.23263	-317.43383	192.86463	1
3336	C	62.41500	74.52080	64.05090	-723.11660	534.39399	151.57985	1
3337	H	61.57500	73.84080	64.30990	1894.43547	-1399.81738	-2085.62983	1
3338	H	63.09600	74.03980	63.31690	1019.44980	2208.15760	1995.74255	1
3339	H	62.01300	75.46580	63.62590	-1982.24411	1150.22911	2155.43673	1
3340	C	66.62700	74.71180	67.33690	574.44850	-552.29807	-443.20059	1
3341	O	66.22400	73.62780	67.63590	488.90100	-608.17075	121.37288	1
3342	N	67.94400	74.80680	67.04190	412.83426	217.61314	703.48041	1

3343	H	68.38100	75.69680	66.93390	-1566.75032	1034.45141	2524.56529	1
3344	C	68.78100	73.65580	66.86890	-596.84400	82.97288	684.35644	1
3345	H	68.16600	72.78480	66.69290	1497.15614	726.10748	2670.11566	1
3346	C	69.72500	73.87980	65.70990	-175.62620	-821.42401	-354.78026	1
3347	H	70.51200	74.64080	65.89490	2171.35181	2255.82464	-307.75434	1
3348	C	70.49500	72.60180	65.37190	378.51733	52.02063	-827.93085	1
3349	H	71.16400	72.77680	64.50290	-1830.41880	-1926.89381	1683.70826	1
3350	H	71.16100	72.19280	66.16290	-1694.63056	-1036.21179	-2439.81938	1
3351	H	69.76400	71.82480	65.06090	1340.02925	2669.43549	-988.26212	1
3352	C	69.01400	74.34080	64.41390	-814.01391	-209.93561	-353.21297	1
3353	H	68.75000	75.40280	64.60590	-2507.13629	1875.32597	309.26749	1
3354	H	69.68600	74.31480	63.52990	-1945.45291	-2290.22985	-931.81889	1
3355	H	68.06000	73.80680	64.21390	2327.78054	2116.14265	40.05353	1
3356	C	69.60800	73.28180	68.10590	732.54018	-357.93091	408.31525	1
3357	O	69.97600	72.13480	68.30190	1.35383	-550.82225	-565.88006	1
3358	N	69.88600	74.25980	68.99390	363.03646	-731.62391	213.54921	1
3359	H	69.62600	75.21180	68.84890	1755.34152	-2608.48845	-113.09448	1
3360	C	70.53000	73.95480	70.25190	897.70081	-103.05256	-122.32915	1
3361	H	70.92300	74.92080	70.53490	-36.69836	-2570.59466	-1813.53869	1
3362	H	71.34000	73.25280	70.12490	2707.14142	1502.01009	559.97968	1
3363	C	69.62700	73.38380	71.24690	-455.10011	563.46771	553.93053	1
3364	O	70.00600	72.62580	72.09890	-186.37563	-688.24524	339.42575	1
3365	N	68.35400	73.82580	71.22490	311.11183	604.43295	500.54223	1
3366	H	67.99000	74.44980	70.53890	1526.07374	630.11928	-2678.11031	1
3367	C	67.42000	73.44580	72.28490	488.89665	-662.84659	-391.23583	1
3368	H	67.91200	72.76780	72.96590	-202.70806	-176.52103	-3134.64129	1
3369	C	66.91300	74.68680	73.11490	284.28868	637.56471	586.63634	1
3370	H	66.12200	75.16780	72.50090	636.15078	1541.45354	-2667.85671	1
3371	H	67.73000	75.39380	73.37290	-1152.87383	-1009.69575	-2747.65767	1
3372	C	66.30000	74.35180	74.45690	529.35420	598.48763	-439.37193	1
3373	H	65.60900	73.48980	74.34190	-1404.50143	1893.60025	2083.23788	1
3374	C	67.30900	73.99080	75.58390	-356.46527	191.87426	-817.04821	1
3375	H	67.94500	74.88180	75.77790	-2886.42813	-572.73393	1112.98460	1
3376	H	67.87700	73.11080	75.21290	1554.72610	1907.30855	1960.41503	1
3377	H	66.84500	73.70680	76.55190	1700.32173	-1757.92658	1979.09737	1
3378	C	65.46100	75.57580	74.92890	-556.85359	-709.22100	135.53838	1
3379	H	66.10500	76.45080	75.16190	2764.59040	962.11966	1153.07932	1
3380	H	64.93300	75.42080	75.89390	-647.66229	-1903.03744	-2420.16700	1
3381	H	64.70300	75.83080	74.15790	-726.31647	962.86753	-2905.78333	1
3382	C	66.18200	72.68480	71.76890	-551.55292	145.25812	-711.43549	1
3383	O	65.92800	71.57280	72.17990	660.67273	-87.87243	423.57669	1
3384	N	65.43300	73.25880	70.81490	350.86310	-95.77548	-761.83622	1
3385	H	65.71600	74.14280	70.44990	-1155.90570	2419.27216	1645.97402	1
3386	C	64.18200	72.72380	70.30190	-367.08880	-590.07583	590.34509	1
3387	H	63.58800	72.69080	71.20390	-2345.06017	1344.25605	-1609.93625	1
3388	C	63.33000	73.64380	69.47090	-881.45777	-148.18660	-180.34394	1
3389	H	63.72500	73.82480	68.44790	-1263.21552	-2863.19262	-323.48226	1
3390	C	61.92300	73.14780	69.18390	-162.98024	889.47281	-117.16040	1
3391	H	61.36800	72.94880	70.12590	1868.77692	2273.08058	1113.10544	1
3392	H	61.30500	73.85280	68.58890	-2062.91018	1098.60995	-2106.10635	1
3393	H	61.96700	72.21880	68.57590	2163.49839	-1231.78059	-1923.59494	1
3394	C	63.22400	75.10980	70.05690	-710.87993	-201.85737	534.18567	1
3395	H	62.72800	74.93580	71.03590	-1722.85908	-2220.69218	-1413.68633	1
3396	H	64.20300	75.58080	70.29190	74.49284	-2991.69774	-970.78406	1
3397	C	62.38800	76.05980	69.16990	-901.93412	-89.79683	-99.51065	1
3398	H	62.69600	75.86280	68.12090	-2194.98692	-1319.68458	-1827.20860	1
3399	H	62.61200	77.12580	69.38790	-2958.87587	943.55482	502.97527	1
3400	H	61.29600	75.86780	69.23290	615.59011	228.60696	-3076.85130	1
3401	C	64.17900	71.32780	69.69790	615.77418	-500.64708	449.02746	1
3402	O	63.61300	70.39280	70.22690	672.86755	410.51495	-48.51765	1
3403	N	64.84000	71.21580	68.46890	30.93819	-690.30030	-484.97486	1
3404	H	65.25800	71.95580	67.94690	2834.41771	-1125.42655	773.12196	1

3405	C	64.86800	69.95580	67.69390	598.91025	-664.56113	176.39734	1
3406	H	63.81200	69.72680	67.68790	-2265.49285	-1205.97625	1819.72241	1
3407	C	65.36600	70.19380	66.22890	-475.69890	749.97196	206.64852	1
3408	H	66.39600	70.60980	66.18990	1947.96506	-2077.23152	1337.44816	1
3409	H	65.22500	69.21180	65.72890	-1103.00333	-1704.59296	2403.32535	1
3410	C	64.53200	71.18780	65.44590	645.79796	-525.54372	-371.75234	1
3411	H	64.74800	72.23680	65.73890	1034.52187	-432.58778	-2939.53373	1
3412	C	64.82900	71.16480	63.94490	-193.44510	495.40262	740.67958	1
3413	H	64.37600	72.06480	63.47790	1030.41163	-2830.14617	-909.25835	1
3414	H	64.51100	70.21780	63.45690	-1788.09069	1872.10513	-1787.78642	1
3415	H	65.92000	71.13280	63.73590	-2319.69691	430.01972	2081.42152	1
3416	C	63.01800	70.99680	65.50990	337.28319	463.18300	-709.33247	1
3417	H	62.67500	69.94880	65.36790	-2169.81831	-2099.82564	883.65550	1
3418	H	62.52000	71.27080	66.46390	1287.11327	-1973.07056	2085.31969	1
3419	H	62.58300	71.55980	64.65590	933.05301	2308.53467	-1923.09802	1
3420	C	65.59900	68.81180	68.33190	-487.30356	405.89265	-655.16212	1
3421	O	65.01500	67.77580	68.08990	51.76259	752.96699	-232.35441	1
3422	N	66.67700	68.82680	69.08290	716.34479	-416.55290	161.26411	1
3423	C	67.51000	69.99280	69.37990	-313.75432	-698.84754	494.59211	1
3424	H	67.00000	70.92280	69.70990	-1118.00607	2940.43275	46.30239	1
3425	H	68.07300	70.27080	68.46290	344.03567	2906.48788	-1154.20703	1
3426	C	67.20100	67.63480	69.73590	-534.45817	709.77158	205.01164	1
3427	H	67.07000	66.78880	69.07690	-857.55567	3023.80252	139.43755	1
3428	C	68.66500	68.04580	70.17490	481.33696	391.24665	668.35005	1
3429	H	69.12400	67.49880	71.02590	-2140.94963	-2003.45149	1140.50123	1
3430	H	69.38400	67.82280	69.35690	672.80993	2140.77173	2205.14159	1
3431	C	68.55100	69.51580	70.42490	-696.14943	-406.90384	-425.74198	1
3432	H	69.49600	70.06980	70.24090	-962.55716	2608.97393	1471.38199	1
3433	H	68.18300	69.79180	71.43690	-2261.40855	-1927.18248	-1034.51694	1
3434	C	66.39300	67.26680	71.00390	-453.74341	739.56402	280.38006	1
3435	O	66.32900	66.10480	71.31490	-137.54694	639.53244	442.38708	1
3436	N	65.84600	68.26680	71.68190	525.19233	644.56059	-146.24280	1
3437	H	65.99600	69.19580	71.35290	2330.43331	683.90243	-1999.89607	1
3438	C	64.95700	68.17180	72.79490	399.79504	-677.76227	460.70949	1
3439	H	64.63100	69.17880	73.00590	2056.58315	1120.06637	2100.98627	1
3440	H	65.55800	67.86280	73.63690	1733.48591	94.92812	-2623.78381	1
3441	C	63.76000	67.32980	72.57190	-10.08677	-839.03243	-356.89472	1
3442	O	63.42600	66.47880	73.44190	-437.01769	-217.15932	-620.87406	1
3443	N	63.06200	67.53680	71.42990	766.41190	160.47857	315.48648	1
3444	H	63.28600	68.31780	70.85290	-1861.68302	1369.43190	2134.71751	1
3445	C	61.89500	66.79280	71.11990	134.00087	-583.58071	687.69784	1
3446	H	61.24900	66.80980	71.98490	-1363.52244	-2722.36357	-792.31898	1
3447	C	61.08100	67.31480	69.93990	593.24576	-688.29568	-75.89158	1
3448	H	60.31700	66.55780	69.66190	1194.47358	2577.93466	-1351.18910	1
3449	C	60.20100	68.50380	70.43690	-62.19399	-708.20101	570.99408	1
3450	H	59.64400	68.05180	71.28490	1664.45034	1183.95113	2392.92520	1
3451	H	59.37700	68.71880	69.72290	-665.70437	3054.70418	-351.91805	1
3452	H	60.89200	69.32080	70.73390	1496.61065	-1903.13702	-2009.09239	1
3453	C	61.97000	67.64580	68.73790	-4.01097	820.47718	-397.80915	1
3454	H	62.59600	68.53580	68.96190	-5.14008	-236.63247	3137.22885	1
3455	H	62.67200	66.81080	68.52690	1511.82584	-448.24004	2722.44187	1
3456	C	61.18200	67.81180	67.43490	-828.62534	-319.95147	-206.06334	1
3457	H	61.83300	68.03080	66.56190	2986.70743	-737.51338	-658.69488	1
3458	H	60.42100	68.61980	67.48290	1471.44982	615.18607	2711.93800	1
3459	H	60.54100	66.91780	67.27590	1969.38797	-2313.68546	816.45382	1
3460	C	62.10100	65.27780	70.85890	542.50498	-411.58330	606.41449	1
3461	O	61.32600	64.41780	71.31790	-90.26999	-196.22098	-759.58929	1
3462	N	63.17400	64.90480	70.18990	-117.44128	375.04606	747.14141	1
3463	H	63.73500	65.66780	69.88090	734.43151	-2823.65248	-1177.20995	1
3464	C	63.66700	63.56780	70.06490	-589.92492	639.39638	-273.15172	1
3465	H	62.88200	62.91180	69.71890	1868.20173	2187.26408	-1274.33290	1
3466	C	64.85000	63.46980	69.11790	73.22357	-747.66018	516.81095	1

3467	H	65.76400	63.92480	69.55590	-60.91869	-1130.28062	-2935.46945	1
3468	C	65.11100	61.98380	68.79790	588.28790	-568.72396	-402.39460	1
3469	H	65.53400	61.39180	69.63790	2129.49122	1687.30096	1586.35080	1
3470	H	65.93800	61.98080	68.05590	869.28117	-2724.29525	1311.78956	1
3471	H	64.16200	61.56580	68.39990	-1383.60622	-1787.62488	-2188.20871	1
3472	C	64.66600	64.18280	67.82090	-511.99294	745.72906	114.90170	1
3473	H	64.71900	65.29080	67.87690	1588.00486	-188.69905	-2709.40205	1
3474	H	65.40800	63.84580	67.06590	1800.67259	-1935.62399	1705.62723	1
3475	H	63.66800	64.06080	67.34590	1347.81269	2032.19053	-1987.92073	1
3476	C	64.06000	63.02280	71.47490	-1.70514	752.11570	-515.52892	1
3477	O	63.68600	61.86980	71.71690	714.84410	-93.59885	-322.27999	1
3478	N	64.69800	63.81880	72.35490	551.30940	-398.39206	500.01400	1
3479	H	64.92200	64.75380	72.09190	1065.39191	2431.51348	-1688.46336	1
3480	C	64.99500	63.39580	73.70990	84.22080	855.54583	-303.97236	1
3481	H	65.58600	62.49180	73.72390	-1378.58275	-2174.01324	-1808.70182	1
3482	C	65.90700	64.41680	74.47290	-548.75752	-723.60389	81.93657	1
3483	H	65.40800	65.40280	74.35890	-798.90751	-3003.86307	486.60013	1
3484	C	65.96600	64.10380	75.97690	121.52595	468.18448	772.97202	1
3485	H	64.99500	64.04380	76.51390	1064.66948	1358.25911	-2630.55837	1
3486	H	66.52400	63.15380	76.11390	728.27879	-2508.23114	1754.02759	1
3487	H	66.62700	64.80880	76.52590	-2157.82906	216.12575	2279.31780	1
3488	C	67.28900	64.30380	73.77390	749.51981	-457.40855	-245.86273	1
3489	H	67.15200	64.24880	72.67190	-420.13663	-1908.78261	-2465.41282	1
3490	H	67.80800	63.36280	74.05590	1292.12572	-2513.34894	-1382.64763	1
3491	C	68.16400	65.49680	74.02690	-394.49375	463.21539	-679.15918	1
3492	H	67.70100	66.33980	73.47090	2086.51082	1736.69889	-1590.14961	1
3493	H	68.23500	65.67980	75.11990	2822.74157	-548.77616	1276.40157	1
3494	H	69.22100	65.29580	73.74790	1926.09764	-1485.74778	1995.22621	1
3495	C	63.73700	63.05580	74.48490	493.45836	-499.32038	-581.91839	1
3496	O	63.59500	61.94380	75.01890	-732.30512	90.81087	281.26470	1
3497	N	62.71100	63.97680	74.42690	-388.37517	-500.86328	-557.64953	1
3498	H	62.97700	64.85880	74.04390	1950.96197	-1152.01113	-2182.85226	1
3499	C	61.40000	63.89880	75.00690	-65.73122	687.61042	595.24979	1
3500	H	61.51400	63.67880	76.05790	-1951.21468	1538.10409	-1930.08375	1
3501	C	60.66100	65.21180	74.74190	522.64942	726.40915	-174.98094	1
3502	H	60.92700	65.60280	73.73690	-1874.72242	1772.08866	-1800.92861	1
3503	H	59.56300	65.07380	74.83190	-3107.24857	303.11924	-389.03888	1
3504	C	61.13800	66.33980	75.75290	-526.39631	-297.91956	682.35025	1
3505	H	62.24600	66.39680	75.69090	-1296.29539	1075.82747	-2657.14880	1
3506	C	60.60400	67.72780	75.32790	559.65290	571.52751	-437.71674	1
3507	H	60.92600	68.06380	74.31990	2176.88016	889.15141	2090.17434	1
3508	H	59.49500	67.79180	75.33190	-1717.87920	-2187.24171	-1470.74505	1
3509	H	60.93400	68.51280	76.04190	939.06574	2087.33093	-2158.57160	1
3510	C	60.79400	66.15080	77.20290	793.52293	-219.55549	-391.87721	1
3511	H	61.31900	65.24480	77.57390	-581.17914	1168.77396	-2862.59051	1
3512	H	60.95400	67.10180	77.75390	-2954.60589	506.49745	954.98199	1
3513	H	59.72800	65.90580	77.39990	1752.84334	232.71534	2602.23174	1
3514	C	60.68300	62.63780	74.55090	-422.82354	680.47202	435.46422	1
3515	O	60.15800	61.87580	75.38690	507.75188	597.42849	-94.31041	1
3516	N	60.66600	62.35580	73.27790	-572.47222	389.58514	482.87811	1
3517	H	61.20100	62.96480	72.69590	1749.94152	-2014.18665	-1667.02820	1
3518	C	60.10100	61.11180	72.65490	146.14881	299.24040	-848.85023	1
3519	H	59.04500	61.08180	72.87990	778.60536	-2130.16337	2180.45957	1
3520	C	60.12500	61.11180	71.07890	-81.54435	640.83186	643.53403	1
3521	H	59.92400	60.10280	70.65790	2240.83455	-2098.16604	688.90203	1
3522	H	61.15700	61.42380	70.81190	1734.81488	-2487.23910	-838.02460	1
3523	O	59.30200	62.05380	70.45490	-354.37435	-48.53850	704.05260	1
3524	H	58.40200	61.85880	70.72590	-972.02832	2985.12033	-206.01886	1
3525	C	60.70300	59.78680	73.11590	596.28258	-631.56435	277.53299	1
3526	O	59.91400	58.83680	73.29290	-337.54624	-10.70752	713.84530	1
3527	N	62.04400	59.67780	73.24190	215.16837	-355.06463	-735.05372	1
3528	H	62.55400	60.48180	72.94690	-1113.47260	-2283.51931	-1855.78678	1

3529	C	62.74300	58.45280	73.65390	-412.71609	-249.10353	773.99216	1
3530	H	62.41300	57.69680	72.95690	-618.05730	2898.96796	-1054.61660	1
3531	C	64.26900	58.73380	73.87290	-728.96113	259.56186	482.38398	1
3532	H	64.76100	57.78280	74.17290	901.55280	931.36218	-2866.70425	1
3533	H	64.35500	59.49580	74.67690	-1452.49062	-2621.83855	956.27393	1
3534	S	64.98900	59.21680	72.26490	-194.13488	-76.32355	517.39441	1
3535	H	64.69800	60.50780	72.31790	-681.37477	-1452.89683	2706.11261	1
3536	C	62.19100	57.92080	74.99590	116.85271	739.49730	-520.51915	1
3537	O	61.86400	56.75380	75.16990	182.68119	593.14954	488.29135	1
3538	N	62.14600	58.80680	76.01990	45.70287	804.95113	-250.27427	1
3539	H	62.48500	59.73680	75.89890	-674.89009	-2327.51731	-2006.34313	1
3540	C	61.69700	58.38880	77.38590	-740.98950	-479.25022	-229.57526	1
3541	H	62.07100	57.41880	77.67990	-2645.96527	1517.62944	770.64577	1
3542	C	62.30100	59.29480	78.44190	757.50892	468.49620	-195.30118	1
3543	H	61.96400	58.85080	79.40290	2406.12827	1321.26137	-1537.21872	1
3544	H	61.85500	60.29480	78.25690	2782.91557	1102.01246	969.11076	1
3545	C	63.83700	59.35180	78.28390	-803.14102	140.99230	408.08906	1
3546	C	64.38900	60.56680	77.83490	569.90361	535.86548	-468.51795	1
3547	H	63.80300	61.43580	77.57490	901.26748	2307.51083	1939.41664	1
3548	C	65.78200	60.60780	77.65190	-37.77197	-597.50180	-687.76150	1
3549	H	66.16600	61.51380	77.20790	-904.88168	1353.36004	2692.17978	1
3550	C	66.60500	59.53580	77.92290	-817.15962	-16.96333	-404.24424	1
3551	O	67.97300	59.58680	77.66090	-653.44068	-391.55089	208.15958	1
3552	H	68.15200	60.22280	76.96390	1760.09192	-2576.95817	-399.48619	1
3553	C	64.61200	58.27280	78.57190	-385.75690	437.13966	701.10737	1
3554	H	64.11800	57.43480	79.04090	2260.45440	-996.47659	1948.23164	1
3555	C	66.01500	58.33080	78.34490	-476.74657	-368.24947	684.51153	1
3556	H	66.62900	57.44280	78.37690	958.68698	-2912.64048	-704.03901	1
3557	C	60.22600	58.36380	77.44290	40.66128	834.47524	-365.30637	1
3558	O	59.63100	57.65280	78.25890	-322.55860	526.28303	-492.55391	1
3559	N	59.50100	59.13780	76.59090	188.73066	-563.22900	-599.85508	1
3560	H	59.91300	59.78880	75.95890	-2203.55087	1691.57533	1476.87599	1
3561	C	58.09000	58.99580	76.38390	-901.54697	-95.99147	97.20962	1
3562	H	57.66200	59.15280	77.36290	1913.20878	-2197.06582	1187.75425	1
3563	C	57.49900	60.00280	75.39790	-3.91098	-816.22786	406.45762	1
3564	H	57.89000	60.99280	75.71490	-1932.81911	-1896.28298	-1602.04474	1
3565	H	57.90100	59.81880	74.37790	730.76234	-3020.63486	489.87516	1
3566	S	55.72300	60.08580	75.22290	-8.62032	-298.44196	471.24165	1
3567	H	55.62900	59.09380	74.34990	-2337.76039	1913.19876	879.07513	1
3568	C	57.68600	57.57480	75.97290	-725.82512	212.06652	-509.56519	1
3569	O	56.79800	56.98380	76.56690	-675.41180	-371.42640	-171.72231	1
3570	N	58.36000	56.95880	75.04090	12.16073	-815.10765	-219.37167	1
3571	H	58.91300	57.53180	74.44090	-727.88212	2445.23033	1840.99497	1
3572	C	58.10400	55.59180	74.61790	-590.94656	130.60970	682.03685	1
3573	H	57.05600	55.50580	74.37190	1979.92371	-2441.04385	-139.40326	1
3574	C	58.88400	55.19280	73.32890	626.26332	-583.85032	-313.63045	1
3575	H	59.96700	55.39580	73.47690	-2093.11751	1786.25521	-1525.24674	1
3576	C	58.75700	53.70380	73.07890	-704.92997	108.48903	568.11519	1
3577	H	59.12800	53.48880	72.05390	2482.17114	1404.67173	-1328.13778	1
3578	H	59.29400	53.04680	73.79590	2783.72384	-1395.70830	-448.44861	1
3579	H	57.68400	53.41180	73.07590	2819.67443	1395.41107	22.14147	1
3580	C	58.35700	55.95380	72.10590	625.30349	-64.59327	-660.51060	1
3581	H	57.42400	55.51380	71.69390	1383.39231	2825.00579	-61.59749	1
3582	H	58.03500	56.99480	72.32590	2392.04041	2043.19427	41.54653	1
3583	C	59.39500	56.11680	70.97890	697.09019	-527.59108	-259.16004	1
3584	H	59.93700	55.16780	70.78090	1909.84300	-1424.44627	2054.67242	1
3585	H	59.03200	56.60880	70.05190	1920.85389	178.12630	2485.32042	1
3586	H	60.04100	56.97780	71.25290	2526.20734	1579.75436	1010.38550	1
3587	C	58.48800	54.59080	75.69290	-672.90234	35.56105	-614.31983	1
3588	O	57.74000	53.60180	75.90990	-478.48117	-400.52770	-484.00470	1
3589	N	59.64700	54.78980	76.37390	-594.65392	-518.80353	-299.83646	1
3590	H	59.99800	55.71780	76.27190	-2801.41960	-1160.56416	838.66875	1

3591	C	60.34200	53.84080	77.29690	-465.92880	-632.01678	-463.59049	1
3592	H	60.57700	52.90980	76.80290	2104.64880	-1398.78162	-1874.05700	1
3593	C	61.81500	54.30380	77.78890	563.73452	-478.79226	533.30326	1
3594	H	61.72400	55.38780	78.01790	-180.62567	2661.80876	-1667.44557	1
3595	C	62.20200	53.43880	79.01190	-735.72828	495.54516	211.16321	1
3596	H	62.13300	52.35980	78.75490	1744.68210	1919.39457	1780.51539	1
3597	H	63.25500	53.63080	79.30990	-2455.01550	-1863.10778	-632.41956	1
3598	H	61.54700	53.49980	79.90690	-3074.15489	510.41792	-432.74879	1
3599	C	62.82100	54.15980	76.66190	-535.57079	392.91337	-624.68714	1
3600	H	62.32800	54.42880	75.70290	2535.16225	-1816.52634	-414.01766	1
3601	H	63.23200	53.13380	76.55490	637.95677	-2996.20685	-716.92531	1
3602	C	64.08400	54.91880	76.90390	-180.83755	852.62476	267.91753	1
3603	H	63.83200	55.97580	77.13390	-2162.95064	-237.77774	-2272.29675	1
3604	H	64.72100	54.56480	77.74290	-681.95603	-2936.95997	-898.57017	1
3605	H	64.80100	54.81880	76.06190	-102.88974	-380.35460	-3121.37314	1
3606	C	59.39500	53.38480	78.45890	365.42209	-771.75666	319.85834	1
3607	O	59.23700	52.19880	78.85690	-130.96376	-582.10112	-517.33356	1
3608	N	58.74100	54.39080	79.02790	-580.04826	-497.83537	358.29632	1
3609	H	58.82900	55.33080	78.70690	-2465.17050	1949.98831	136.77065	1
3610	C	57.95400	54.24980	80.20890	552.93237	-538.66922	485.33727	1
3611	H	58.55600	53.66780	80.89190	-1936.24275	1681.77355	1822.31390	1
3612	C	57.67700	55.58980	80.88790	-544.96510	524.50920	-509.26825	1
3613	H	57.07200	55.33580	81.78590	2316.46170	-1887.20468	-985.23598	1
3614	C	58.98100	56.16480	81.44990	634.75023	581.47036	300.72474	1
3615	H	58.79600	57.04280	82.10490	2074.77167	-1603.44444	1738.53809	1
3616	H	59.55900	55.40180	82.01390	-3027.53279	730.20764	-446.17064	1
3617	H	59.56000	56.60080	80.60790	492.25962	-3013.89594	756.53021	1
3618	C	56.89100	56.57580	80.03690	-735.50513	-67.82815	-534.67985	1
3619	H	57.59600	57.08480	79.34490	-2011.17990	2111.92388	1180.32164	1
3620	H	56.23000	55.99780	79.35490	-1755.26170	1810.64938	1881.17820	1
3621	C	56.10400	57.58680	80.84990	614.68626	74.55363	669.36803	1
3622	H	55.43400	57.04080	81.54790	2510.66828	1886.50010	189.44233	1
3623	H	55.39900	58.12580	80.18290	-12.55402	61.42276	-3145.51997	1
3624	H	56.80600	58.30380	81.32690	2078.87938	-1735.19968	1601.73931	1
3625	C	56.78400	53.35880	80.02290	-743.53414	511.49723	-130.30185	1
3626	O	56.23600	52.76380	80.96890	588.39911	524.92125	43.25962	1
3627	N	56.27700	53.27880	78.79190	13.28607	588.62638	604.99153	1
3628	H	56.73500	53.86180	78.12490	946.06818	-1978.89572	2255.47178	1
3629	C	55.13000	52.49880	78.47790	-295.89285	791.67877	-342.26182	1
3630	H	54.47900	52.42980	79.33690	843.43458	1701.42202	2508.38742	1
3631	C	54.26500	53.22480	77.40490	754.02901	511.08116	-41.07688	1
3632	H	53.70300	54.02080	77.93790	-1909.60232	-2485.84722	268.71691	1
3633	H	53.51500	52.55080	76.93890	-2511.76953	-1578.68953	1047.36786	1
3634	O	55.06400	53.77880	76.36790	-400.51945	635.55216	-243.48482	1
3635	H	55.77900	53.17280	76.16290	126.75732	3123.91475	351.16297	1
3636	C	55.34500	51.08080	78.13790	729.63697	-446.46594	315.83076	1
3637	O	54.38400	50.33480	77.74290	442.93773	-651.90520	-49.52781	1
3638	N	56.56600	50.60580	78.30390	-107.75884	-765.91461	338.28262	1
3639	H	57.18900	51.23380	78.76590	-203.77245	1794.70073	-2575.99540	1
3640	C	56.93000	49.22180	78.07690	649.67172	-639.82059	2.69468	1
3641	H	56.17700	48.60980	78.54990	-1683.53299	-2008.38757	1740.78209	1
3642	C	56.90500	48.80080	76.58590	550.37529	503.16102	524.75426	1
3643	H	55.84500	48.89880	76.26890	-1913.41416	2467.82422	383.29633	1
3644	H	57.16400	47.73180	76.43290	1246.14911	2688.02245	1058.24095	1
3645	C	57.61500	49.74880	75.55590	-524.85807	656.88756	352.80837	1
3646	H	58.66700	49.92380	75.86590	53.68440	-3097.36282	-549.26111	1
3647	H	57.07500	50.71580	75.64090	813.94205	1730.01573	-2498.55361	1
3648	C	57.50000	49.15880	74.14190	-220.05618	494.47871	733.83724	1
3649	H	58.09000	49.79580	73.44890	-2571.25717	-1811.98947	59.64017	1
3650	H	58.01800	48.17680	74.12790	2258.20433	443.46897	-2145.24468	1
3651	C	56.08000	49.16180	73.63190	570.19697	-673.94438	228.30983	1
3652	H	55.39300	48.50380	74.20690	1472.61415	-1731.58635	-2175.14195	1

3653	H	55.70700	50.20880	73.64390	2314.10831	134.62230	-2127.20610	1
3654	N	56.00100	48.71280	72.26790	-364.77716	-342.77374	-679.79120	1
3655	H	56.26500	49.45680	71.59090	165.10505	-2618.56232	1736.11575	1
3656	H	55.01000	48.47780	72.05990	1485.64317	2105.19406	1805.33891	1
3657	H	56.61600	47.89280	72.09290	2555.77940	-661.07959	-1711.48814	1
3658	C	58.25800	48.62980	78.70690	530.68986	545.42282	502.32780	1
3659	O	58.67000	47.50480	78.41790	-483.71484	-550.91079	293.50382	1
3660	N	58.87400	49.39780	79.67090	-9.30974	-840.03168	83.26103	1
3661	H	58.55300	50.33080	79.81490	2297.01815	2051.55425	-642.69667	1
3662	C	60.05300	49.01480	80.43090	-738.17546	52.50969	532.72011	1
3663	H	60.85900	48.83280	79.73490	-210.22144	1446.03697	2786.21791	1
3664	C	60.48400	50.11080	81.40890	-591.45373	419.26880	-553.03451	1
3665	H	60.55300	51.07380	80.85790	-1981.72135	-900.86016	2271.44396	1
3666	H	59.62900	50.22680	82.10890	-1607.70201	-1667.68815	-2128.92854	1
3667	C	61.81200	49.86180	82.09690	-16.13933	55.14233	910.02739	1
3668	H	61.77700	48.88480	82.62590	487.95653	2621.51135	1669.67149	1
3669	C	62.94700	50.01980	81.06690	705.18292	-576.44655	-43.32926	1
3670	H	62.97300	51.01480	80.57190	-2305.40820	1828.95797	1112.75874	1
3671	H	62.94200	49.14980	80.37590	-378.26055	-366.92465	-3101.69494	1
3672	H	63.86500	49.83680	81.66490	2805.76968	1332.24762	-500.99800	1
3673	C	61.98100	50.95380	83.20990	-529.26154	-527.10529	-522.96582	1
3674	H	61.11500	50.89480	83.90290	-2600.06500	-10.89578	1771.37503	1
3675	H	62.95000	50.78680	83.72690	-2857.22398	-1163.83868	-616.42263	1
3676	H	62.00600	51.98380	82.79390	-1978.21852	-1094.01348	2188.15270	1
3677	C	59.83400	47.69080	81.19690	29.37427	590.26214	-694.39093	1
3678	O	60.73700	46.80980	81.21890	-395.33304	-155.10882	665.79296	1
3679	N	58.64700	47.46780	81.86090	190.50952	-793.34384	-216.75786	1
3680	H	57.93700	48.16280	81.93990	-2342.89876	-2093.71748	159.36980	1
3681	C	58.32400	46.20480	82.43990	-697.54255	580.86657	-86.48359	1
3682	H	59.16000	45.72380	82.92390	-135.59744	-1219.89506	2896.84235	1
3683	C	57.25300	46.40580	83.55490	439.01971	-366.94824	709.97302	1
3684	H	56.46500	47.09480	83.18390	-2983.55025	-793.80366	-605.41709	1
3685	H	56.84700	45.42880	83.89290	-1528.44556	2391.22976	-1357.97666	1
3686	O	57.79400	47.05480	84.72390	-58.33021	-271.59339	-739.23058	1
3687	H	58.33600	46.39680	85.16390	-3067.75475	-104.94495	689.99534	1
3688	C	57.74300	45.15880	81.47690	-760.62354	368.20265	-342.53415	1
3689	O	57.44700	44.02980	81.86390	658.98494	-55.19269	-431.64782	1
3690	N	57.64000	45.44880	80.18090	-27.63665	-200.09890	-819.67612	1
3691	H	57.87600	46.33480	79.79090	-2405.58554	1968.51410	486.14470	1
3692	C	57.07300	44.51080	79.22090	223.58277	529.74666	-707.69359	1
3693	H	56.64100	43.64980	79.70890	-2194.21227	2069.53962	894.79860	1
3694	C	55.93600	45.12680	78.34290	-518.88023	-145.33223	735.59014	1
3695	H	56.29600	45.99180	77.74590	2184.72905	100.66614	2261.64797	1
3696	H	55.54800	44.49680	77.51490	1248.43424	-602.57619	-2824.27692	1
3697	N	53.71900	46.31980	78.70290	-450.62011	535.76950	-471.76779	1
3698	H	53.67500	46.71180	77.78490	2145.22324	692.26068	-2194.77074	1
3699	C	54.76900	45.59380	79.19390	747.60014	320.33242	412.22830	1
3700	C	52.84700	46.50780	79.73890	-653.78111	361.98540	522.48238	1
3701	H	51.89400	47.02380	79.61890	821.71042	-3004.28058	-444.20312	1
3702	N	53.29900	45.96080	80.86590	-521.14493	-363.93868	555.54378	1
3703	C	54.52600	45.35480	80.48390	151.03952	173.87420	882.27310	1
3704	H	55.14700	44.83680	81.20490	-1933.72550	1915.08321	1578.41320	1
3705	C	58.04800	44.00880	78.19490	737.17950	260.16697	469.39380	1
3706	O	57.88200	42.94680	77.55890	260.74621	-502.24469	550.80751	1
3707	N	59.14200	44.76280	78.02990	-229.19614	-767.26064	-267.30605	1
3708	H	59.21600	45.65280	78.47390	2722.75767	-1531.41429	-373.61368	1
3709	C	60.37000	44.45780	77.32690	475.53858	-634.38824	450.40607	1
3710	H	60.06600	43.86780	76.47490	1926.73388	-1447.61399	-2022.45804	1
3711	C	61.19700	45.73880	76.87590	-753.09062	-29.10756	513.28186	1
3712	H	62.10800	45.47580	76.29590	-203.08343	-2886.69370	1234.49700	1
3713	H	61.43300	46.19080	77.86290	-2217.83936	860.91246	-2058.69972	1
3714	O	60.39300	46.65880	76.10090	299.48177	657.88616	317.99952	1

3715	H	59.93500	47.30180	76.64590	-931.22968	1921.92466	2310.24742	1
3716	C	61.25600	43.57680	78.15690	-178.70763	-160.85079	879.56899	1
3717	O	61.74400	44.02380	79.23190	668.96290	409.43745	92.06977	1
3718	O	61.55900	42.43480	77.70390	607.49542	-496.86289	-87.77135	1
3719	N	68.09800	39.69880	83.86190	571.61285	349.91433	513.31374	1
3720	H	68.31400	38.85080	84.42290	910.08563	2169.10908	2089.24296	1
3721	H	68.24600	39.59180	82.83790	1776.01328	-2241.62595	1311.15071	1
3722	H	67.12500	40.02180	84.03590	1021.37160	1012.12330	-2798.32677	1
3723	C	68.95200	40.75780	84.30590	777.55891	146.67247	453.14493	1
3724	H	68.94300	40.82480	85.38390	1946.09249	226.04804	2461.67677	1
3725	C	70.47100	40.56280	83.91090	-111.61165	613.31428	665.46182	1
3726	H	70.98000	41.53880	84.06090	2031.28577	2399.19909	-126.28571	1
3727	H	70.47900	40.45980	82.80490	230.72473	-2499.99811	-1896.04900	1
3728	C	71.15500	39.33080	84.51890	-126.72152	-755.37306	494.77692	1
3729	H	72.17500	39.10180	84.14190	2817.21167	-1316.06727	479.07368	1
3730	H	70.62200	38.43880	84.12690	2586.76849	178.09807	-1781.89115	1
3731	C	71.32300	39.38980	86.03290	463.17499	681.60177	-390.30625	1
3732	H	70.30800	39.45380	86.48090	140.17274	-556.15974	-3093.42273	1
3733	H	71.82700	40.34380	86.29990	-1194.98471	1307.19899	2600.28240	1
3734	C	71.99000	38.13380	86.56490	192.57395	-856.97157	244.87956	1
3735	H	71.54000	37.18180	86.20890	2223.30287	-2111.73266	704.08501	1
3736	H	73.02200	38.05280	86.16090	-2223.17803	-1828.22959	1270.15048	1
3737	N	72.01700	38.08680	88.06190	-231.46637	312.51116	749.28792	1
3738	H	72.40100	38.94980	88.49690	-1219.09390	2187.79300	-1904.10033	1
3739	H	71.06600	37.95380	88.46190	-1435.97863	-1999.74162	-1958.88362	1
3740	H	72.60700	37.30680	88.41590	2885.33725	1136.02598	-531.50744	1
3741	C	68.42100	42.10180	83.76190	-828.88752	-98.95561	366.88455	1
3742	O	67.82500	42.17680	82.71690	-522.37256	-577.22668	-132.52735	1
3743	N	68.61900	43.27580	84.43490	-646.96390	541.01008	-37.65773	1
3744	H	69.20800	43.27780	85.23890	2269.17026	2048.11863	744.51504	1
3745	C	67.99400	44.54780	83.99690	242.27881	241.13978	-845.34229	1
3746	H	68.34000	44.71780	82.98890	859.63306	-1423.90944	-2670.53162	1
3747	H	66.91700	44.46680	83.96490	-771.66451	-605.82432	-2989.27031	1
3748	C	68.37200	45.68480	84.92590	184.66813	-321.36860	833.10918	1
3749	O	68.20000	46.83880	84.64490	-682.82653	-368.19143	147.68288	1
3750	N	68.83800	45.43480	86.17690	-151.80695	593.35009	-581.00139	1
3751	H	69.14100	44.52880	86.46290	2037.25410	2010.44992	1306.10606	1
3752	C	69.04600	46.53980	87.06590	-543.62316	-345.00075	-645.67743	1
3753	H	68.12300	47.09580	87.14390	66.33524	-2802.41070	1428.39775	1
3754	C	69.42500	45.95680	88.48290	-272.01223	-709.62501	-503.87766	1
3755	H	69.61000	46.79780	89.18490	-409.90894	2764.32361	-1445.23903	1
3756	H	70.26400	45.23680	88.37490	2379.73334	927.90655	1836.86822	1
3757	N	68.12900	45.25980	90.58990	460.74564	311.05029	-635.32154	1
3758	H	68.44200	46.05880	91.10290	-330.13030	2963.30336	1004.02859	1
3759	C	68.28000	45.18480	89.23290	519.54692	329.33351	-673.09839	1
3760	C	67.11100	44.45380	90.92790	644.40650	-337.95750	549.52342	1
3761	H	66.88800	44.18780	91.96090	1809.78404	2565.69366	-200.30982	1
3762	N	66.50500	43.97780	89.88790	-540.84101	466.07973	-450.48082	1
3763	C	67.24500	44.40280	88.80090	233.82681	632.05969	614.22844	1
3764	H	67.06100	44.12980	87.76890	2200.32966	771.33471	-2112.30168	1
3765	C	70.13100	47.50080	86.71590	173.45819	439.65766	-779.78484	1
3766	O	69.95600	48.68880	86.84090	222.39656	-627.13672	425.28406	1
3767	N	71.22300	46.97380	86.14590	204.60913	810.01953	121.14355	1
3768	H	71.30800	45.98380	86.05590	1395.58742	-1035.56346	2622.62660	1
3769	C	72.34500	47.79380	85.73390	660.80815	628.31392	2.28335	1
3770	H	72.45100	48.61880	86.42290	-1545.53051	576.21836	-2679.09202	1
3771	C	73.65200	47.05680	85.70090	-425.79057	48.13732	804.88272	1
3772	H	73.55600	46.00080	85.36790	3039.25537	630.53926	-513.39387	1
3773	H	74.35000	47.50180	84.95990	-1972.72698	1038.17948	-2220.08060	1
3774	C	74.30700	47.04680	87.09390	480.53013	151.83766	759.92574	1
3775	H	74.48500	48.04780	87.54190	2370.68197	2029.45804	-399.24092	1
3776	H	75.34400	46.64680	87.06490	1467.22559	-1259.41518	2481.80352	1

3777	C	73.53900	46.29480	88.22990	58.71735	865.85843	279.80790	1
3778	O	73.14300	46.94180	89.21590	700.56881	-336.87543	-139.08814	1
3779	N	73.26100	44.98580	88.05190	-505.79474	159.24044	-656.87629	1
3780	H	73.59700	44.45680	87.27190	3144.97068	8.48997	-85.51932	1
3781	H	72.71800	44.56680	88.77890	2893.42752	214.46368	-1216.67940	1
3782	C	72.00600	48.49580	84.37690	-652.05618	177.10620	-612.29661	1
3783	O	72.38900	49.64980	84.14890	350.99120	170.81571	-686.47971	1
3784	N	71.16500	47.88080	83.49290	-302.53106	-766.33903	-184.04277	1
3785	H	70.90700	46.92780	83.63290	364.44118	-1764.43515	2579.18155	1
3786	C	70.59400	48.62080	82.36290	-862.50171	-289.28886	-62.07866	1
3787	H	71.41900	49.01280	81.78590	1036.01167	2208.48577	-1986.83081	1
3788	C	69.70100	47.63480	81.51590	-164.55527	-344.16843	-828.20327	1
3789	H	69.09700	47.05380	82.24590	658.45871	-2145.97582	2204.41515	1
3790	H	69.01800	48.11480	80.78390	2985.10277	-664.84523	738.49069	1
3791	C	70.56200	46.67680	80.62690	283.54917	211.53191	840.41961	1
3792	H	71.33500	46.24680	81.29890	-1916.84059	822.55660	-2355.28109	1
3793	H	71.11300	47.16180	79.79190	-944.70943	-446.17113	2967.60537	1
3794	C	69.74500	45.52780	80.02090	524.29088	-391.76342	634.89487	1
3795	H	69.31500	44.92580	80.84990	-1229.57383	1844.48205	2232.54572	1
3796	H	70.38800	44.89380	79.37490	1015.63131	-780.23833	-2873.66446	1
3797	C	68.59400	45.99380	79.11190	-663.46686	-12.73768	-625.38027	1
3798	H	67.85700	46.48980	79.77890	2253.08905	-497.15486	-2138.84385	1
3799	H	68.97400	46.63180	78.28490	916.62625	-2520.24030	1645.11743	1
3800	N	68.02900	44.78280	78.47990	-646.67135	411.61989	353.63473	1
3801	H	67.98800	44.08980	79.25490	456.55696	-1691.11499	2613.41005	1
3802	H	67.10500	44.86980	78.00990	1932.75723	1360.21106	2076.65635	1
3803	H	68.67200	44.54580	77.69790	417.66651	2948.47236	1015.03285	1
3804	C	69.71700	49.79980	82.79390	-617.67290	-324.69073	586.94729	1
3805	O	69.79800	50.86580	82.22390	540.16093	474.80293	-326.21401	1
3806	N	68.85600	49.66080	83.84290	594.48378	432.66991	-414.79883	1
3807	H	68.79800	48.77280	84.29290	-978.53363	2663.26302	-1359.31167	1
3808	C	68.00000	50.77580	84.28590	715.14807	-556.17579	103.35727	1
3809	H	67.57400	51.25780	83.41790	2428.98298	1120.09530	1656.39803	1
3810	C	66.81200	50.11480	85.12790	-332.12868	-304.81920	792.60759	1
3811	H	67.22400	49.50880	85.96190	-139.30877	1651.25559	-2674.35493	1
3812	H	66.27300	50.96480	85.59790	-1694.81756	919.65983	2485.96972	1
3813	C	65.87200	49.30880	84.17590	395.52658	651.74012	-500.24449	1
3814	H	66.45800	48.61780	83.53290	-1809.92321	376.01599	2545.78400	1
3815	H	65.40700	50.13980	83.60490	-2338.21175	-441.51441	-2058.16838	1
3816	C	64.58100	48.69080	84.76490	226.48407	674.72310	570.00413	1
3817	H	63.91200	48.26980	83.98490	-2066.60647	-2145.83371	-1011.31678	1
3818	H	64.00700	49.44380	85.34690	2912.66198	1184.58333	106.71804	1
3819	N	64.98200	47.51680	85.61290	-664.91099	244.64166	-459.03826	1
3820	H	64.97100	46.61780	85.17490	-2236.99295	368.58991	2181.33680	1
3821	C	64.91300	47.44980	86.91190	515.92537	620.47959	-424.59050	1
3822	N	65.22000	46.31280	87.50190	290.27672	-635.12157	-474.37570	1
3823	H	65.23700	45.48880	86.93590	-2931.03971	-12.51396	1143.27417	1
3824	H	64.79200	46.14780	88.39090	-219.68945	1131.84790	2927.26546	1
3825	N	64.55700	48.39180	87.74590	366.70747	732.70913	203.31074	1
3826	H	64.32200	49.30080	87.40390	1717.53574	-1465.36163	2191.12129	1
3827	H	64.48300	48.15980	88.71590	896.89385	606.79751	2953.91341	1
3828	C	68.76300	51.77380	85.17190	-285.50188	631.16787	-592.93069	1
3829	O	68.31700	52.89480	85.38790	455.07951	-469.12633	-443.22720	1
3830	N	69.99200	51.44480	85.66490	3.21938	-338.54617	773.33590	1
3831	H	70.22400	50.48180	85.78290	-2461.25588	946.01213	-1716.24788	1
3832	C	71.03900	52.33780	86.14090	-581.44329	507.81909	485.27773	1
3833	H	70.60600	52.99280	86.88290	-1990.57360	-1242.27221	-2095.85370	1
3834	C	72.06500	51.49980	86.96290	573.91930	-554.52735	441.09757	1
3835	H	72.56500	50.79680	86.26290	-1932.81945	2229.60763	-1091.46003	1
3836	H	71.46100	50.99980	87.75090	560.37078	3084.03253	-270.10028	1
3837	C	73.17300	52.34480	87.63990	60.06995	701.82141	-579.04172	1
3838	H	73.64300	52.97080	86.85090	1255.68737	-183.46375	2878.85681	1

3839	H	74.04000	51.75980	88.01390	319.95097	2014.62973	2395.22956	1
3840	C	72.66500	53.24480	88.79790	-478.15527	563.67583	533.93642	1
3841	H	72.29600	54.16380	88.29490	-1899.60117	-2176.04413	1246.82540	1
3842	H	71.81600	52.78380	89.34490	-611.93222	2480.08668	-1836.55526	1
3843	C	73.72900	53.65480	89.76990	779.41680	-154.22984	447.40765	1
3844	H	74.54200	54.24280	89.29390	-2182.45431	-1070.66177	1997.19874	1
3845	H	74.15700	52.71680	90.18490	-258.53165	184.47061	3130.07319	1
3846	N	73.08500	54.51480	90.80690	-312.61414	-447.45925	643.99139	1
3847	H	72.42900	53.95380	91.38690	1690.89145	-1863.86110	-1888.15628	1
3848	H	72.53100	55.23180	90.29690	245.16499	3099.80847	478.86093	1
3849	H	73.73600	55.06480	91.40390	2155.19886	-2109.17509	897.06441	1
3850	C	71.68500	53.15880	85.00390	623.75668	-425.37872	-511.30378	1
3851	O	71.94000	54.39380	85.13790	210.32796	-64.02608	758.47877	1
3852	N	72.06400	52.55680	83.85790	-512.68802	-561.07426	367.44925	1
3853	H	72.02800	51.56080	83.83890	-1340.09802	-2231.07034	-1767.67889	1
3854	C	72.45900	53.18580	82.59290	272.44450	717.63508	492.16348	1
3855	H	73.31700	53.82280	82.75190	-2566.36552	740.82608	-1662.27885	1
3856	C	72.73700	52.17980	81.49090	-525.34461	-458.00046	587.96226	1
3857	H	73.16400	52.69180	80.60190	-869.76759	-2305.19100	-1956.48282	1
3858	H	73.43100	51.39180	81.85490	1353.06864	498.04678	-2796.31559	1
3859	H	71.81100	51.66480	81.15690	-241.38724	2448.10649	-1961.30901	1
3860	C	71.42300	54.10280	82.09390	-689.97708	-585.91715	109.92600	1
3861	O	71.72400	55.20980	81.62890	-552.83839	-246.67264	507.09915	1
3862	N	70.15100	53.68580	82.18190	-342.29331	458.75259	-620.52691	1
3863	H	69.93300	52.74080	82.41190	-2053.05600	-911.11173	2202.96680	1
3864	C	69.05200	54.61880	81.81290	-661.84217	377.23300	501.10998	1
3865	H	69.27300	54.93580	80.80490	2243.27517	930.64832	-1999.95911	1
3866	C	67.72000	53.76380	81.88590	639.20273	-551.70776	344.22291	1
3867	H	67.86000	52.87180	81.23890	-2063.73426	-2288.81104	632.90689	1
3868	H	67.52600	53.54180	82.95690	-1559.68592	-2705.88566	379.19502	1
3869	C	66.42000	54.44080	81.37090	430.20625	-46.35091	-802.63639	1
3870	H	66.26400	55.30580	82.05090	-681.97645	-583.37952	3015.42744	1
3871	C	66.51600	54.88780	79.91790	-173.14037	-434.96732	782.48121	1
3872	H	67.34800	55.61980	79.84090	-803.72996	-2374.21637	-1901.40501	1
3873	H	66.83700	54.05780	79.25390	1898.90846	2069.68757	-1417.30952	1
3874	H	65.61300	55.35880	79.47290	-1667.41036	-79.12497	2666.77861	1
3875	C	65.08700	53.64980	81.60090	-731.35607	301.24535	-453.67448	1
3876	H	64.19400	54.26480	81.35690	-2511.54906	1572.20663	1057.59817	1
3877	H	65.13500	52.68680	81.04990	-595.74175	-3073.77495	-308.58642	1
3878	H	65.04700	53.31080	82.65790	-2822.71283	-1352.70024	317.36508	1
3879	C	68.94000	55.86580	82.65390	-70.47272	-828.70885	373.79973	1
3880	O	68.94800	56.97480	82.06590	-446.80757	137.32904	636.49899	1
3881	N	68.95500	55.70480	84.03490	279.57794	-554.94538	571.44036	1
3882	H	68.90000	54.78480	84.41390	1046.08587	-532.20686	2919.02149	1
3883	C	69.01700	56.76980	84.97390	-534.55167	-434.10288	597.71247	1
3884	H	68.18000	57.41880	84.76190	-1645.94003	-1799.36271	-1987.81324	1
3885	C	68.98700	56.10080	86.37390	385.92827	769.98546	-299.38731	1
3886	H	67.97000	55.65380	86.34790	1889.06635	1409.96097	2083.66615	1
3887	H	69.84200	55.41280	86.55090	-1619.21534	815.70040	2571.18664	1
3888	C	69.01600	57.12980	87.55390	-623.59984	585.04799	316.69085	1
3889	H	68.64300	58.10980	87.18590	2090.21703	-1164.78809	-2042.66681	1
3890	H	70.04000	57.51080	87.75690	2155.28233	1395.29939	-1818.27499	1
3891	C	68.28500	56.64680	88.80690	-56.65648	-649.82734	-637.15420	1
3892	H	67.27800	56.32580	88.46590	-516.46076	-2477.12087	-1869.58998	1
3893	H	68.78000	55.77180	89.27990	-2708.29037	-130.47564	1595.73357	1
3894	C	68.18300	57.76180	89.88990	-301.37460	-720.47852	470.67511	1
3895	H	67.70500	58.60680	89.34890	-1411.07974	-1846.54891	2120.69265	1
3896	H	69.18300	58.07080	90.26390	2505.33603	-21.34407	1902.90884	1
3897	N	67.28600	57.24180	90.94090	-427.52308	-725.09425	-64.30115	1
3898	H	67.23400	57.85680	91.77790	-2217.36352	404.32433	-2195.00503	1
3899	H	66.34800	56.94180	90.60490	2024.90662	1892.46171	-1488.81432	1
3900	H	67.76700	56.37380	91.25190	2451.35277	-664.42586	1856.78058	1

3901	C	70.26400	57.65280	84.87290	243.27956	-474.74816	-739.51352	1
3902	O	70.14300	58.87780	84.98790	-350.36558	642.74227	-296.23228	1
3903	N	71.49100	57.15780	84.71690	525.38516	-576.92895	322.17342	1
3904	H	71.63100	56.17080	84.69590	192.96560	-1746.91109	-2609.46204	1
3905	C	72.71900	57.94580	84.52690	-330.22362	621.77168	579.48541	1
3906	H	72.79500	58.56780	85.40690	-1952.93453	2422.54589	-464.26757	1
3907	C	74.01800	57.10780	84.51390	-88.98608	856.89754	298.76258	1
3908	H	74.13900	56.57280	83.54790	1097.55944	-2284.88143	-1863.57355	1
3909	O	74.08600	56.29880	85.65490	-367.30544	-694.24777	82.06081	1
3910	H	73.52300	55.52680	85.55590	2455.66144	-868.21927	-1764.69500	1
3911	C	75.19200	58.07780	84.76890	20.29836	-909.46653	-62.52683	1
3912	H	75.21200	58.81580	83.93790	3118.96169	66.95838	-407.21098	1
3913	H	76.17100	57.55180	84.75690	2081.85373	-2327.17554	-385.18214	1
3914	H	75.14700	58.74180	85.65790	1243.13381	322.57344	-2872.07085	1
3915	C	72.59200	58.81480	83.22690	-330.46249	261.44679	-808.63534	1
3916	O	73.01500	59.98280	83.18890	-340.56796	-20.52919	-712.19326	1
3917	N	72.00200	58.27580	82.17390	268.31858	-474.22387	-644.81715	1
3918	H	71.78800	57.30480	82.23390	1714.59334	745.53730	-2530.33002	1
3919	C	71.67800	58.96180	80.92490	197.77714	-849.81669	-264.85240	1
3920	H	72.62500	59.27280	80.50790	164.43913	870.78194	3018.76213	1
3921	C	71.09500	58.12480	79.80190	-407.85511	-507.48595	-638.40678	1
3922	H	70.05700	57.80880	80.03990	-2605.82938	1041.61792	1422.29096	1
3923	O	71.89200	56.91180	79.71290	480.89195	457.24105	428.13641	1
3924	H	71.56000	56.30780	80.38190	-2278.15747	2128.42482	-421.93905	1
3925	C	71.17200	58.81080	78.46790	509.30657	20.67635	756.06237	1
3926	H	72.19700	59.09080	78.14290	1932.07419	920.80895	2305.95456	1
3927	H	70.51100	59.70180	78.53390	-407.85607	3061.21716	600.69058	1
3928	H	70.87600	58.20880	77.58290	637.30372	-1572.87634	-2649.17538	1
3929	C	70.83300	60.20580	81.08790	-909.86007	-35.78903	-48.21613	1
3930	O	71.24500	61.35880	80.80990	298.18598	-476.17007	554.95443	1
3931	N	69.70300	59.95480	81.76090	-226.13355	-415.64329	699.12557	1
3932	H	69.43500	59.01180	81.94290	-1315.49295	1570.02918	2388.03537	1
3933	C	68.79200	60.93480	82.26090	-456.02518	37.45616	-788.72624	1
3934	H	68.27700	61.41580	81.44290	-286.12146	1164.47398	2908.66999	1
3935	C	67.64800	60.18880	82.90290	570.37181	-682.81244	-199.73525	1
3936	H	68.05500	59.43180	83.60690	-1276.19407	2174.53921	1881.73700	1
3937	C	66.77000	61.10180	83.78390	326.57539	660.06675	-537.69081	1
3938	H	65.86900	60.56480	84.14890	2409.09134	642.70293	1918.70740	1
3939	H	66.36600	61.97780	83.23390	-1844.74327	2366.54682	-945.83543	1
3940	H	67.30500	61.44380	84.69590	-2707.66627	1602.04970	-14.36530	1
3941	C	66.87700	59.43380	81.79990	-552.19502	-579.97955	-436.06809	1
3942	H	65.98800	58.91880	82.22390	1821.96405	-2564.38861	50.83576	1
3943	H	67.56900	58.76680	81.24290	2706.18772	-1097.80482	-1170.29860	1
3944	H	66.48400	60.21480	81.11490	1610.79832	-15.96195	-2702.46188	1
3945	C	69.33700	61.96280	83.14390	171.94929	749.49115	-490.04842	1
3946	O	69.12900	63.14880	82.91090	-217.41480	-646.23898	398.41338	1
3947	N	70.16800	61.60980	84.15190	639.72837	-179.72673	520.69012	1
3948	H	70.42600	60.68180	84.41090	574.47676	-1720.67927	2570.49908	1
3949	C	70.81100	62.52780	85.05990	765.64765	-88.77459	487.18964	1
3950	H	70.02500	63.10980	85.51790	-1690.19238	-1785.53545	-1962.99238	1
3951	C	71.57800	61.78180	86.15290	-646.68575	67.45467	639.29524	1
3952	H	72.12500	60.95180	85.65690	-2582.64648	1101.73039	-1419.27923	1
3953	C	72.63700	62.69880	86.91090	509.85807	454.90297	-603.78725	1
3954	H	73.14200	62.11380	87.70790	-1397.43705	-1333.21994	2483.52985	1
3955	H	72.14800	63.58180	87.37590	-35.65275	3117.99305	-418.41898	1
3956	H	73.44600	62.89480	86.17490	-1420.38108	-1983.24603	-1986.82636	1
3957	C	70.63500	61.17080	87.20590	553.34893	534.02336	489.97451	1
3958	H	69.64800	60.89180	86.77890	-1578.04832	140.24373	2718.14669	1
3959	H	70.45800	61.96580	87.96190	2868.32007	896.40040	931.36058	1
3960	C	71.26700	59.95680	87.91890	85.39618	-811.05417	-407.85981	1
3961	H	70.48700	59.54080	88.59190	-1870.51271	-1676.22946	-1894.64066	1
3962	H	71.59500	59.21580	87.15890	-1924.64270	-1979.66680	1508.27586	1

3963	H	72.13800	60.22880	88.55390	-2473.46250	-76.71059	1942.76220	1
3964	C	71.66200	63.52580	84.35490	438.07441	633.69871	-487.81940	1
3965	O	71.52800	64.71780	84.59990	-443.34025	-349.46283	552.22494	1
3966	N	72.44000	63.06280	83.35390	-624.40211	557.05801	-111.71691	1
3967	H	72.41000	62.08380	83.16990	386.38993	-135.32627	3119.39351	1
3968	C	73.23300	63.90780	82.52590	365.35043	-426.39720	718.43962	1
3969	H	73.88400	64.42880	83.21190	550.96647	1392.34146	2766.95635	1
3970	C	74.22100	63.07780	81.65290	-146.04760	808.90844	-394.70019	1
3971	H	73.76600	62.28180	81.02690	-2505.44589	-11.68796	1902.84800	1
3972	H	74.79000	62.50380	82.41590	2273.04631	-1218.22742	1802.05678	1
3973	C	75.19500	63.90380	80.72890	-542.81902	264.10424	683.40871	1
3974	H	74.55500	64.48980	80.03390	-767.21379	2580.81773	1627.57152	1
3975	C	76.09000	64.93880	81.32490	14.20169	-878.17541	-245.06582	1
3976	H	76.90300	64.44380	81.89790	1439.76558	-2322.83709	1558.75886	1
3977	H	75.62900	65.65480	82.03890	-739.09741	2217.17861	2106.20043	1
3978	H	76.67100	65.48180	80.54890	-1948.68896	-2390.62720	621.07902	1
3979	C	76.03300	62.90280	79.89590	-458.99115	-255.15187	745.43655	1
3980	H	76.48300	62.22980	80.65690	2600.30754	1525.48479	-899.73501	1
3981	H	76.84200	63.38880	79.30890	1497.07460	-1397.33276	2388.40010	1
3982	H	75.43400	62.30680	79.17490	2301.56355	-2144.06834	-63.26486	1
3983	C	72.43700	64.90980	81.66490	-222.19629	779.00499	418.60606	1
3984	O	72.81300	66.08780	81.57690	-433.56174	-600.34748	-274.28881	1
3985	N	71.36300	64.44380	80.99590	-324.41239	573.49571	527.76089	1
3986	H	71.19000	63.46780	81.10790	1198.28039	1442.96826	2525.90438	1
3987	C	70.42600	65.14580	80.24290	-623.76666	556.66821	363.98716	1
3988	H	71.03900	65.71780	79.56190	-2613.07726	-1465.26358	-960.75809	1
3989	C	69.50000	64.18580	79.47790	248.39544	-8.29385	877.31518	1
3990	H	69.27400	63.33580	80.15590	17.57965	1064.64299	-2960.48180	1
3991	C	68.14600	64.84580	79.02290	719.99373	-206.78992	-519.90188	1
3992	H	67.51200	65.16380	79.87790	860.76847	-3026.02063	22.42768	1
3993	H	67.58600	64.15180	78.35890	-522.75864	2584.60160	-1716.03735	1
3994	H	68.45800	65.75480	78.46590	-660.30959	-2856.39409	1141.59112	1
3995	C	70.28000	63.43880	78.39190	-471.10765	-680.19178	383.20717	1
3996	H	70.44600	64.25280	77.65390	-148.63059	2023.65396	-2404.36266	1
3997	H	71.27200	63.03780	78.69290	-1939.54892	2067.38678	-1364.65679	1
3998	C	69.41000	62.39680	77.58790	27.87344	617.60138	670.25563	1
3999	H	68.96100	61.73580	78.35990	-2867.19630	554.91047	-1170.25039	1
4000	H	68.57700	62.83380	76.99690	977.52840	-2604.20158	1469.96550	1
4001	H	70.16900	61.86880	76.97190	-1503.18671	-2078.04153	-1822.19629	1
4002	C	69.70600	66.19980	80.98090	615.56666	-32.45129	-671.91935	1
4003	O	69.55800	67.36380	80.51690	444.73037	316.86583	570.47189	1
4004	N	69.14000	65.92480	82.22190	-560.34921	575.99168	258.67863	1
4005	H	69.22700	64.99080	82.55990	-2543.67384	-1684.65722	-768.03624	1
4006	C	68.75000	66.92180	83.19690	-549.25090	-557.48047	467.96364	1
4007	H	67.89500	67.41080	82.75390	-1202.66214	2108.85369	2001.14120	1
4008	C	68.34200	66.10180	84.47590	406.38210	-489.19738	653.44511	1
4009	H	68.06800	66.67780	85.38590	743.46099	-750.85036	-2963.39598	1
4010	H	69.24300	65.50480	84.73090	-2010.00971	-2073.72596	-1248.09769	1
4011	C	67.11800	65.15880	84.29590	-81.02934	-73.17877	-905.27903	1
4012	H	67.27600	64.54180	83.38490	-1070.74360	-2563.83302	-1475.97244	1
4013	C	67.17400	64.17980	85.52090	463.14448	-513.33840	-594.50137	1
4014	H	66.20600	63.64480	85.41390	2399.23451	1929.74753	-646.50944	1
4015	H	67.27400	64.75380	86.46590	-2867.84577	1245.42519	-350.14706	1
4016	H	68.06800	63.52580	85.43190	1296.50617	-786.12915	-2756.68260	1
4017	C	65.84000	65.91780	84.21390	870.64524	268.71178	-34.95503	1
4018	H	65.86700	66.56680	83.31290	2138.08734	-2069.27399	-1022.21029	1
4019	H	64.97100	65.22780	84.18490	2231.15667	-824.78726	-2059.09983	1
4020	H	65.68500	66.60280	85.07490	-1727.56287	-1803.47867	-1913.43080	1
4021	C	69.78900	67.93480	83.58990	-666.59651	591.10016	-194.16668	1
4022	O	69.52000	69.15080	83.59590	-327.14884	-500.18694	516.15297	1
4023	N	71.02500	67.45980	83.92190	-668.40418	452.16205	-247.90648	1
4024	H	71.29900	66.50280	83.86090	1266.76997	2405.96981	1582.66527	1

4025	C	72.04000	68.25880	84.44690	15.43303	422.10510	808.10897	1
4026	H	71.72900	68.65180	85.40390	-1702.36420	688.91380	2554.52151	1
4027	C	73.35000	67.44380	84.73490	-744.59771	-367.26277	377.01897	1
4028	H	74.10400	68.14980	85.14490	2988.90615	-697.01464	-691.98039	1
4029	H	73.20500	66.70780	85.55390	-703.87624	-2780.78880	1292.28406	1
4030	H	73.77200	66.98480	83.81490	2028.40491	-2216.74908	932.64316	1
4031	C	72.37500	69.33780	83.44090	-762.43527	-335.32620	-371.07923	1
4032	O	72.35400	70.52480	83.71590	535.09965	467.64694	344.38631	1
4033	N	72.52600	68.93380	82.15690	567.82762	-253.64860	570.88218	1
4034	H	72.48400	67.96680	81.91890	-311.17023	2478.09920	-1913.22338	1
4035	C	72.88600	69.73780	81.06290	281.76155	528.84857	-687.29951	1
4036	H	73.82700	70.20980	81.30690	-2876.31137	100.50283	-1270.81010	1
4037	C	73.15900	68.74380	79.88290	38.65303	903.87174	-113.89831	1
4038	H	72.24600	68.13780	79.70290	2003.80494	-786.29881	-2294.49911	1
4039	H	74.00200	68.08380	80.18090	-1457.38086	2589.07619	-1034.86797	1
4040	C	73.42400	69.35880	78.57890	807.67268	-421.78101	-34.88021	1
4041	C	74.73300	69.62180	78.20490	-887.19590	-172.55521	120.66125	1
4042	H	75.61300	69.41980	78.79790	514.38192	-2657.95822	1602.77746	1
4043	C	74.94800	70.16980	76.88990	506.85242	-148.00777	743.40119	1
4044	H	75.94500	70.40780	76.54990	-2057.27705	-762.85986	-2254.74659	1
4045	C	73.86900	70.43680	76.05490	-115.11739	-903.73521	-38.23159	1
4046	H	74.11800	70.79380	75.06590	-810.10216	2960.38401	-691.43851	1
4047	C	72.34100	69.62080	77.69590	-637.40370	-2.52272	-652.04384	1
4048	H	71.31700	69.47980	78.01090	-913.71889	1686.08332	2494.08641	1
4049	C	72.56000	70.16080	76.43590	-547.91257	-660.70685	-307.74874	1
4050	H	71.70500	70.39580	75.81990	-2798.21263	423.81403	1374.26851	1
4051	C	71.85900	70.76280	80.73490	361.91530	-606.37613	-576.86767	1
4052	O	72.02600	71.98080	80.52490	251.12941	291.83528	689.48779	1
4053	N	70.56600	70.38080	80.67190	-574.94779	539.68619	-301.40694	1
4054	H	70.32800	69.41380	80.71090	1729.56689	2048.77939	-1646.00352	1
4055	C	69.44000	71.27380	80.50690	-831.09200	347.37310	-141.66520	1
4056	H	69.51600	71.89380	79.62590	-663.10323	-2419.00002	-1899.19963	1
4057	C	68.15900	70.43480	80.33790	507.21461	-180.16149	736.02051	1
4058	H	67.91400	69.83780	81.24290	-1462.49686	1425.98534	2392.88424	1
4059	H	68.37400	69.74180	79.49790	1822.66047	2229.26481	-1267.48312	1
4060	C	66.92100	71.17580	80.05790	-383.58289	-227.95308	-795.20599	1
4061	C	66.57200	71.44880	78.74590	-795.50275	442.43117	-53.67529	1
4062	H	67.31800	71.24980	77.98990	982.27208	1484.92119	2593.91150	1
4063	C	65.36200	72.05980	78.40290	-424.62679	560.01409	-580.97100	1
4064	H	65.06300	72.19480	77.37390	2881.47047	177.74285	1250.50455	1
4065	C	64.52500	72.43380	79.47390	287.06335	-522.43045	690.00874	1
4066	H	63.62600	73.01480	79.32790	-1612.45005	2071.34543	1734.28924	1
4067	C	66.02700	71.52980	81.08290	-416.92943	-447.70391	676.15239	1
4068	H	66.30100	71.35380	82.11290	-3035.20177	-817.83505	-130.08575	1
4069	C	64.89600	72.27080	80.79890	306.78485	561.44746	-649.70055	1
4070	H	64.14400	72.56780	81.51590	2267.31498	-343.02556	-2154.02936	1
4071	C	69.33500	72.26180	81.71990	787.55063	-102.23205	-448.06654	1
4072	O	69.08000	73.41680	81.52690	-372.56696	694.58838	48.66286	1
4073	N	69.63000	71.85980	82.96790	433.03109	-325.42850	647.49722	1
4074	H	69.70200	70.91080	83.26390	-1650.72846	-2672.16063	-181.32662	1
4075	C	69.74000	72.75980	84.02890	-875.54912	-117.10418	-226.16667	1
4076	H	68.80600	73.27580	84.19490	2218.07323	-1064.37813	1960.98867	1
4077	C	69.97200	71.99480	85.34890	-255.79290	521.70126	702.74376	1
4078	H	69.16700	71.24180	85.48590	1967.09899	1790.97782	-1679.62681	1
4079	H	70.95100	71.47480	85.41890	-258.16526	-3132.40923	-139.96202	1
4080	H	69.93600	72.73580	86.17590	-1650.24808	1788.44499	1994.08426	1
4081	C	70.81600	73.85580	83.78590	299.93807	614.64045	603.07982	1
4082	O	70.62400	75.02280	84.15090	-635.12172	-331.96871	-331.72942	1
4083	N	71.92800	73.46580	83.15890	219.79269	688.33212	-436.53449	1
4084	H	71.88900	72.59580	82.67490	-2318.58861	-1320.12745	-1667.22423	1
4085	C	73.00100	74.43080	82.80690	-56.28492	505.89737	-756.53874	1
4086	H	73.28100	74.87180	83.75190	560.35807	-260.08162	3084.89588	1

4087	C	74.19600	73.61780	82.23390	-178.32623	-426.60590	-785.91231	1
4088	H	74.96200	74.36980	81.94790	-90.42995	2301.01560	-2143.68278	1
4089	H	73.88900	73.19180	81.25490	-2496.61376	281.72810	-1893.61433	1
4090	S	74.87400	72.35080	83.38990	-391.10506	304.14548	-256.40390	1
4091	H	73.67600	71.91480	83.75190	2085.04461	-1803.58698	1515.87902	1
4092	C	72.62400	75.52980	81.86190	-616.08198	158.70291	653.22843	1
4093	O	72.81800	76.70480	82.13490	782.67298	-104.30276	13.08299	1
4094	N	71.91800	75.07780	80.72890	-223.12259	-529.41462	-618.55376	1
4095	H	71.92300	74.09580	80.55290	-2078.71397	-2344.42619	-284.32429	1
4096	C	71.54200	75.91280	79.63390	160.71277	284.92917	-851.13911	1
4097	H	72.31800	76.64380	79.46390	687.85511	2637.49308	1571.21349	1
4098	C	71.62200	74.98880	78.37290	-14.87462	-544.45953	-731.29581	1
4099	H	71.04500	75.42080	77.52690	546.99020	792.51684	2995.15359	1
4100	H	71.17500	73.99780	78.60090	1747.68890	-1667.58371	-2015.68209	1
4101	C	73.02200	74.78780	77.81290	67.32814	600.59950	682.78706	1
4102	C	73.70700	73.56580	77.87990	108.14474	662.31673	-617.32671	1
4103	H	73.23900	72.61380	78.08190	2252.51218	599.02628	2113.19251	1
4104	N	74.94100	73.72080	77.23790	664.40130	-435.37845	-285.81253	1
4105	H	75.57100	73.04880	76.91690	-2958.82831	-154.63791	-1058.13439	1
4106	C	75.03800	74.99780	76.86390	318.30645	-448.54322	727.28329	1
4107	C	73.88500	75.72880	77.20590	101.30690	-666.07712	-614.43403	1
4108	C	73.84600	77.15180	77.05090	602.07279	-458.97011	508.23793	1
4109	H	72.96800	77.73480	77.28890	-102.26161	3138.63819	191.62225	1
4110	C	74.99200	77.74080	76.45190	-384.88471	-657.20590	-501.39323	1
4111	H	74.97600	78.77380	76.13690	2077.72398	2362.45752	-9.15197	1
4112	C	76.13500	75.64780	76.26290	273.95214	365.00384	-789.41334	1
4113	H	77.00800	75.08280	75.96990	-1844.42720	-2080.93541	-1471.74127	1
4114	C	76.07400	77.02980	76.04390	265.68115	714.65104	500.13841	1
4115	H	76.95300	77.55880	75.70590	-2227.71763	1240.99214	-1842.67167	1
4116	C	70.21200	76.64580	79.76090	-791.09693	346.49207	292.50624	1
4117	O	70.11700	77.79280	79.22390	-397.74122	-250.32718	634.63805	1
4118	N	69.22300	76.15280	80.47990	-738.81374	392.55939	112.79924	1
4119	H	69.32500	75.27080	80.93290	-2383.06337	1963.14052	604.41252	1
4120	C	67.91700	76.79680	80.50690	-228.98232	-612.60296	635.40201	1
4121	H	67.50100	76.72480	79.51290	-2652.48398	586.45764	1587.01682	1
4122	C	67.04200	75.89380	81.32190	253.12686	-868.38801	-115.23913	1
4123	H	67.50300	75.63980	82.29990	1794.50829	-2443.81903	-840.06832	1
4124	H	67.00500	74.91080	80.80590	2392.61939	1490.38827	1397.26214	1
4125	C	65.64000	76.49380	81.61290	-712.02831	-496.01506	280.06384	1
4126	H	65.63400	77.50380	82.07590	-2855.05416	-392.98280	1261.92571	1
4127	C	64.73900	76.55180	80.32490	-185.66717	-392.15166	801.99488	1
4128	H	64.91700	75.65380	79.69490	2031.57726	-631.98670	2317.65245	1
4129	H	63.67100	76.57880	80.62790	-3050.89579	-760.90833	-106.20553	1
4130	H	64.89500	77.50380	79.77390	1268.44632	2145.45816	1919.96860	1
4131	C	64.90600	75.60280	82.61490	217.91727	481.57359	-743.00063	1
4132	H	65.60700	75.23780	83.39590	-1776.92534	1897.96495	1771.57885	1
4133	H	64.05500	76.15680	83.06690	1742.36489	-1253.92117	-2300.01577	1
4134	H	64.60100	74.61180	82.21590	1329.07292	-1922.97514	2105.69656	1
4135	C	67.88300	78.25880	80.97990	-721.79164	-420.42846	-365.66070	1
4136	O	67.19700	79.02380	80.29190	491.88635	473.02935	397.38934	1
4137	N	68.52100	78.78280	82.02490	-50.66107	833.81815	-121.87301	1
4138	C	69.31500	77.97980	82.97190	-774.94738	288.15534	384.54396	1
4139	H	68.96900	76.92580	83.03290	-430.51626	2323.24255	-2077.36036	1
4140	H	70.36000	78.03480	82.59890	-123.70575	-1711.17270	2637.19759	1
4141	C	68.47200	80.19080	82.39590	123.65519	-846.88794	-314.54923	1
4142	H	67.44000	80.42380	82.61490	-718.05829	-2317.42853	-2003.03358	1
4143	C	69.25900	80.17180	83.75390	-400.17499	590.16441	-568.34580	1
4144	H	68.88300	80.87580	84.52690	2876.13069	1213.09254	393.07118	1
4145	H	70.32300	80.40280	83.53390	1018.20321	2831.75888	-917.94886	1
4146	C	69.11600	78.74880	84.28590	826.15565	200.65177	329.63118	1
4147	H	69.94800	78.54280	84.99390	2720.23055	1575.50067	-127.94379	1
4148	H	68.10900	78.61380	84.73490	1975.53506	-1680.30383	1781.02962	1

4149	C	69.05500	81.12380	81.23090	627.27813	121.76532	650.49701	1
4150	O	68.57200	82.24780	81.04590	358.18926	669.48263	217.07301	1
4151	N	70.09900	80.67380	80.54090	-757.99160	-237.76688	285.63601	1
4152	H	70.39500	79.77580	80.85690	1831.42459	-1978.30896	-1621.85199	1
4153	C	70.60700	81.42980	79.40390	-215.14607	876.68391	128.79633	1
4154	H	70.77000	82.44380	79.73990	-1946.65767	-2362.23219	727.05515	1
4155	C	71.94100	80.76680	78.92290	439.12220	-738.99675	-304.14882	1
4156	H	71.86800	79.65880	78.87490	1433.13192	865.53009	-2663.68481	1
4157	H	72.71000	80.96280	79.70090	2497.91656	-1128.30750	1544.52622	1
4158	C	72.44600	81.21980	77.54890	551.45682	363.65370	-628.57169	1
4159	C	73.03200	82.49780	77.40790	126.03326	887.00283	-169.68381	1
4160	H	73.19700	83.12680	78.26990	2997.77976	-929.91023	-216.35544	1
4161	C	73.38000	82.91680	76.12890	-268.62169	687.00284	536.02284	1
4162	H	73.80300	83.90780	76.04790	286.85084	3044.91548	737.85674	1
4163	C	73.21100	82.08580	74.99290	-484.43244	-749.27995	188.03130	1
4164	O	73.66500	82.54480	73.75290	658.54087	-314.36535	-301.87013	1
4165	H	74.19700	83.33680	73.85990	-741.21548	2282.44509	2034.51966	1
4166	C	72.14500	80.45680	76.39290	-380.39147	-828.65090	-9.54060	1
4167	H	71.53000	79.57280	76.46990	-237.42891	-3112.42521	-393.27223	1
4168	C	72.59800	80.86680	75.14790	360.82114	-783.09724	-296.67797	1
4169	H	72.46700	80.20280	74.30690	2569.56100	-1632.10586	-794.86662	1
4170	C	69.60500	81.53480	78.26890	-278.55029	-734.90649	462.35613	1
4171	O	69.34000	82.63880	77.79490	698.00129	-336.44272	152.40644	1
4172	N	68.89900	80.39980	77.87590	717.85149	441.77882	46.82945	1
4173	H	69.15900	79.51980	78.26490	-1642.63553	-2014.54850	-1772.44720	1
4174	C	67.79400	80.35980	76.99690	794.35812	-98.70473	-436.69619	1
4175	H	68.02800	80.90180	76.09190	-809.75792	-1680.34789	-2533.56455	1
4176	C	67.37900	78.88380	76.66290	784.30748	152.04994	-439.53793	1
4177	H	67.35800	78.20080	77.53890	2473.25549	1467.80879	1275.44927	1
4178	H	66.31400	78.74980	76.37590	1805.91656	-974.83447	-2384.65707	1
4179	C	68.31100	78.32080	75.65290	-698.59298	500.17537	-305.35791	1
4180	C	68.11000	78.68280	74.28590	540.67500	540.67818	-496.77827	1
4181	H	67.23800	79.29980	74.12290	1016.32147	2082.23211	2128.29188	1
4182	C	68.99100	78.15880	73.25190	212.00214	-690.14627	556.95980	1
4183	H	68.92600	78.57780	72.25790	-1771.57840	-172.91884	2594.19260	1
4184	C	69.92600	77.15880	73.58790	-488.10877	111.40820	762.09517	1
4185	O	70.77300	76.70680	72.57590	624.88106	256.11046	-409.33888	1
4186	H	70.57700	77.24380	71.80390	-2369.74769	-1734.43725	1128.82661	1
4187	C	69.24800	77.30080	75.92290	399.94764	-446.97378	686.80953	1
4188	H	69.32500	76.81380	76.88390	2438.68726	1984.75587	-108.51194	1
4189	C	70.03300	76.73280	74.90990	274.87732	481.77146	-723.73318	1
4190	H	70.81500	76.02580	75.14390	1698.21567	2136.86009	1564.64652	1
4191	C	66.60900	81.16880	77.39390	-503.59349	535.04360	539.97494	1
4192	O	66.03000	81.91280	76.59390	-555.71653	-31.06093	-560.21566	1
4193	N	66.26200	81.14380	78.69490	-423.91051	460.76442	-566.27583	1
4194	H	66.72900	80.59280	79.38290	231.56496	-420.20322	-3109.34610	1
4195	C	65.22400	82.07880	79.20490	673.00490	-614.10019	-37.36801	1
4196	H	64.38800	81.88480	78.54990	-2063.42445	-1517.23627	-1827.15623	1
4197	C	64.68300	81.72780	80.60790	-832.15514	-43.89968	-370.19135	1
4198	H	65.60700	81.77480	81.22190	-1925.12662	1278.53341	2134.82225	1
4199	C	63.60600	82.80080	81.01090	505.36527	-397.43725	646.60697	1
4200	H	62.70300	82.86080	80.36690	-2007.05635	1127.90983	2144.24123	1
4201	H	63.25600	82.57980	82.04190	-2206.49127	-827.25388	2084.53196	1
4202	H	64.00900	83.83280	81.09290	-2810.47507	-735.62911	-1207.60337	1
4203	C	64.11400	80.29080	80.63890	612.56915	-593.56585	322.31913	1
4204	H	63.25500	80.13980	79.95190	2849.58568	596.58090	-1192.55142	1
4205	H	64.84000	79.61680	80.13490	-1849.77837	-2543.24136	-92.03029	1
4206	C	63.65900	79.83980	81.99690	532.32684	449.11009	-588.53994	1
4207	H	64.50200	79.89380	82.71890	2476.88810	-656.72205	-1825.36783	1
4208	H	63.43900	78.75180	81.95090	2383.43696	-183.50493	2045.42916	1
4209	H	62.80200	80.44580	82.35890	-734.01996	2926.88786	890.37542	1
4210	C	65.58000	83.61280	79.03390	-662.43462	-189.91493	597.12955	1

4211	O	64.77400	84.26080	78.37690	-448.56273	-99.99674	642.19884	1
4212	N	66.82900	84.06580	79.36490	-665.14497	222.68035	-469.75304	1
4213	H	67.45400	83.43180	79.81190	-2950.53399	-175.34435	1077.88206	1
4214	C	67.36000	85.36180	78.94990	-588.82118	446.31850	534.35982	1
4215	H	66.87600	86.21180	79.40790	-1520.49547	35.19402	-2754.10260	1
4216	H	68.40000	85.20580	79.19290	-2997.98735	-883.96427	359.03380	1
4217	C	67.26100	85.73780	77.49590	-579.75952	-504.97981	-490.22984	1
4218	O	66.68600	86.70480	77.07990	253.85435	13.10768	-747.67198	1
4219	N	67.89100	84.89680	76.61290	356.73523	-663.28731	381.39508	1
4220	H	68.32900	84.14080	77.09390	888.15468	2662.37180	1421.68347	1
4221	C	67.85900	85.09480	75.22390	579.06050	400.74256	579.26276	1
4222	H	68.31200	86.06280	75.06790	-497.62359	-3061.05885	-529.63734	1
4223	C	68.53600	83.92580	74.53290	-676.89647	-545.29416	-275.52940	1
4224	H	68.10500	82.98380	74.93690	-1566.49989	1817.76903	-2034.70393	1
4225	C	68.34900	83.93880	73.05490	-859.83284	287.47088	97.46273	1
4226	H	67.38300	83.53880	72.67890	559.45597	-3034.42126	614.42889	1
4227	H	68.68700	84.91880	72.65490	-2379.23533	1914.79470	755.66312	1
4228	H	69.02400	83.17980	72.60690	2573.12642	-623.55059	-1699.53856	1
4229	C	70.05800	83.94780	74.75490	-859.47197	15.31935	304.17799	1
4230	H	70.56200	83.01280	74.42890	-557.06634	2791.46622	1340.00734	1
4231	H	70.17300	83.76380	75.84390	1858.38971	1313.36782	-2172.48219	1
4232	C	70.81700	85.19880	74.41190	468.39538	567.69126	538.31533	1
4233	H	71.72500	85.38780	75.02290	2423.32327	1061.82646	-1702.42625	1
4234	H	71.17000	85.05380	73.36790	-1391.98393	-1495.87398	2392.27256	1
4235	H	70.21200	86.12680	74.49190	-1825.42016	-2272.48838	-1184.00339	1
4236	C	66.41400	85.17680	74.58490	547.85271	327.48064	651.20261	1
4237	O	66.09500	85.96780	73.73790	-613.35023	-199.85188	455.50846	1
4238	N	65.47600	84.30180	75.09290	-415.11655	435.25446	-592.37158	1
4239	H	65.70400	83.60980	75.77290	-77.01283	-2431.77744	1994.68136	1
4240	C	64.05600	84.33580	74.67990	-310.60242	222.51014	-827.92897	1
4241	H	64.10600	84.16680	73.61490	-2580.20351	-1213.99403	-1329.28347	1
4242	C	63.18100	83.19080	75.19690	304.73127	-482.89879	710.91393	1
4243	H	62.22600	83.07180	74.64190	2747.40308	654.17390	1386.38344	1
4244	H	63.77500	82.27180	75.00590	524.28411	-1982.39564	-2386.09722	1
4245	O	62.80900	83.14980	76.55590	289.23783	159.36988	717.33531	1
4246	H	63.47300	83.61580	77.06990	2995.73456	32.18442	-960.60649	1
4247	C	63.34300	85.61080	74.89990	-656.06267	-431.13188	463.85135	1
4248	O	62.67600	86.19280	74.08490	502.92737	-462.55454	-395.89719	1
4249	N	63.54200	86.18680	76.12590	-408.17442	-673.09304	304.97819	1
4250	H	63.94200	85.72380	76.91290	-3039.24047	276.65651	-764.65990	1
4251	C	63.04400	87.46780	76.40390	44.70488	455.93402	-788.40132	1
4252	H	61.96800	87.39480	76.34390	-1667.93073	2647.00364	331.06652	1
4253	C	63.35300	87.79980	77.87690	-598.46551	647.21875	-233.23361	1
4254	H	64.45200	87.72880	78.01890	-278.17736	-309.07368	3118.54406	1
4255	C	62.94900	89.29880	78.18190	606.71934	-594.83637	-330.92649	1
4256	H	63.57100	90.00980	77.59890	-1132.92528	2028.61754	-2121.18302	1
4257	H	63.03800	89.62780	79.23990	586.02889	-902.88286	2956.28126	1
4258	H	61.86000	89.47680	78.05590	2126.22108	-767.41858	-2188.25933	1
4259	C	62.60100	86.80080	78.81690	367.53153	-446.54527	704.96021	1
4260	H	62.53600	85.76480	78.42190	-1942.42350	-2208.91700	-1116.20020	1
4261	H	61.56000	87.13080	79.01890	837.13409	-1604.10293	-2573.76893	1
4262	C	63.36500	86.71780	80.15690	-425.39329	-530.02168	607.92152	1
4263	H	62.93200	86.02680	80.91090	-3126.52227	-254.11949	-241.88426	1
4264	H	64.35900	86.24380	80.00790	2339.91868	648.99618	2000.45264	1
4265	H	63.35000	87.69880	80.67790	-2132.14493	2044.44772	1082.78241	1
4266	C	63.62200	88.55180	75.49490	-777.04139	389.13413	-276.10200	1
4267	O	62.90700	89.44980	75.09090	-623.18562	357.24860	328.08590	1
4268	N	64.93800	88.51180	75.25590	535.72064	-628.81794	173.96459	1
4269	H	65.58600	87.90280	75.70590	-2387.27561	2046.77673	-99.22908	1
4270	C	65.57500	89.44880	74.36590	144.86321	443.59837	-783.38122	1
4271	H	65.34500	90.45980	74.66690	-2769.77704	-411.56968	-1434.28441	1
4272	C	67.14800	89.20280	74.37090	-688.59560	247.79742	-543.95178	1

4273	H	67.44500	88.23180	73.91890	-2274.23592	-1380.20099	1679.61972	1
4274	H	67.47200	89.10980	75.42890	2155.13779	1737.92999	-1494.39176	1
4275	C	67.91700	90.44380	73.95490	-334.06105	814.45484	237.73417	1
4276	O	69.15300	90.38580	73.78690	-667.95610	393.77320	149.68150	1
4277	O	67.30500	91.53180	73.82090	-561.65531	473.79940	289.28303	1
4278	C	65.14400	89.32380	72.90190	372.50462	-49.14678	-830.82845	1
4279	O	64.90300	90.28580	72.17490	583.88468	-74.22430	-526.49469	1
4280	N	64.79100	88.07980	72.53990	-241.74926	-305.80538	-748.80749	1
4281	H	65.07900	87.29980	73.08990	1028.72721	2880.29732	737.45095	1
4282	C	64.05000	87.77080	71.30790	-381.90911	-806.75133	186.41008	1
4283	H	64.54100	88.24280	70.46990	-2646.60051	-1684.85058	234.54313	1
4284	C	64.03200	86.26380	70.91690	-480.12005	509.59444	584.16543	1
4285	H	63.45300	85.74580	71.71090	368.86763	2307.58677	2106.46770	1
4286	H	63.59700	86.24480	69.89490	-190.21284	44.93046	3140.06792	1
4287	O	65.28700	85.69280	70.81490	475.91158	428.92284	-461.69318	1
4288	H	65.74900	85.77980	71.65090	-577.08106	-2276.39413	2093.61731	1
4289	C	62.61000	88.31980	71.28190	496.40988	544.83045	-536.83146	1
4290	O	62.05800	88.75280	70.22290	777.96265	-10.66516	-135.23163	1
4291	N	61.82700	88.28880	72.38990	718.02271	425.55357	126.56950	1
4292	H	62.31400	87.88780	73.16190	-2039.59803	925.04983	2209.64905	1
4293	C	60.49700	88.86780	72.56790	356.19728	-566.43827	619.45314	1
4294	H	59.95400	88.60980	71.67090	-2487.96707	453.02335	1871.63456	1
4295	C	59.71400	88.52580	73.88190	898.54614	-154.90224	8.43378	1
4296	H	58.66500	88.88680	73.93990	-1300.38834	-1001.29396	2684.14359	1
4297	H	60.24300	88.94580	74.76490	1247.02449	2887.54142	-72.53085	1
4298	C	59.61000	87.05380	74.08590	-511.65030	-560.09113	505.92776	1
4299	C	59.50900	86.23880	72.95590	452.02409	-550.02019	-569.73942	1
4300	H	59.52300	86.56480	71.92690	-2176.88894	-1346.75866	1829.10412	1
4301	C	59.30100	84.85880	73.12290	25.30453	-618.46486	669.56098	1
4302	H	59.12100	84.20580	72.28090	1154.23989	2424.67675	1639.17636	1
4303	C	59.18800	84.30980	74.35190	550.80277	-533.65806	493.23056	1
4304	H	59.20900	83.23180	74.40590	-120.72906	-1414.18726	-2807.79720	1
4305	C	59.53100	86.46980	75.36190	598.14968	440.98937	-528.39032	1
4306	H	59.61000	87.05880	76.26390	-2928.88016	253.02367	1120.65440	1
4307	C	59.32900	85.10380	75.47890	414.74357	-762.39785	279.62170	1
4308	H	59.40800	84.60080	76.43090	499.78648	3074.09538	445.39565	1
4309	C	60.57300	90.36780	72.47590	436.61691	785.06542	156.48951	1
4310	O	59.69300	91.01980	71.88190	430.69699	-370.22122	548.69261	1
4311	N	61.61200	91.00880	73.03090	470.13990	-413.92238	565.95851	1
4312	H	62.26600	90.52480	73.60690	-2740.88441	-1269.73649	879.51583	1
4313	C	61.98300	92.38380	72.83590	367.50565	654.02190	-518.31067	1
4314	H	61.06200	92.92380	73.00090	1959.92137	1776.09116	-1703.65332	1
4315	C	62.99500	92.85080	73.91290	-198.05729	880.31189	131.43552	1
4316	H	63.71500	92.00380	73.92790	-3114.93931	411.84340	160.51277	1
4317	C	63.69900	94.14680	73.48490	157.77493	552.46376	708.05498	1
4318	H	64.24300	94.07580	72.51890	1195.18092	2790.02674	827.96111	1
4319	H	63.00600	94.98380	73.25290	-2573.91313	1146.18715	1399.80443	1
4320	H	64.33500	94.69180	74.21490	-1940.69466	-2305.82958	902.81803	1
4321	C	62.33300	92.81780	75.33690	-179.94500	562.41271	694.81130	1
4322	H	61.96200	91.77980	75.47190	-509.21854	1673.33294	2615.12515	1
4323	H	61.49500	93.54180	75.42490	96.74515	2211.27671	2235.87162	1
4324	C	63.29200	93.07080	76.48090	-199.74951	-261.89426	-850.27204	1
4325	H	62.74900	92.97680	77.44590	-1413.72772	-1792.56813	2164.78628	1
4326	H	63.67800	94.11280	76.48690	-2387.85302	2048.47276	-11.98002	1
4327	H	64.14200	92.35980	76.40090	-2485.99538	-274.11740	1908.64162	1
4328	C	62.32600	92.76680	71.39490	-49.24127	-765.60269	492.82737	1
4329	O	61.76600	93.71080	70.85690	476.70310	269.15676	-569.15378	1
4330	N	63.11700	91.91480	70.68990	686.68948	-345.49041	348.95018	1
4331	H	63.47100	91.13780	71.20390	-2023.53646	-943.86499	-2216.44880	1
4332	C	63.42100	91.92980	69.22690	-284.34473	-810.44076	-306.24312	1
4333	H	63.88600	92.87780	69.00090	1766.57290	-1355.40181	2222.68584	1
4334	C	64.48700	90.89480	68.84690	-308.06672	96.57155	-852.77185	1

4335	H	64.02300	90.03680	68.31490	-1699.33147	2162.14703	-1528.27321	1
4336	H	65.03700	90.51580	69.73490	-2666.31805	-769.34019	-1482.25839	1
4337	C	65.55300	91.46880	67.92090	904.72499	58.38217	97.54597	1
4338	H	65.88900	92.36180	68.49090	-1413.37723	2175.77700	-1779.49023	1
4339	C	66.74300	90.55080	67.77190	659.96935	-437.60804	452.09585	1
4340	H	66.70500	89.77780	66.97590	1794.26758	-2584.25429	21.44302	1
4341	H	67.04300	90.04280	68.71390	-1761.65116	-1460.27037	2159.26420	1
4342	H	67.68000	91.13080	67.63490	1724.67085	-2619.58559	248.00812	1
4343	C	64.99000	92.02780	66.62490	812.45115	300.03345	285.22632	1
4344	H	64.39000	92.93380	66.85590	2225.25523	324.28708	2200.29617	1
4345	H	65.78300	92.40380	65.94390	2952.33407	1076.43689	-152.42505	1
4346	H	64.40900	91.25080	66.08390	2054.98316	-1999.50370	1295.08895	1
4347	C	62.22200	91.80780	68.30290	-511.02145	598.77157	-460.19636	1
4348	O	62.08600	92.56080	67.36590	-732.03870	30.85435	-294.60919	1
4349	N	61.34400	90.81980	68.58590	-137.52035	-125.26974	823.44881	1
4350	H	61.49700	90.14980	69.30790	2625.39759	170.09980	1725.27672	1
4351	C	60.25300	90.53480	67.66990	-908.48253	-56.74423	-53.76416	1
4352	H	60.49700	90.84480	66.66490	958.44099	2762.76686	-1160.48972	1
4353	C	59.80500	89.01380	67.63290	-77.98446	837.93255	351.05338	1
4354	H	58.96000	88.88580	66.92290	-1628.59390	1608.24391	2158.57816	1
4355	H	59.39100	88.62780	68.58790	2203.20574	614.73801	2160.14070	1
4356	C	60.97000	88.07680	67.26890	253.91082	742.44824	-464.48995	1
4357	H	61.92200	88.30480	67.79390	1475.13688	-2598.50945	984.85840	1
4358	C	60.64600	86.53780	67.53890	-751.68450	-513.33146	53.96512	1
4359	H	61.58000	85.93980	67.48090	2936.79641	-326.08156	-1080.33510	1
4360	H	59.86300	86.24980	66.80490	-957.49656	644.10162	-2926.86858	1
4361	H	60.31500	86.54780	68.59990	2959.72686	241.99668	1039.07689	1
4362	C	61.22200	88.19580	65.74490	354.96439	-422.35485	725.99426	1
4363	H	62.08300	87.54380	65.48490	810.74681	-2204.10055	-2093.52731	1
4364	H	60.28400	87.83380	65.27190	1991.78702	1591.56674	-1843.34642	1
4365	H	61.54500	89.20880	65.42090	883.86084	1973.04114	2285.63446	1
4366	C	59.02200	91.36880	68.05590	361.20375	791.18508	-273.87776	1
4367	O	58.06000	91.49180	67.27790	-162.46777	-380.12080	-672.85929	1
4368	N	59.09400	92.15380	69.13390	-769.07544	199.47098	285.31839	1
4369	H	59.94300	92.03980	69.64290	2245.11343	1250.57882	1814.86763	1
4370	C	58.27900	93.28280	69.53090	-521.15520	738.01222	-123.23241	1
4371	H	58.91100	93.87680	70.17490	-2281.03347	-35.68296	2166.52700	1
4372	C	58.07200	94.37680	68.44190	141.58468	-386.29826	-813.74347	1
4373	H	57.58200	94.03080	67.50590	435.60624	2471.35445	-1897.59864	1
4374	H	57.34300	95.11580	68.83890	-687.92666	2247.46218	-2091.38635	1
4375	C	59.37100	95.22880	68.23990	-58.45589	-777.88053	-472.16077	1
4376	H	60.11800	94.59680	67.71390	-2448.74411	-1583.94155	1180.25745	1
4377	H	59.87800	95.63380	69.14190	2832.33529	868.90613	-1058.82254	1
4378	C	59.00200	96.42980	67.42990	215.41922	151.87551	872.91431	1
4379	O	58.24300	97.34480	67.84890	-454.54374	466.44157	446.59767	1
4380	O	59.36800	96.47080	66.23290	546.80057	349.08473	450.30681	1
4381	C	57.02900	92.96280	70.36990	-718.01438	561.60954	-22.38493	1
4382	O	56.13800	93.83780	70.46390	-571.70451	540.68598	-66.63222	1
4383	N	56.98000	91.76780	70.91190	9.26674	692.79998	482.30136	1
4384	H	57.72300	91.10880	70.83290	90.31959	-2201.23711	2246.02400	1
4385	C	55.88300	91.32880	71.76290	-100.60129	-608.55914	-671.55503	1
4386	H	55.00300	91.49780	71.15990	-1776.98377	1184.77817	2310.16354	1
4387	C	56.15900	89.81180	72.05990	-92.96948	-263.79740	-867.88168	1
4388	H	57.14500	89.73180	72.56590	2737.29581	-183.30220	-1540.07733	1
4389	C	55.05100	89.32380	72.95190	363.49373	-833.06919	72.93171	1
4390	H	55.05500	88.22180	73.09590	1524.23176	2746.28700	181.24982	1
4391	H	55.19400	89.75780	73.96490	985.47413	1980.04105	2237.52193	1
4392	H	54.04400	89.58180	72.55990	-2619.55744	1712.79383	-320.12862	1
4393	C	56.34800	89.02380	70.73890	-286.60934	651.20748	-570.29371	1
4394	H	57.24700	89.32080	70.15890	1136.48729	1642.34113	2430.91310	1
4395	H	55.58800	89.36780	70.00490	-2292.05810	-2134.41636	298.26612	1
4396	C	56.50200	87.49080	70.85790	744.48531	-235.20460	-471.03230	1

4397	H	56.73200	86.94080	69.92090	-402.36676	2622.43372	-1690.90763	1
4398	H	57.31500	87.25580	71.57690	-1236.15168	-2871.10828	-356.21972	1
4399	H	55.50300	87.14480	71.20190	2153.89519	-1474.75064	-1756.15270	1
4400	C	55.76600	92.25280	72.96690	134.31473	-568.52658	700.13433	1
4401	O	54.65300	92.72280	73.33990	113.09774	-162.58944	764.46112	1
4402	N	56.88400	92.58880	73.50690	380.05954	-682.57389	-319.87486	1
4403	H	57.73700	92.27980	73.09290	1693.25364	-436.33977	-2615.47815	1
4404	C	57.01300	93.31680	74.76590	406.01346	440.19272	687.62959	1
4405	H	56.03600	93.61680	75.11690	2479.87840	1934.54434	-77.25001	1
4406	C	57.46400	92.44880	75.95490	-726.97172	-137.95170	532.85312	1
4407	H	57.55200	93.08580	76.86090	-2067.71498	2356.65572	262.59246	1
4408	C	56.41600	91.42680	76.31290	-31.39083	-887.09872	-208.61803	1
4409	H	55.37100	91.71680	76.07290	-2476.26877	-1846.46220	-597.40820	1
4410	H	56.58000	90.43780	75.83390	2203.12138	1077.81493	1970.48151	1
4411	H	56.50200	91.14880	77.38490	-666.97644	-2930.26221	-931.09186	1
4412	C	58.87700	91.85880	75.79190	793.70700	435.86914	-107.23005	1
4413	H	59.62000	92.66980	75.63290	520.20988	2252.86080	-2133.59465	1
4414	H	58.76600	91.36580	74.80190	-1609.62309	941.31790	-2534.02059	1
4415	C	59.44300	90.91480	76.88690	-505.18802	632.31375	420.01832	1
4416	H	60.48200	90.69380	76.56190	-683.53794	2896.37661	-1020.78628	1
4417	H	58.85100	89.98080	76.99690	473.10784	-2241.19085	2156.72408	1
4418	H	59.57900	91.43880	77.85790	-666.46335	-3074.42538	-44.28782	1
4419	C	57.83900	94.51480	74.62190	-494.92836	714.30571	276.15987	1
4420	O	58.88000	94.49180	73.99490	334.39491	-511.97831	499.68538	1
4421	N	57.43500	95.63580	75.27990	-92.15096	754.15181	368.01568	1
4422	H	56.52300	95.78680	75.65390	-905.72856	2520.55901	-1650.65571	1
4423	C	58.25800	96.83880	75.22690	844.78454	-231.50281	-253.37033	1
4424	H	59.20600	96.64080	74.74990	-843.31977	2783.22906	1200.28079	1
4425	C	57.58400	97.93780	74.39090	219.47670	-178.65264	866.81268	1
4426	H	58.24300	98.83180	74.37090	2799.11058	1207.34245	-778.15835	1
4427	H	56.59600	98.21880	74.81490	1912.41463	-1540.89628	-1966.35072	1
4428	C	57.42100	97.46980	72.89890	581.89159	-306.29449	631.69365	1
4429	H	58.44600	97.33480	72.48990	2743.78894	363.10605	-1495.99548	1
4430	H	56.78500	96.56080	72.84690	2185.89880	411.46194	2225.03297	1
4431	C	56.77400	98.51580	72.03390	-392.49675	779.90036	262.96907	1
4432	H	57.23300	99.49080	72.30390	2113.82102	-1802.78182	-1476.47032	1
4433	H	55.68700	98.57780	72.25190	1936.97873	-318.32427	-2458.66006	1
4434	C	56.95100	98.32980	70.53290	-256.14584	-870.89224	85.94778	1
4435	H	56.19100	98.90980	69.96590	-2792.73516	836.04161	-1183.16988	1
4436	H	56.80600	97.25080	70.31390	2380.20070	462.98942	-2004.62257	1
4437	N	58.24300	98.82280	70.07890	269.42694	702.65764	-382.56195	1
4438	H	58.40600	98.41180	69.13790	-1088.41930	2343.68214	1794.63747	1
4439	H	58.32600	99.85380	69.96590	2466.54525	-1470.99767	1284.73600	1
4440	H	59.00800	98.48680	70.69790	-2898.84773	1204.56099	-209.62082	1
4441	C	58.57400	97.24380	76.66790	-621.34123	-127.45546	655.08868	1
4442	O	57.69300	97.31680	77.49190	506.82086	-71.37615	601.38614	1
4443	N	59.87100	97.37780	76.93290	-362.31753	-195.55717	736.99097	1
4444	H	60.59300	97.31280	76.24790	-2778.00772	-1318.17235	665.82354	1
4445	C	60.44500	97.48380	78.27490	393.16436	-561.94487	600.90828	1
4446	H	59.65900	97.62580	79.00190	-2131.49500	-1717.19315	-1551.19405	1
4447	C	61.26600	96.19680	78.67890	-609.35985	-508.40593	-449.06011	1
4448	H	61.68100	96.35180	79.69790	-1080.04612	2703.63969	-1192.50116	1
4449	H	62.16300	96.06980	78.03490	2147.16784	1855.36260	-1358.50143	1
4450	C	60.44600	94.85480	78.66090	-91.62198	-633.26907	649.63582	1
4451	H	59.94200	94.74080	77.67690	2004.87724	-917.90028	2244.13738	1
4452	H	61.09700	93.95880	78.74790	-1846.75850	-1569.59195	2006.01355	1
4453	C	59.44500	94.78580	79.82490	-429.34184	699.98786	-396.40078	1
4454	O	58.22300	94.90280	79.62490	685.67099	-232.79582	-315.10098	1
4455	N	59.93100	94.46580	81.06390	498.11152	672.86346	108.68287	1
4456	H	60.91600	94.51480	81.23090	-2542.61648	69.24054	-1851.62993	1
4457	H	59.20800	94.33680	81.74290	-1065.19003	2525.37634	-1544.69115	1
4458	C	61.34100	98.72380	78.30790	303.76043	-694.25907	-507.13405	1

4459	O	61.82800	99.19480	77.29590	413.80603	-499.77224	450.13276	1
4460	N	61.58800	99.25980	79.51490	386.03956	-521.49301	540.08405	1
4461	H	61.24200	98.89480	80.37590	-1364.92434	1888.69026	2113.77786	1
4462	C	62.61800	100.32780	79.69390	-803.35923	284.74248	324.01647	1
4463	H	62.67200	100.57080	80.74490	238.34568	-327.90415	-3119.91930	1
4464	H	62.35800	101.15980	79.05690	2675.80429	15.16577	1654.71074	1
4465	C	63.99200	99.94280	79.36590	629.10956	-658.07772	-51.04782	1
4466	O	64.38600	98.79380	79.32990	-672.53849	-407.94647	69.99204	1
4467	N	64.77500	101.00880	79.16790	492.08962	-594.47331	-342.23029	1
4468	H	64.32700	101.89080	79.03990	-360.83645	2185.87360	2233.82629	1
4469	C	66.24800	101.05880	78.91790	-537.72735	492.34922	547.62446	1
4470	H	66.37700	100.57780	77.95990	-1208.33463	866.62565	-2772.56445	1
4471	C	66.79800	102.45580	78.81090	591.95417	-488.75801	-492.09438	1
4472	H	67.79900	102.35780	78.33790	2031.23839	-2349.62109	501.57510	1
4473	H	66.90700	103.00680	79.76990	-2047.39412	1288.41154	2011.56637	1
4474	S	65.81700	103.59380	77.81590	-515.34854	-26.50207	211.95313	1
4475	C	66.99300	100.29880	79.98790	-306.99949	115.12686	-850.85141	1
4476	O	67.88000	99.47380	79.77390	-567.17695	173.32166	-521.43757	1
4477	N	66.54400	100.51380	81.27890	-401.10325	-435.01105	602.12445	1
4478	H	65.83100	101.17780	81.48990	455.12354	-2523.91253	1822.34858	1
4479	C	67.02000	99.88180	82.51790	-576.96346	558.08937	432.55107	1
4480	H	68.09700	99.96080	82.54290	2074.18141	1975.37048	1301.50266	1
4481	C	66.41100	100.64180	83.75890	407.94169	730.32140	-362.85704	1
4482	H	65.35100	100.81480	83.47490	-2239.46140	-1264.23948	-1812.38445	1
4483	H	66.89900	101.63880	83.80190	851.36305	-1080.65734	2829.41459	1
4484	C	66.54800	99.88680	85.09890	-504.07707	749.61930	-124.21035	1
4485	H	65.85400	99.02280	85.18090	-892.64623	-2909.71836	-796.83625	1
4486	H	67.51100	99.33480	85.13890	-213.12526	2504.55416	-1892.09204	1
4487	C	66.28900	100.87080	86.19690	683.05188	165.99099	580.80816	1
4488	O	67.32800	101.19980	86.84990	-136.38829	-280.21718	-725.60581	1
4489	O	65.16300	101.30180	86.50690	488.89598	-379.67191	490.36435	1
4490	C	66.79500	98.34580	82.63090	886.72408	84.15160	-195.16639	1
4491	O	67.69400	97.57980	83.10990	-541.19789	573.40571	-44.02227	1
4492	N	65.61600	97.84880	82.17690	721.91217	-387.58309	203.21036	1
4493	H	64.80900	98.39780	81.97690	-1858.76061	2369.05327	-911.49426	1
4494	C	65.33400	96.43080	81.99190	-829.63214	226.75513	-302.89212	1
4495	H	65.52200	95.82880	82.86790	2343.03941	2070.51780	-348.35126	1
4496	C	63.77200	96.26080	81.74690	-117.59870	773.92979	-467.60478	1
4497	H	63.24200	96.70480	82.61690	-2548.47429	-1654.52005	816.13017	1
4498	H	63.44900	96.78180	80.81990	-164.26450	-1334.80667	2844.21071	1
4499	C	63.35700	94.81080	81.66990	772.90078	10.18220	483.70623	1
4500	C	62.80900	94.10180	82.79790	523.00936	-420.34241	617.43378	1
4501	H	62.63100	94.62380	83.72690	-2716.64045	-1419.01509	-710.27255	1
4502	C	62.39200	92.77480	82.62990	311.39012	-821.47456	-244.26776	1
4503	H	62.00500	92.28580	83.51190	-1549.67754	-1858.50510	2010.64282	1
4504	C	62.62400	92.09880	81.42490	-116.25282	-579.89728	-694.01400	1
4505	H	62.26000	91.08280	81.39790	1248.81659	2315.15295	-1725.90561	1
4506	C	63.54400	94.11580	80.48690	-180.62298	672.16442	-589.08516	1
4507	H	63.94400	94.68880	79.66390	2349.07241	1916.45918	-840.99300	1
4508	C	63.21900	92.80580	80.33990	512.23643	556.47921	-509.30907	1
4509	H	63.36400	92.28080	79.40790	2405.06051	1090.59627	-1710.11987	1
4510	C	66.22000	95.81380	80.94590	587.13112	-424.77149	-553.44127	1
4511	O	66.65800	94.68880	81.18290	-433.30365	-349.67624	560.00152	1
4512	N	66.39900	96.46680	79.80590	-378.96959	-303.45803	-690.62838	1
4513	H	65.93900	97.33380	79.63390	-2740.48121	-1317.03747	-808.33239	1
4514	C	67.29500	95.96780	78.75290	-523.32395	654.59471	-359.28932	1
4515	H	66.93300	94.96880	78.55890	-826.69346	72.22315	-3034.73029	1
4516	C	67.06200	96.78780	77.47690	779.89052	-312.14183	354.66782	1
4517	H	67.18400	97.87680	77.66490	1775.24687	-2170.05852	1427.43505	1
4518	H	67.78700	96.49380	76.68690	-1848.52398	-2536.00268	223.32879	1
4519	C	65.64500	96.51380	76.88790	892.27510	130.37498	-135.27197	1
4520	H	64.89400	97.05180	77.50390	-2492.32341	-1917.99827	88.50355	1

4521	H	65.48400	95.41480	76.91390	525.92815	2034.88297	2341.12732	1
4522	C	65.47300	96.99180	75.50790	854.37408	-197.50180	-249.97796	1
4523	O	66.20800	96.42980	74.63790	601.86227	-133.33160	493.57038	1
4524	O	64.61400	97.86580	75.15490	-700.63094	361.70562	-43.73277	1
4525	C	68.72300	95.85580	79.13490	630.02516	590.06238	-293.84637	1
4526	O	69.44300	94.87880	78.86890	-604.34468	-228.20875	-454.21966	1
4527	N	69.24100	96.86280	79.91290	31.23487	306.04149	-786.15220	1
4528	H	68.82800	97.76980	79.93290	-741.83341	-3017.75172	491.00302	1
4529	C	70.56400	96.79380	80.57090	54.96050	712.40195	566.49254	1
4530	H	71.32700	96.63980	79.82290	946.57754	-1959.41970	2272.19974	1
4531	C	70.83400	98.12880	81.32590	-797.20287	-440.87872	-39.30068	1
4532	H	70.03100	98.34680	82.06290	-1168.23346	2583.42648	-1363.58514	1
4533	H	70.80400	98.94380	80.57190	-2104.96005	2262.06444	591.97457	1
4534	C	72.15200	98.17780	82.12990	-542.24403	-576.70649	-452.58374	1
4535	O	71.96400	97.99580	83.33490	-736.90470	202.24862	199.23401	1
4536	N	73.31500	98.45480	81.58790	-776.19999	83.93123	321.15636	1
4537	H	73.43300	98.38680	80.59690	-1383.01634	2757.98116	615.65571	1
4538	H	74.09200	98.74380	82.14690	2921.37174	-315.68092	-1124.34823	1
4539	C	70.66400	95.62680	81.57990	638.67776	-508.31582	406.39483	1
4540	O	71.63400	94.88780	81.55090	369.84116	-455.37454	528.65752	1
4541	N	69.57000	95.38880	82.35190	803.66949	-239.38050	97.38902	1
4542	H	68.96800	96.18380	82.34090	-2589.51248	-1310.92543	-1214.13583	1
4543	C	69.53900	94.32680	83.36790	227.23494	552.83012	-688.61756	1
4544	H	70.45500	94.44680	83.92590	2560.88098	-475.18417	1764.74215	1
4545	C	68.35200	94.52480	84.31790	87.53090	727.64337	-542.51680	1
4546	H	67.36300	94.44580	83.81990	-659.21951	-1877.00824	-2437.31326	1
4547	O	68.41100	95.81580	84.87890	-664.26496	135.27103	405.06918	1
4548	H	68.22700	96.47080	84.20190	-1867.79321	1268.57734	2190.95556	1
4549	C	68.40700	93.51880	85.52090	334.58799	259.61003	807.52988	1
4550	H	69.39000	93.63880	86.02390	-1287.43396	-2565.55837	1287.88598	1
4551	H	68.34500	92.45380	85.21090	-2476.00148	-792.48542	-1771.89440	1
4552	H	67.62300	93.68880	86.28990	-1667.92656	2667.01738	57.14440	1
4553	C	69.47200	92.96480	82.78390	-358.07958	-543.20095	-638.87616	1
4554	O	70.18300	92.01380	83.16790	-348.99905	488.97297	-512.57422	1
4555	N	68.69300	92.74580	81.70290	-109.01704	-621.71391	-560.58843	1
4556	H	68.07500	93.45380	81.37090	-730.30748	2639.49080	-1548.53658	1
4557	C	68.70100	91.53980	80.88390	-662.93073	114.45947	-615.52651	1
4558	H	68.48700	90.74380	81.58090	-2914.49762	-382.24865	-1121.52389	1
4559	C	67.46700	91.52180	79.94790	620.59277	629.21794	-224.50032	1
4560	H	67.43600	92.48480	79.39390	-2501.80883	-860.28054	-1702.67325	1
4561	C	67.58700	90.35180	78.97190	535.72959	-464.83957	-573.03489	1
4562	H	68.31500	90.60880	78.17290	2142.21755	-1801.19393	1436.95185	1
4563	H	67.83000	89.44380	79.56390	365.45387	-3097.29171	414.06972	1
4564	H	66.63000	90.11080	78.46090	19.85469	2330.68766	2113.22670	1
4565	C	66.22300	91.42980	80.81690	-707.73477	15.43062	574.73854	1
4566	H	66.46200	90.58180	81.49390	311.26424	2840.24579	-1316.94521	1
4567	H	65.95000	92.31380	81.43190	-2978.16376	394.76408	934.30623	1
4568	H	65.35400	91.25480	80.14690	-497.98330	798.72272	-3002.04612	1
4569	C	69.96800	91.16980	80.22890	-188.01956	-683.09886	-573.99965	1
4570	O	70.47700	90.03780	80.42490	-516.56066	134.50138	581.98084	1
4571	N	70.63000	92.18480	79.60790	-8.12667	4.64669	-844.14729	1
4572	H	70.22000	93.09380	79.61990	1523.40750	1233.98071	-2460.63964	1
4573	C	71.92800	91.98880	78.97590	724.33748	22.69976	-553.41751	1
4574	H	71.80600	91.16980	78.28290	-1470.38710	-1832.10135	-2092.74763	1
4575	C	72.28500	93.29280	78.21890	681.65803	232.56653	559.20134	1
4576	H	72.23900	94.14980	78.92390	652.18002	358.61990	3056.84138	1
4577	H	71.45200	93.48680	77.50990	2058.21365	2371.17056	198.82898	1
4578	N	73.90700	92.75580	76.30690	64.67433	628.99855	-559.33027	1
4579	C	73.69000	93.34780	77.52990	-638.33125	-339.06739	555.89344	1
4580	C	75.18200	92.83380	76.13690	826.59966	-137.74320	359.45906	1
4581	H	75.67100	92.43480	75.24890	423.03514	-1181.67822	2884.94438	1
4582	N	75.77500	93.60580	77.05090	344.91991	200.20735	744.05615	1

4583	H	76.65800	94.06280	76.94590	-1917.73075	2493.55337	-52.21686	1
4584	C	74.81900	93.91180	77.94990	678.46801	-128.43498	595.51375	1
4585	H	75.04900	94.45280	78.85990	774.59397	2493.51352	1755.16972	1
4586	C	73.04300	91.56380	79.87290	571.84372	618.60609	-348.95883	1
4587	O	73.74200	90.57580	79.61790	-197.21200	523.09428	-557.76969	1
4588	N	73.21000	92.24180	81.05590	291.77962	-277.67722	-741.91125	1
4589	H	72.64300	93.05680	81.13690	2270.83949	-1480.64662	-1596.62138	1
4590	C	74.29500	91.86580	81.98990	879.52314	114.28282	-211.72974	1
4591	H	75.18400	91.84580	81.37690	3132.16728	291.18965	-54.43283	1
4592	C	74.49600	92.83180	83.17390	78.17615	588.24346	692.32154	1
4593	H	74.67900	93.79680	82.65490	-1426.37341	-1249.81477	-2510.30838	1
4594	H	75.41600	92.54880	83.72790	2186.68951	-1572.98743	-1625.52323	1
4595	C	73.24000	93.09080	84.05290	662.55941	-622.36375	71.61974	1
4596	H	72.39000	93.37280	83.39590	1014.02519	-748.94488	-2882.54414	1
4597	H	72.91000	92.17080	84.58190	-2715.90045	-1346.48108	-842.08058	1
4598	C	73.48100	94.11680	85.15190	683.93941	403.93374	447.78948	1
4599	H	74.37300	93.91880	85.78490	-1782.77323	-757.13202	2479.25331	1
4600	H	72.53000	94.04580	85.72190	-1822.53489	-1756.39145	-1868.60426	1
4601	C	73.73200	95.54680	84.66290	545.29584	421.51497	597.01640	1
4602	H	74.72900	95.68580	84.19190	-1318.14961	-1395.73166	2492.51699	1
4603	H	73.03400	95.83680	83.84890	-2464.75156	-1620.10531	1094.75328	1
4604	N	73.60600	96.46680	85.77390	561.38981	247.02334	-580.08037	1
4605	H	74.04900	97.33580	85.41290	1370.40643	2602.82682	-1116.02195	1
4606	H	72.64200	96.65680	86.11590	2090.48050	1654.70179	1670.35310	1
4607	H	74.11500	96.04880	86.57890	-1191.70596	1390.46465	-2558.25550	1
4608	C	74.20000	90.47680	82.54090	-487.72473	-733.52937	235.60615	1
4609	O	75.22000	89.85080	82.71690	-64.51248	165.60396	769.44181	1
4610	N	72.94000	89.98980	82.82990	-148.33868	752.92200	-351.81869	1
4611	H	72.15000	90.54180	82.57590	2035.76327	-1173.54162	-2092.05502	1
4612	C	72.77300	88.66980	83.39290	-879.23319	-48.37224	-236.77022	1
4613	H	73.52500	88.46980	84.14290	-1609.14643	2702.54311	-71.65699	1
4614	C	71.49900	88.70180	84.21990	37.83587	910.21525	-39.08526	1
4615	H	71.14700	87.66280	84.38990	1.38984	2099.06627	2343.53261	1
4616	H	70.72900	89.15680	83.55990	-1754.78517	-2513.90825	-706.55541	1
4617	C	71.47600	89.29880	85.56990	476.93117	-776.51260	-31.87236	1
4618	C	70.77800	90.40080	85.96290	-110.62230	274.39981	-862.50707	1
4619	H	70.21900	90.99680	85.25690	-1962.41917	-1198.03341	2147.52257	1
4620	N	70.97100	90.65280	87.28890	402.81749	-571.48394	-473.09245	1
4621	H	70.71100	91.40380	87.85690	-719.28466	346.24748	3043.18394	1
4622	C	71.85300	89.77980	87.78790	292.22307	507.77742	698.72654	1
4623	C	72.27800	88.91180	86.70390	-431.23208	292.37630	-748.33548	1
4624	C	73.18300	87.88980	86.97590	110.92114	-779.99310	459.08416	1
4625	H	73.42800	87.26580	86.12990	2287.71933	-289.27582	2140.30045	1
4626	C	73.70000	87.73080	88.28690	750.75952	468.30409	-220.23266	1
4627	H	74.41700	86.99880	88.62790	3082.43382	241.78196	-581.69534	1
4628	C	72.45600	89.67880	89.07590	-701.25082	-569.31201	124.82837	1
4629	H	72.15800	90.33180	89.88290	1529.77907	-1868.58338	-2016.53128	1
4630	C	73.40800	88.65980	89.24590	-650.35960	-636.88868	53.44349	1
4631	H	73.93400	88.44380	90.16390	1857.00231	-163.59676	-2534.36476	1
4632	C	72.69700	87.57380	82.32990	658.27244	-45.77019	629.31192	1
4633	O	72.97000	86.37880	82.59190	-694.70592	143.09943	347.17930	1
4634	N	72.52100	87.89680	81.03990	453.39732	-467.60282	-537.07612	1
4635	H	72.43400	88.83280	80.70790	-393.16373	-1866.50407	2501.96145	1
4636	C	72.62800	86.81380	80.01690	-458.79092	447.13632	-648.86902	1
4637	H	71.96700	86.00480	80.28890	1427.84479	-2257.51374	1662.26267	1
4638	C	72.23300	87.26580	78.62290	-794.34215	395.95106	-209.03184	1
4639	H	72.65300	88.28780	78.50190	-632.15630	1171.48271	-2850.65482	1
4640	C	72.84300	86.40880	77.46290	-492.29276	743.76479	-189.50668	1
4641	H	73.95100	86.34980	77.52190	1111.17608	1705.86769	-2398.65157	1
4642	H	72.65800	86.89280	76.48090	-508.42400	-2045.45502	2335.77504	1
4643	H	72.31200	85.43280	77.48490	-2905.79766	-561.37702	-1067.43712	1
4644	C	70.68700	87.36480	78.40590	474.61880	-778.50760	-10.67300	1

4645	H	70.17800	87.61580	79.36090	2505.63229	-493.60750	1837.49413	1
4646	H	70.28600	86.36180	78.14590	-2088.49886	2257.64032	662.91699	1
4647	C	70.16400	88.41780	77.37290	-137.92445	-819.75694	-374.73511	1
4648	H	70.16200	89.45380	77.77490	1957.10291	-2458.53115	153.61966	1
4649	H	70.78400	88.37580	76.45190	1932.01789	2179.48750	-1189.69212	1
4650	H	69.12400	88.13080	77.10890	-2594.16435	416.06165	1730.73113	1
4651	C	74.09800	86.35680	79.99190	-45.64211	821.74823	-392.55273	1
4652	O	74.44300	85.17380	79.88790	-352.34390	397.93196	-584.06434	1
4653	N	75.07900	87.26580	80.13590	737.87333	-276.43125	-302.98680	1
4654	H	74.93300	88.23280	80.33190	-2233.39283	-1780.45828	1319.14783	1
4655	C	76.53100	86.84580	80.13590	653.50581	439.88827	459.21615	1
4656	H	76.71700	86.27180	79.24090	-1159.23066	-1613.09012	-2439.74400	1
4657	C	77.40900	88.11280	80.22090	-576.65164	700.18875	-93.05699	1
4658	H	77.21600	88.75580	81.10590	2183.85902	-1768.74676	1414.39771	1
4659	H	78.45900	87.76480	80.12190	2384.49466	930.86428	-1829.18101	1
4660	O	77.20500	88.90880	79.06090	-144.64983	220.02156	744.50935	1
4661	H	77.49200	88.41880	78.28790	-857.99633	639.18082	-2958.63421	1
4662	C	76.88800	85.98480	81.37890	423.49418	466.81827	-658.92669	1
4663	O	77.68100	85.04580	81.27590	-303.67832	-657.44464	-314.91785	1
4664	N	76.30800	86.30980	82.50890	-341.63208	771.76511	-18.39636	1
4665	H	75.81500	87.17280	82.58490	2671.56451	957.79820	-1357.78934	1
4666	C	76.52700	85.56580	83.70690	473.79959	-775.19806	-77.67188	1
4667	H	77.58500	85.35280	83.73190	1757.41538	1548.54438	2100.41132	1
4668	C	76.04800	86.41380	84.93190	-224.86717	416.92979	-779.13754	1
4669	H	74.99000	86.70980	84.76990	2129.80883	463.56755	-2268.75422	1
4670	C	76.15300	85.60480	86.26390	693.97884	573.33548	-145.36439	1
4671	H	75.89400	86.33780	87.05790	1022.76268	-2880.91752	-743.30139	1
4672	H	75.51400	84.69780	86.20590	-1205.53578	-2376.94491	1671.83810	1
4673	H	77.18100	85.20780	86.40790	2510.26980	-613.46551	-1794.55616	1
4674	C	76.77600	87.79080	84.99490	-652.83463	175.22999	-612.00686	1
4675	H	76.92500	88.38780	84.06990	-3061.43237	402.46148	603.22699	1
4676	H	76.25800	88.42580	85.74490	-1191.17830	-1617.91519	2421.08879	1
4677	C	78.21500	87.72780	85.60790	-755.02085	449.50697	-243.59392	1
4678	H	78.16500	87.32980	86.64390	-1608.59590	-2035.69557	-1779.49122	1
4679	H	78.53000	88.77680	85.79690	1713.38234	-2446.06988	-989.59048	1
4680	H	78.85800	87.16780	84.89690	-1758.95051	-2594.07582	274.02545	1
4681	C	75.78700	84.21280	83.67290	785.59210	-41.69588	-461.03959	1
4682	O	76.22800	83.19180	84.17690	-760.26374	-47.55351	208.24251	1
4683	N	74.61500	84.11980	83.04490	568.63411	-188.08241	-594.93911	1
4684	H	74.13500	84.95480	82.78790	-339.13717	2869.24803	-1245.24213	1
4685	C	73.91400	82.81280	82.88690	-714.12081	390.46939	411.11572	1
4686	H	74.00400	82.22380	83.78790	627.52040	2153.46706	-2206.13327	1
4687	C	72.40500	82.98880	82.63790	728.78165	-305.49799	-454.97175	1
4688	H	71.80800	82.06780	82.46190	-1939.59620	-1719.67361	1782.95134	1
4689	O	72.05500	83.93480	81.60190	-711.95499	-76.44498	333.02175	1
4690	H	72.41500	84.72780	82.00590	2028.88158	-1577.80108	-1814.49979	1
4691	C	71.88900	83.50080	83.95390	610.30246	-359.87625	573.99564	1
4692	H	72.21200	84.53380	84.20790	2197.15808	-1938.77183	-1145.37609	1
4693	H	72.03100	82.81280	84.81390	1808.91683	84.80891	-2572.71327	1
4694	H	70.78500	83.62080	83.92590	-1622.85904	-2138.11175	-1641.04629	1
4695	C	74.57400	81.90580	81.81590	620.58496	-666.18084	50.28313	1
4696	O	74.51000	80.70880	81.83790	-641.08760	129.02499	442.70360	1
4697	N	75.20800	82.54480	80.80190	479.05021	677.55215	155.26194	1
4698	H	75.17800	83.52780	80.63590	-837.16039	-1004.73959	2861.44842	1
4699	C	76.14000	81.91880	79.89590	163.53308	867.18234	229.57076	1
4700	H	75.54400	81.19980	79.35290	2581.68508	1356.24594	-1180.56144	1
4701	C	76.52300	82.92480	78.72290	281.23824	729.14528	-469.79061	1
4702	H	75.62500	83.11680	78.09690	2071.08828	-1560.73574	-1781.27019	1
4703	H	76.66500	83.94280	79.14390	2175.09361	-2265.87376	-181.68689	1
4704	C	77.84600	82.66780	77.99590	-611.28743	136.94309	662.58982	1
4705	H	77.88700	81.63180	77.59590	-1864.58453	2010.47920	-1542.57063	1
4706	H	78.72200	82.60580	78.67690	3008.43310	-858.42995	332.64770	1

4707	C	78.18500	83.71880	76.95690	-100.08441	-888.55719	178.60636	1
4708	O	77.71100	83.55580	75.80090	695.97028	2.01554	373.16019	1
4709	O	78.82900	84.76080	77.27790	526.81165	293.53919	509.83473	1
4710	C	77.35300	81.31380	80.52590	123.66998	725.30763	538.59594	1
4711	O	77.70100	80.15980	80.26390	-47.60118	737.08425	-279.40682	1
4712	N	77.95800	82.09480	81.38790	501.09383	643.90192	-216.72006	1
4713	H	77.75900	83.05180	81.58290	-1879.33957	-2215.99323	-1206.51688	1
4714	C	79.11300	81.64780	82.15290	-452.63025	499.63369	-613.95687	1
4715	H	79.84000	81.34180	81.41590	786.17076	-2556.41567	-1656.77418	1
4716	C	79.73600	82.80780	82.92590	554.46504	-703.14981	172.04613	1
4717	H	79.00500	83.27380	83.62090	2004.73176	-30.22616	2424.53360	1
4718	H	80.07200	83.58180	82.20390	1772.73343	-1970.85715	1694.51011	1
4719	H	80.64900	82.46280	83.45690	2.80618	2331.74634	-2112.14993	1
4720	C	78.82700	80.48580	83.13890	-364.78748	-599.64303	-582.07331	1
4721	O	79.55900	79.51980	83.22390	155.80951	287.15421	718.95277	1
4722	N	77.64800	80.51980	83.78290	449.33258	348.72806	623.82791	1
4723	H	77.05800	81.29980	83.58990	1784.10871	2072.15124	-1556.07570	1
4724	C	77.12500	79.38880	84.44290	-295.09981	-726.39276	465.53266	1
4725	H	77.86300	79.04080	85.15090	-2727.53363	-1206.29691	-1001.81550	1
4726	C	75.91800	79.80180	85.39390	-757.97348	-220.69563	-456.31201	1
4727	H	75.08100	80.21480	84.79090	1548.95543	-1156.06598	2482.43323	1
4728	H	75.49200	78.90680	85.89490	1945.07207	1925.55312	-1551.50444	1
4729	C	76.28200	80.82580	86.48490	-429.60876	81.85717	800.11669	1
4730	H	76.98000	81.55880	86.02790	3043.05091	527.76234	-599.61179	1
4731	C	74.98200	81.56780	86.85190	-739.86855	-312.57104	-431.67682	1
4732	H	75.18900	82.57080	87.28190	-2660.18509	-1222.97732	-1151.50683	1
4733	H	74.37200	80.96780	87.56090	447.33926	-2204.42072	2199.69159	1
4734	H	74.21300	81.76580	86.07590	-2694.53847	-1171.12975	-1125.23053	1
4735	C	77.11200	80.14080	87.64290	469.81814	-361.58067	-692.80686	1
4736	H	78.19900	80.15580	87.41590	-732.39479	-2433.87245	-1854.20845	1
4737	H	76.72400	79.10680	87.76490	765.36022	-721.81661	-2965.03469	1
4738	H	77.02300	80.76480	88.55790	-1923.97086	-2479.18462	224.06694	1
4739	C	76.81200	78.16480	83.60190	-22.31535	583.42087	700.40925	1
4740	O	76.88800	77.02780	84.09590	685.45654	-368.42810	-134.30301	1
4741	N	76.40900	78.34580	82.33290	119.54106	-327.95053	-768.65511	1
4742	H	76.25200	79.28280	82.02990	-478.66696	1307.72408	-2821.16322	1
4743	C	76.00000	77.24280	81.44990	226.40760	-710.74026	524.44150	1
4744	H	75.30300	76.60780	81.97590	-1972.63729	1232.05443	2118.71901	1
4745	C	75.34000	77.71080	80.16190	-746.49746	356.20258	-383.81280	1
4746	H	74.36600	78.17280	80.43090	-560.59934	2524.15006	-1792.37861	1
4747	H	76.02600	78.35680	79.57290	2904.65159	-1130.66475	427.57756	1
4748	H	75.07000	76.89780	79.45490	-1751.90925	-2497.87211	767.90308	1
4749	C	77.21500	76.45580	81.18090	254.29364	646.04355	591.11207	1
4750	O	77.05800	75.22780	81.01690	85.78053	472.65664	626.78914	1
4751	N	78.42600	76.99280	81.18490	358.51261	-73.79128	760.72061	1
4752	H	78.51000	77.98480	81.24190	2131.35755	-951.09259	2109.73081	1
4753	C	79.72500	76.37280	80.94990	790.95648	-213.49684	400.32231	1
4754	H	79.67100	75.84580	80.00890	-2579.11328	-1694.61832	-612.10266	1
4755	C	80.84500	77.40480	80.87490	-626.90113	612.71879	-251.04114	1
4756	H	81.81300	76.89780	80.67290	1830.89959	-2197.76584	-1309.90773	1
4757	H	80.83100	77.90280	81.86790	-790.79718	1507.55025	2645.78122	1
4758	C	80.72800	78.48680	79.85590	479.70328	135.08583	-763.60172	1
4759	C	79.79900	78.45180	78.78390	-183.74456	-156.55681	-879.30592	1
4760	H	79.19800	77.57480	78.59390	1926.01378	2015.95197	1457.61271	1
4761	C	79.71500	79.51180	77.92990	-489.63198	-675.39204	368.18083	1
4762	H	78.93100	79.51880	77.18690	-2290.19744	314.94731	2134.01736	1
4763	C	80.60300	80.61280	78.00890	-880.95828	130.84427	195.55891	1
4764	H	80.63700	81.41480	77.28690	-1401.23023	-534.01084	-2765.79328	1
4765	C	81.56500	79.61080	80.03390	-30.08665	719.81308	558.94089	1
4766	H	82.29100	79.66680	80.83190	-3115.34577	373.38735	231.14680	1
4767	C	81.49000	80.62980	79.09190	-431.76577	-325.69810	-734.13219	1
4768	H	82.21500	81.42980	79.14390	989.86037	1265.28560	-2705.07949	1

4769	C	80.06500	75.30780	81.89290	31.90069	-619.47539	-668.34391	1
4770	O	80.91900	74.45080	81.59690	674.12057	393.73415	119.00462	1
4771	N	79.44000	75.24380	83.07190	604.30545	-486.62010	-332.69820	1
4772	H	78.65900	75.82680	83.28190	105.38128	2691.56887	1625.60081	1
4773	C	79.63100	74.13880	83.98890	-66.99465	63.58043	907.14952	1
4774	H	80.68900	74.07380	84.19190	2817.10129	-1089.75806	880.11018	1
4775	C	78.87000	74.41180	85.37190	-411.44980	-610.69340	-537.78586	1
4776	H	78.83600	73.47280	85.96590	-1799.52483	-1148.24537	-2311.16187	1
4777	H	77.82200	74.75780	85.24390	738.91547	2930.71442	873.58066	1
4778	C	79.70500	75.33080	86.30090	16.30274	410.88287	813.85533	1
4779	C	79.44800	76.73280	86.29990	328.68061	-573.89021	-627.75002	1
4780	H	78.60500	77.12880	85.75290	2073.69103	1839.07786	1488.56453	1
4781	C	80.18400	77.60480	87.17890	-239.16738	833.38714	-282.33993	1
4782	H	79.91800	78.64980	87.23690	-69.32709	882.12279	-3019.15209	1
4783	C	81.22300	77.03480	87.99790	-586.87850	17.73531	-697.64610	1
4784	H	81.76900	77.73080	88.61790	22.20190	-2098.03390	2344.35216	1
4785	C	80.73400	74.83380	87.05290	-299.66440	445.90339	-736.76483	1
4786	H	80.89600	73.77180	87.15890	-2127.09584	-1154.87293	-2009.96469	1
4787	C	81.50200	75.61880	87.92690	-213.40335	885.98350	30.71242	1
4788	H	82.33500	75.21480	88.48390	-441.49341	2000.91161	-2387.39660	1
4789	C	79.16300	72.79280	83.47990	-512.18341	551.44290	-514.81054	1
4790	O	79.55200	71.72080	84.04290	546.98955	-434.99900	-367.70305	1
4791	N	78.30700	72.68380	82.44790	-838.63012	80.80121	53.31956	1
4792	H	77.94400	73.50180	82.00890	1039.05760	-615.25822	2905.17518	1
4793	C	78.01100	71.39980	81.79690	-309.55387	391.59378	-763.07386	1
4794	H	77.51000	70.87580	82.59890	1354.97506	1384.02390	-2479.26333	1
4795	C	77.14300	71.47680	80.57290	-596.12525	-477.18205	498.38036	1
4796	H	76.78100	70.46380	80.29490	-985.45094	-236.74442	-2978.43327	1
4797	H	76.21100	71.97380	80.91690	-387.48183	-1088.87301	2926.16466	1
4798	N	77.72300	73.44280	79.04490	341.93191	-771.55333	-21.45493	1
4799	H	77.43600	74.19280	79.63990	-1938.80414	-1989.10208	-1477.40910	1
4800	C	77.73900	72.10080	79.28290	344.02764	657.14981	530.33019	1
4801	C	78.21500	73.63280	77.79190	-501.13935	-650.85986	-395.84316	1
4802	H	78.09200	74.62580	77.35890	2928.43007	-608.88172	975.59552	1
4803	N	78.44100	72.46680	77.21390	490.42239	-384.41680	-569.54534	1
4804	C	78.16100	71.51680	78.14890	-688.54299	-588.20201	106.66745	1
4805	H	78.36500	70.47680	77.92590	1216.27355	1923.67520	-2172.18291	1
4806	C	79.20000	70.61280	81.39290	735.05954	475.77954	254.50403	1
4807	O	79.29400	69.44680	81.75690	-83.43832	41.34332	-784.19131	1
4808	N	80.23700	71.24080	80.70990	572.91786	430.53569	-446.17982	1
4809	H	80.12400	72.15080	80.31990	-1145.03920	-2406.47985	-1672.11428	1
4810	C	81.53600	70.68980	80.37790	262.62537	-782.51813	-387.48458	1
4811	H	81.30400	69.88380	79.69790	319.28447	-2656.90068	-1654.43720	1
4812	C	82.43700	71.71380	79.66390	595.61793	253.45936	-642.22165	1
4813	H	82.58700	72.59480	80.32390	637.66042	936.40154	2935.09243	1
4814	H	83.49300	71.39880	79.52090	1359.47320	-2172.67367	-1824.70490	1
4815	S	81.70000	72.38080	78.16590	99.41861	-448.52625	316.46604	1
4816	H	80.97600	71.33580	77.79290	1224.90468	-1566.27297	2438.15991	1
4817	C	82.28600	70.13480	81.59390	-536.82951	549.70559	491.00799	1
4818	O	82.97200	69.12480	81.49390	-432.37493	390.92855	532.77952	1
4819	N	82.03700	70.65580	82.81090	10.04037	-152.43001	830.26295	1
4820	H	81.50900	71.49380	82.92690	-1332.28925	1918.42969	2107.80908	1
4821	C	82.76200	70.16280	84.01490	-508.81131	510.36718	-558.64783	1
4822	H	83.68700	69.72280	83.67190	2442.91795	1691.13637	-1034.61871	1
4823	C	82.99500	71.37380	84.95390	747.48769	-516.64910	76.07140	1
4824	H	83.61300	70.98680	85.79290	-2661.14238	1489.24911	773.74709	1
4825	H	82.07200	71.89880	85.27890	-560.36490	-2073.15394	-2299.18467	1
4826	S	83.97900	72.63280	84.11290	-393.35366	170.28612	357.05201	1
4827	H	85.18200	72.12980	84.34390	-934.84142	706.51112	-2919.78420	1
4828	C	81.93800	69.10780	84.71990	-663.17384	500.13723	376.18375	1
4829	O	82.51800	68.29280	85.42290	-489.82023	-377.73486	-490.93762	1
4830	N	80.65300	69.10580	84.45990	620.55471	-132.67695	556.75935	1

4831	H	80.19800	69.73580	83.83490	-2555.32480	-1828.15402	-162.46305	1
4832	C	79.68700	68.14480	85.04490	-411.87352	253.31633	-773.07312	1
4833	H	80.05800	67.92580	86.03490	-1436.50210	-2775.98866	-358.57345	1
4834	C	78.28300	68.75380	85.06290	-345.68825	763.58357	359.01361	1
4835	H	77.45500	68.03180	85.23190	2182.10346	2181.03833	616.21628	1
4836	H	78.09100	69.16680	84.04990	1968.74098	-958.03083	-2259.30567	1
4837	C	78.00400	69.82480	86.20890	21.66441	198.75540	889.65046	1
4838	H	78.90500	70.47180	86.14290	-1124.67544	653.13390	-2864.74213	1
4839	C	76.81100	70.73680	85.85990	-442.51807	603.47208	521.00884	1
4840	H	76.67900	71.41480	86.72990	-1424.58125	2302.51876	-1602.24900	1
4841	H	77.14500	71.31780	84.97290	-1675.25388	735.45172	-2559.46507	1
4842	H	75.93600	70.06580	85.72890	2457.59394	1188.55643	1563.90277	1
4843	C	77.83700	69.07980	87.51390	259.07306	560.55749	670.90048	1
4844	H	76.86500	68.54180	87.53190	2630.65550	885.60610	1481.07384	1
4845	H	77.89600	69.81380	88.34590	1042.12469	-1661.88916	-2459.74120	1
4846	H	78.56200	68.26680	87.73190	100.03453	2293.77046	2151.00823	1
4847	C	79.65200	66.80780	84.29190	-497.04322	-497.78045	580.18417	1
4848	O	79.37600	65.74280	84.89590	483.03343	-539.98788	-314.19584	1
4849	N	79.98800	66.80280	82.99990	630.53445	-66.55911	557.37642	1
4850	H	80.13000	67.65680	82.50490	1403.00927	-2147.30901	-1821.77255	1
4851	C	80.27200	65.57980	82.21990	348.30010	-448.08950	-713.69030	1
4852	H	79.38000	64.97580	82.30090	1653.53871	1518.54351	-2204.10108	1
4853	C	80.25600	65.98080	80.69390	-330.36906	570.92528	629.56462	1
4854	H	80.91000	66.86380	80.53090	2649.74001	-536.50494	1609.11980	1
4855	H	79.24200	66.28180	80.35290	28.02504	-800.85526	-3042.37928	1
4856	C	80.67100	64.84780	79.76590	95.16582	863.10047	278.30207	1
4857	O	80.29900	63.70080	79.96890	494.90230	508.91229	345.98732	1
4858	N	81.33000	65.20580	78.66090	438.82548	-590.04873	-414.66491	1
4859	H	81.30100	66.17680	78.42390	-88.44591	2770.89819	-1487.45648	1
4860	H	81.92300	64.53680	78.21290	-1620.76387	-664.79494	2613.31177	1
4861	C	81.38000	64.62380	82.85090	827.58549	-12.68046	382.61268	1
4862	O	81.10700	63.45380	83.05790	-128.54851	778.97455	-17.35391	1
4863	N	82.53700	65.11480	83.31390	-336.41963	-722.01654	279.61803	1
4864	C	83.22100	66.26080	82.69590	545.21241	-111.42309	722.34294	1
4865	H	82.94100	67.16080	83.28390	1549.02701	-2008.63643	1861.21499	1
4866	H	82.92800	66.49280	81.64990	909.45614	-1204.18131	-2760.62730	1
4867	C	83.43800	64.25680	84.07790	-238.07708	-339.70476	-812.01661	1
4868	H	83.55400	63.29780	83.59490	2126.73239	-1230.34476	1965.06675	1
4869	C	84.69700	65.12580	84.13990	-794.25120	-125.86467	429.85360	1
4870	H	85.61200	64.50480	84.24490	2282.02598	693.88454	2051.61105	1
4871	H	84.61000	65.77680	85.03590	-1598.53836	-1253.88925	2402.22045	1
4872	C	84.69800	65.91280	82.85790	-745.90164	-524.29326	-14.08283	1
4873	H	85.34200	66.81680	82.82290	1915.70789	-1911.19203	-1604.87836	1
4874	H	85.02000	65.31480	81.97890	2196.43781	-1270.72493	1859.87777	1
4875	C	82.95000	63.89680	85.48290	699.85510	-16.64032	-584.27471	1
4876	O	83.29800	62.85680	86.07890	430.43769	-589.05475	-302.26665	1
4877	N	82.18500	64.85480	86.18890	647.91516	-462.28353	281.37551	1
4878	H	82.04200	65.79680	85.89690	-1847.35312	-2155.36681	-1356.43157	1
4879	C	81.67900	64.58180	87.53990	887.62622	204.82628	40.21058	1
4880	H	82.46700	64.31080	88.22590	1310.86746	1453.57780	-2463.12085	1
4881	C	80.99100	65.83580	88.13590	-474.95018	757.05842	-180.93058	1
4882	H	80.39700	66.35780	87.35590	2521.47463	1877.07192	130.35679	1
4883	C	80.07500	65.51980	89.33090	-484.17800	742.03202	215.43246	1
4884	H	79.23600	64.80180	89.20790	-1420.43333	-679.00593	2723.88442	1
4885	H	79.60200	66.50280	89.53890	-348.43063	1610.18341	-2680.32306	1
4886	H	80.59200	65.06380	90.20190	-2652.82464	1246.87961	1142.82060	1
4887	C	82.10400	66.82480	88.54790	342.79674	752.15329	384.97640	1
4888	H	82.94700	66.77280	87.82690	1060.16392	253.18339	2951.30088	1
4889	H	82.54800	66.39380	89.46990	211.16541	-1465.18218	2776.12618	1
4890	C	81.75600	68.27980	88.67090	768.55745	474.63903	-124.45175	1
4891	H	81.18400	68.37880	89.61690	-1083.06842	-2623.20134	1357.94100	1
4892	H	82.69900	68.86180	88.75190	-1627.98157	-1946.31068	1860.04758	1

4893	H	81.16100	68.59880	87.78890	-1718.41937	-506.04212	2586.34539	1
4894	C	80.71800	63.40580	87.53890	685.09411	526.56062	291.25758	1
4895	O	80.75900	62.52280	88.33690	-297.37391	285.74901	-673.45637	1
4896	N	79.82600	63.35580	86.53090	-564.81906	398.55425	-484.56808	1
4897	H	79.63700	64.12880	85.92890	1420.45157	-2166.26829	-1785.44820	1
4898	C	78.94800	62.20480	86.22690	3.46571	435.45703	-801.13430	1
4899	H	78.49300	61.75780	87.09790	1788.16026	-1479.33231	2124.21398	1
4900	C	77.77100	62.67180	85.34990	-247.32046	-653.19514	-586.19084	1
4901	H	78.14500	63.09380	84.39290	-1169.14294	2061.70156	2068.98953	1
4902	H	77.13300	61.79380	85.11490	2696.87489	115.39037	1616.09935	1
4903	C	76.80000	63.71180	86.07290	-89.35583	-902.76136	92.13284	1
4904	H	77.33300	64.63980	86.37290	241.23475	258.76471	-3126.19143	1
4905	C	75.74100	64.25280	85.11390	508.89365	-686.87176	-317.30970	1
4906	H	76.09600	64.59780	84.11990	1290.22365	-2286.51655	-1733.60642	1
4907	H	74.99800	63.47780	84.82990	-1470.30461	176.98919	-2775.80717	1
4908	H	75.09800	65.00780	85.61490	2434.08427	-1731.40928	987.76611	1
4909	C	76.08600	63.16980	87.28090	-698.92658	-473.00164	-345.28551	1
4910	H	75.75700	62.14180	87.01690	-444.39435	-2545.30035	1795.04485	1
4911	H	76.70900	63.27280	88.19590	1112.26189	2060.49673	2101.29792	1
4912	H	75.17000	63.75080	87.51990	-1081.19711	-1744.84542	2384.27211	1
4913	C	79.71000	61.03980	85.48290	407.63862	567.41295	-585.93883	1
4914	O	79.10700	60.24680	84.78490	-160.11677	548.56613	545.03674	1
4915	N	81.05000	60.89580	85.67690	535.16889	-564.79892	-327.51905	1
4916	H	81.56300	61.63580	86.10390	1084.70637	-1558.34142	2508.62718	1
4917	C	81.67900	59.58380	85.48290	568.02070	-235.90330	673.16649	1
4918	H	80.94000	58.86180	85.16790	-1777.96583	935.53677	2421.12261	1
4919	C	82.84300	59.77880	84.44790	539.89634	-555.84947	480.61868	1
4920	H	83.72900	59.14880	84.67490	1893.32725	1319.30710	2138.44966	1
4921	H	83.19000	60.83380	84.42090	1060.88305	2829.74290	874.81911	1
4922	C	82.46800	59.21580	83.06090	638.82962	-68.15783	-647.07204	1
4923	C	82.09700	57.87180	82.98090	-614.41689	664.29035	-112.52206	1
4924	H	82.06500	57.29180	83.89090	-1039.31101	257.72386	-2958.31663	1
4925	C	81.76000	57.32380	81.74990	-200.07316	-400.13889	794.55057	1
4926	H	81.57400	56.26280	81.67190	1132.54480	2819.76813	-815.15411	1
4927	C	81.73300	58.12080	80.62590	794.88340	-446.15328	-23.63556	1
4928	O	81.35100	57.56780	79.39290	474.27188	613.47937	-149.45392	1
4929	H	80.98200	56.68280	79.44890	-2193.12138	-319.55392	-2233.00921	1
4930	C	82.57200	59.98580	81.93490	662.44523	-600.59580	-178.61133	1
4931	H	82.88300	61.01080	82.07090	2145.09316	-1742.62567	-1503.34871	1
4932	C	82.18800	59.43480	80.71690	-585.85399	-486.28005	-501.75474	1
4933	H	82.27300	60.00980	79.80690	-2931.97802	-993.46169	561.03920	1
4934	C	82.20300	59.06980	86.83590	541.32979	112.43807	725.10050	1
4935	O	82.67700	57.91880	86.94890	332.09874	31.53896	715.78136	1
4936	N	82.03300	59.88880	87.89690	-705.35059	-270.74143	-376.63232	1
4937	H	81.63800	60.79980	87.80690	-2286.10306	230.95421	2149.09730	1
4938	C	82.49000	59.51680	89.18790	-428.60429	-658.60830	-462.58456	1
4939	H	83.47100	59.07480	89.09290	-656.54819	-2944.77325	891.89752	1
4940	C	82.64400	60.75380	90.06890	594.76028	562.03824	-402.27382	1
4941	H	83.36700	60.50080	90.87390	1955.73995	-1226.39319	2137.58443	1
4942	H	81.69200	61.08180	90.53790	2705.22946	-863.29827	1354.50209	1
4943	H	83.13700	61.58380	89.51890	-2831.04941	-1372.20502	-20.94952	1
4944	C	81.62000	58.45680	89.91790	690.61544	503.73551	317.41432	1
4945	O	80.36400	58.52880	89.88090	473.31981	534.42028	-337.62487	1
4946	N	82.22900	57.62180	90.79390	-74.95390	-710.43364	449.82023	1
4947	H	83.21700	57.48780	90.80390	-2531.29487	1335.52380	1306.57900	1
4948	C	81.49200	56.95580	91.86190	-485.07052	583.70129	505.42101	1
4949	H	82.21900	56.51580	92.52890	415.96401	-2019.59418	-2376.22379	1
4950	C	80.59000	57.87080	92.75390	-491.30625	-658.90044	394.86630	1
4951	H	79.86600	58.38380	92.08590	1816.04908	1152.37066	2296.13454	1
4952	H	80.09300	57.24080	93.52290	2201.76944	-1700.96961	-1468.72051	1
4953	C	81.46100	58.86380	93.52190	-583.73211	606.76237	-350.06750	1
4954	C	82.52500	58.47380	94.32090	-97.74378	-758.65384	496.32802	1

4955	H	82.86400	57.44780	94.30990	2840.28852	-959.12381	954.49927	1
4956	C	83.30600	59.40880	95.01490	402.20585	465.13548	673.29818	1
4957	H	84.13400	59.10480	95.63690	2263.76029	-1687.84156	-1387.37393	1
4958	C	82.96400	60.78380	94.84590	562.69367	510.87950	503.81442	1
4959	H	83.47000	61.57380	95.38290	2290.66345	1104.58151	1852.29232	1
4960	C	81.16500	60.24680	93.35090	630.27321	595.89160	281.28258	1
4961	H	80.29800	60.48480	92.75290	-1224.04756	2160.53694	-1931.84211	1
4962	C	81.88600	61.18680	94.02290	-516.25570	734.96358	157.35180	1
4963	H	81.69100	62.24580	93.93990	-141.20022	-1686.02368	2652.47297	1
4964	C	80.76400	55.70980	91.43490	-500.67091	191.22002	-737.70899	1
4965	O	79.70800	55.31080	91.95290	-20.76668	609.16259	502.11245	1
4966	N	81.30300	54.90280	90.49790	-613.53821	139.25076	-562.89642	1
4967	H	82.18100	55.22180	90.14890	-1239.73952	2117.27393	1969.37129	1
4968	C	80.71900	53.68480	89.94390	612.00407	597.23992	-316.55411	1
4969	H	79.65100	53.83680	89.97990	2833.75944	-1174.44528	-699.07934	1
4970	C	81.27100	53.31280	88.53290	-560.37603	454.47798	-557.56567	1
4971	H	80.83700	52.33080	88.24890	1578.57404	-2692.15327	398.29759	1
4972	H	82.36400	53.11580	88.57390	1257.69372	-2241.60671	-1814.28556	1
4973	C	80.98500	54.38180	87.51690	-841.99760	349.42617	19.80891	1
4974	H	81.51500	55.32680	87.76390	2395.44139	-729.31323	-1904.78056	1
4975	C	81.53700	54.10480	86.08490	671.95339	-472.07004	396.33259	1
4976	H	81.59600	55.10380	85.60390	-965.80976	2726.10573	1238.46084	1
4977	H	82.55700	53.69280	86.23790	-2210.97216	-2224.80784	-245.06818	1
4978	H	81.03200	53.33780	85.45890	-1644.81482	-2509.38904	946.45502	1
4979	C	79.54200	54.65580	87.23390	-438.41855	552.71613	-577.70672	1
4980	H	79.04100	54.79480	88.21590	-1489.29346	-1960.43075	-1958.81150	1
4981	H	79.34300	55.38180	86.41690	-2620.30005	1269.85404	1191.52198	1
4982	H	79.14800	53.69780	86.83090	-875.74175	-2192.85269	2079.11032	1
4983	C	80.97300	52.63780	90.95190	-295.42717	226.19485	832.47203	1
4984	O	82.06500	52.10580	91.11790	-627.35600	133.17096	460.77888	1
4985	N	79.89800	52.16980	91.66690	699.98022	-390.63673	264.76956	1
4986	H	78.97800	52.45280	91.40590	-682.54242	2389.00221	-1930.03381	1
4987	C	80.08900	51.23780	92.72590	-238.89617	603.03427	640.88165	1
4988	H	79.15000	50.75680	92.95390	2214.23644	-2229.66527	-154.84179	1
4989	H	80.83200	50.52280	92.40490	-1666.71564	2604.77001	-579.18770	1
4990	C	80.71500	51.67880	93.95290	774.96208	-244.92028	-413.39912	1
4991	O	81.35700	50.96780	94.71090	241.13544	-647.48386	382.42068	1
4992	N	80.54900	52.96080	94.25390	210.37923	-723.05530	381.58078	1
4993	H	80.17900	53.60180	93.58590	2801.91022	231.30967	1412.09814	1
4994	C	81.11800	53.58680	95.39990	-687.52660	598.73800	16.46173	1
4995	H	82.06300	53.10980	95.61590	-2114.34932	-2272.06003	515.26344	1
4996	C	81.44900	55.05980	95.20090	14.46586	-473.49130	779.13268	1
4997	H	82.12800	55.25980	94.34390	-3143.66611	68.32620	104.50435	1
4998	H	80.47800	55.52680	94.93090	1235.10165	-2883.76761	237.98003	1
4999	H	81.73900	55.58780	96.13490	-2909.47399	-1185.33090	-167.86302	1
5000	C	80.21700	53.42580	96.59890	723.55233	-554.90228	-2.54632	1
5001	O	79.01700	53.23880	96.46890	631.29480	-307.86580	360.98858	1
5002	N	80.81200	53.47280	97.79790	-256.05364	543.33727	593.20607	1
5003	H	81.79700	53.59180	97.89590	-556.24216	1897.09413	2447.41798	1
5004	C	80.10400	53.53380	99.00590	-86.72511	664.13658	618.75064	1
5005	H	79.05200	53.39680	98.80390	-475.19793	2330.06184	-2059.90897	1
5006	C	80.72100	52.50880	100.05290	230.36682	-429.05876	-770.90253	1
5007	H	81.81400	52.47280	99.85790	1869.39229	-1429.11700	-2088.35420	1
5008	H	80.40300	52.62580	101.11090	2229.68911	-1199.15006	1867.82008	1
5009	C	80.28200	51.06780	99.72490	737.32720	385.05736	373.53773	1
5010	H	80.89900	50.69980	98.87790	-910.52263	-2102.76751	-2155.81621	1
5011	H	80.52600	50.40280	100.58090	1206.09344	-2445.06171	1570.10765	1
5012	C	78.78400	50.94080	99.35690	-220.94944	-409.60827	-784.12589	1
5013	H	78.65100	51.25080	98.29890	592.24843	643.37699	-3022.17373	1
5014	H	78.23800	51.66280	100.00090	-865.79467	1998.83832	2270.08175	1
5015	C	78.18400	49.58980	99.52590	655.94020	477.55902	-416.08993	1
5016	H	78.30600	49.19080	100.55490	2211.02539	2206.23220	-377.00458	1

5017	H	78.65300	48.87980	98.81090	2548.99670	-723.66099	1696.21839	1
5018	N	76.74200	49.65680	99.25790	416.26646	494.79098	542.74894	1
5019	H	76.66100	49.91580	98.25390	-1361.29987	743.28023	2737.26568	1
5020	H	76.41300	50.36980	99.93990	2244.37531	-1615.88694	1499.97171	1
5021	H	76.27200	48.73580	99.36890	-544.92497	471.79777	3062.46467	1
5022	C	80.22600	54.95980	99.62690	-378.19203	-96.29545	-824.10495	1
5023	O	81.26600	55.62880	99.55690	-515.08317	-299.62246	-518.21129	1
5024	N	79.06500	55.53180	100.15290	70.80141	-566.95695	-621.46542	1
5025	H	78.24600	54.96680	100.20890	2164.26931	2075.14709	952.85317	1
5026	C	78.96600	56.92180	100.51590	-589.40826	-553.58529	-421.41694	1
5027	H	79.79100	57.47180	100.08790	-1675.87924	-833.15247	-2528.93495	1
5028	C	77.72400	57.53680	99.83390	623.27081	199.74475	-634.89096	1
5029	H	76.80700	57.08980	100.27490	1411.86485	-2624.29912	-1008.91922	1
5030	H	77.67100	58.59880	100.15690	-2148.84816	713.62940	-2184.35595	1
5031	C	77.84300	57.42380	98.31090	-242.60111	-876.89297	60.45187	1
5032	C	78.61700	58.35580	97.58790	105.34580	-787.70608	447.07090	1
5033	H	79.29400	59.02580	98.09690	-525.39720	2291.80635	-2090.40849	1
5034	C	78.64100	58.25080	96.16690	851.10042	-138.40312	-296.51924	1
5035	H	79.20400	58.96380	95.58290	-2920.42460	1090.93755	423.32218	1
5036	C	77.93600	57.23580	95.50590	-630.03242	-493.47572	437.02616	1
5037	H	78.04600	57.12480	94.43790	1998.86955	251.13034	-2416.54305	1
5038	C	77.15700	56.45480	97.64590	577.85381	-618.90545	338.36670	1
5039	H	76.68800	55.65580	98.20190	-267.36934	-1292.25015	2856.01635	1
5040	C	77.20800	56.31680	96.28190	561.30100	446.83096	-562.79151	1
5041	H	76.74300	55.47580	95.78890	-2001.23461	2387.81635	437.74347	1
5042	C	78.97800	57.25380	102.00090	-768.63764	349.27438	344.46275	1
5043	O	79.06900	58.41480	102.47090	125.32698	449.02694	637.41289	1
5044	N	78.95100	56.16180	102.83090	540.14932	-557.66368	-331.54521	1
5045	H	78.58300	55.30280	102.48390	-2360.81145	1736.90962	-1143.65227	1
5046	C	78.88800	56.33080	104.26790	675.31176	-597.84226	-134.12552	1
5047	H	78.72600	57.37580	104.48790	2697.96271	376.01024	1574.11554	1
5048	C	77.73800	55.52780	104.91990	583.94266	-608.02770	-347.51156	1
5049	H	77.73700	55.67180	106.02190	-2152.12641	2287.11714	188.87393	1
5050	H	78.02200	54.47280	104.71790	854.06480	-2371.74791	-1882.44824	1
5051	C	76.39500	56.07880	104.37490	-387.71609	-456.11444	-687.81310	1
5052	H	76.33400	56.03080	103.26590	2421.74602	-1977.78675	-348.90118	1
5053	H	76.43600	57.17880	104.52490	2443.08952	841.08750	1795.02413	1
5054	C	75.12500	55.41780	105.00790	97.14733	-453.00127	-785.36823	1
5055	H	74.21200	55.89580	104.59090	-829.78562	-2235.84412	-2051.99492	1
5056	H	75.24900	55.59280	106.09790	-2546.31834	-786.16770	-1672.25282	1
5057	C	75.05000	53.89580	104.84890	-167.98973	-550.29803	-707.39136	1
5058	H	75.91600	53.36880	105.30390	2465.04029	-386.94185	-1916.26684	1
5059	H	74.88900	53.64780	103.77790	-1773.59602	2596.47137	104.49781	1
5060	N	73.87300	53.41980	105.56690	-551.26435	350.18367	-534.93112	1
5061	H	74.07600	53.58480	106.57290	2814.68176	-460.90583	-1327.91516	1
5062	H	73.01100	53.99980	105.60990	-241.20627	2579.86855	-1784.46744	1
5063	H	73.73800	52.42180	105.30890	1431.47478	1835.82938	2116.32622	1
5064	C	80.16700	55.94380	104.98190	-566.28741	-635.08442	327.77637	1
5065	O	80.39300	56.21780	106.18890	-474.92593	-350.84747	-524.38406	1
5066	N	81.09000	55.32780	104.18990	-623.65888	50.73588	566.69900	1
5067	H	80.83000	54.95680	103.30190	-1478.77195	1668.88869	2219.52028	1
5068	C	82.53200	55.16980	104.40690	222.09073	827.13953	312.99667	1
5069	H	82.59600	54.28380	105.02190	-3144.52774	-72.28619	70.32920	1
5070	C	83.29300	54.91580	103.09090	63.11093	744.29227	-522.96944	1
5071	H	82.81500	54.08480	102.53090	-1224.14638	-2204.00011	1882.04021	1
5072	O	84.67700	54.54080	103.24590	-725.06844	-109.93823	-292.94466	1
5073	H	84.78500	53.96080	104.00290	-304.29553	-2261.69628	-2165.72399	1
5074	C	83.23200	56.06680	102.10790	-556.50453	-374.31243	617.77335	1
5075	H	83.45200	55.63380	101.10790	-1792.42401	-2551.05235	421.39563	1
5076	H	83.82700	56.93980	102.45090	-1821.08005	-628.06650	2487.45375	1
5077	H	82.23100	56.54280	102.03790	1180.34726	2425.35769	-1619.45875	1
5078	C	83.20700	56.25880	105.24790	-485.58654	578.43675	-510.94779	1

5079	O	83.00500	57.44880	105.00190	547.13124	-567.29965	-49.45441	1
5080	N	83.99000	55.88980	106.24490	529.58547	240.29309	-611.94015	1
5081	H	84.16600	54.94980	106.52790	88.04386	-84.20542	3143.78497	1
5082	C	84.73700	56.88680	106.99290	821.10572	-384.26135	-97.87550	1
5083	H	84.96900	57.66880	106.28490	-2004.76628	1616.49215	-1807.23311	1
5084	C	83.91500	57.42980	108.20490	901.59265	121.77557	-61.25690	1
5085	H	84.21500	58.48080	108.40390	58.48733	-2968.54791	1040.44643	1
5086	H	82.85200	57.49980	107.89190	1198.21386	1397.51495	2551.36468	1
5087	O	83.89700	56.69080	109.40790	-31.33697	777.03860	137.31799	1
5088	H	83.44200	57.18580	110.09290	1292.49466	1810.80216	2224.56272	1
5089	C	86.04500	56.31880	107.48390	910.25559	-53.67074	2.28316	1
5090	O	86.23700	55.11080	107.49890	224.73168	386.38818	-651.02003	1
5091	N	86.96200	57.19680	107.92490	592.41732	-115.38395	-590.25465	1
5092	H	86.55800	58.10780	107.88190	-196.95547	-3017.49164	868.43480	1
5093	C	88.24100	56.92680	108.44490	-44.60705	39.58217	-909.88706	1
5094	H	88.79900	56.31480	107.75190	-2313.53670	-391.48440	2095.83257	1
5095	C	88.99900	58.27680	108.62790	528.28372	275.33553	-690.33156	1
5096	H	88.48300	58.99280	109.30190	1616.71985	2514.68091	980.21583	1
5097	H	90.03800	57.98680	108.89590	2278.22391	-1515.91739	-1552.39059	1
5098	H	89.10200	58.71980	107.61390	-2193.15855	-1988.53404	1064.90103	1
5099	C	88.23700	56.08880	109.70490	636.87901	275.86417	591.38404	1
5100	O	89.01500	55.11480	109.84290	668.78163	-409.00382	95.25881	1
5101	N	87.28400	56.41280	110.61790	542.61366	463.04814	-451.47439	1
5102	H	86.91200	57.33580	110.56290	2022.12249	-1412.01961	1953.31705	1
5103	C	86.97200	55.47480	111.74990	-589.19915	-411.36289	-561.31626	1
5104	H	87.90700	55.26180	112.24790	2295.20594	491.90314	-2094.82391	1
5105	C	85.97400	56.15380	112.70390	-440.56961	335.32811	724.50292	1
5106	H	85.55200	55.42080	113.42490	-2658.59194	-436.23655	1624.75006	1
5107	H	85.16200	56.58080	112.07790	1386.42037	-1331.91514	2490.39492	1
5108	C	86.51500	57.41880	113.51390	-524.96174	589.96805	455.85510	1
5109	H	85.63700	57.75580	114.10590	-403.58530	-2866.71174	-1231.79094	1
5110	H	86.86800	58.20880	112.81690	3080.02555	295.04673	569.75107	1
5111	C	87.65700	56.97980	114.46190	-379.69386	543.51629	-625.99810	1
5112	O	87.51800	56.06080	115.23690	-568.76345	-231.43650	-496.56068	1
5113	N	88.78900	57.67580	114.32290	105.92758	837.51450	-4.59422	1
5114	H	88.76800	58.52780	113.79990	-1547.03354	-1699.33908	2148.75782	1
5115	H	89.56800	57.40480	114.88790	25.26782	-2350.18093	-2091.46775	1
5116	C	86.38100	54.13380	111.32290	180.00555	27.32998	-893.47752	1
5117	O	86.84900	53.05580	111.69790	-204.81051	-507.76855	569.07907	1
5118	N	85.41700	54.13580	110.31590	-576.83895	-497.44063	-363.98067	1
5119	H	85.05700	54.93680	109.84490	1266.94635	-2491.28727	1444.49330	1
5120	C	84.85500	52.81180	109.85490	416.52979	487.10829	-648.59807	1
5121	H	84.53200	52.34680	110.77490	299.29514	-727.32019	-3046.25245	1
5122	C	83.70500	53.01180	108.93090	-15.29436	-675.26288	-612.56601	1
5123	H	84.01300	53.65080	108.07590	1428.91896	-2800.76377	-110.17758	1
5124	H	83.34100	52.09480	108.41990	2239.82015	-1322.46097	-1769.89517	1
5125	N	82.20500	53.38680	110.95190	-135.16195	-113.48893	-825.54455	1
5126	H	82.76300	52.85980	111.59290	2109.15876	335.39947	-2310.23435	1
5127	C	82.52300	53.64980	109.61990	-546.29797	-362.55731	633.68899	1
5128	C	81.11100	54.09780	111.23090	-452.77879	119.68693	782.37932	1
5129	H	80.61100	53.96480	112.18990	515.65026	-1085.65638	-2907.52150	1
5130	N	80.67200	54.79180	110.20390	-672.10464	-496.37782	120.65113	1
5131	C	81.57800	54.50080	109.14890	-415.10380	170.73927	793.71780	1
5132	H	81.39700	54.85780	108.14190	-2409.73621	-1633.57327	1192.82690	1
5133	C	85.90800	51.89980	109.19590	-57.11934	500.76370	759.88427	1
5134	O	85.88900	50.70180	109.38790	747.08667	-254.89254	-22.77120	1
5135	N	86.82900	52.50780	108.42890	434.81749	-696.92036	194.69990	1
5136	H	86.68300	53.45680	108.15990	2062.99251	-2373.89735	-83.06334	1
5137	C	88.02200	51.87180	107.84890	682.44651	538.86219	-274.49097	1
5138	H	87.57200	51.13580	107.19990	-1843.79418	-2538.43053	234.56273	1
5139	C	88.70700	52.92580	106.97790	-743.15574	-519.11314	98.44841	1
5140	H	89.07900	53.71380	107.66690	1482.52963	-2243.39052	-1633.25781	1

5141	H	88.02500	53.45380	106.27890	1598.24750	-2654.66864	544.57836	1
5142	H	89.64100	52.60980	106.46590	-670.78534	1167.49753	2843.45262	1
5143	C	88.99100	51.29980	108.85590	656.08552	-500.36518	-388.12045	1
5144	O	89.45100	50.19180	108.67390	-267.34786	-76.77617	-739.09253	1
5145	N	89.27600	51.98380	109.97890	-430.61950	-549.47687	474.67284	1
5146	H	88.76800	52.80380	110.22890	-911.04899	-2824.16187	1045.14387	1
5147	C	90.10100	51.42580	111.06990	-685.54544	552.14713	237.93275	1
5148	H	91.01100	51.07180	110.60790	-937.79610	2652.29756	-1408.57459	1
5149	C	90.26000	52.46080	112.19890	-150.36184	-552.95767	-709.28142	1
5150	H	90.54900	51.99480	113.16490	-2813.47406	1355.73689	380.22020	1
5151	H	89.29800	53.00080	112.32690	-1967.51298	1885.96383	1571.70587	1
5152	C	91.46800	53.42280	111.91590	547.78928	-534.48686	495.68306	1
5153	H	91.24700	53.92980	110.95190	945.15212	-928.87648	2853.43690	1
5154	C	91.52600	54.66780	112.80790	-324.36065	-543.92493	656.03875	1
5155	H	91.94300	54.47580	113.81990	-1370.29770	-1637.02729	-2310.98510	1
5156	H	92.19500	55.45480	112.39790	-1482.15837	2656.29835	-803.43753	1
5157	H	90.49100	55.02780	112.99190	-1680.46250	1661.10919	-2077.25499	1
5158	C	92.83900	52.70780	111.87190	-401.11306	622.08389	-532.51380	1
5159	H	92.94400	52.02380	111.00290	-152.06164	-2008.65723	2416.69188	1
5160	H	93.60500	53.51180	111.82990	2247.42890	2158.53128	433.62692	1
5161	H	93.04000	52.07480	112.76290	1888.77528	1844.73379	-1711.05564	1
5162	C	89.46100	50.19980	111.71690	-554.61851	177.36824	701.70494	1
5163	O	90.15700	49.23380	112.03990	-668.38767	417.15757	-53.52294	1
5164	N	88.19500	50.21680	112.07190	504.38531	-570.37054	364.61650	1
5165	H	87.72300	51.07580	111.88590	-1725.82391	1957.80252	-1756.91984	1
5166	C	87.47100	49.11180	112.69890	394.57747	402.03212	717.02845	1
5167	H	88.04300	48.79080	113.55590	-2404.20558	-1920.06895	656.77771	1
5168	C	86.10000	49.48680	113.13590	601.96840	-204.01925	-653.80516	1
5169	H	85.43700	48.61080	113.30090	-2440.18554	-196.75757	-1976.10911	1
5170	O	85.50100	50.38680	112.30590	203.56133	657.91341	386.44529	1
5171	H	85.67800	50.08280	111.41290	-2043.42410	390.47843	-2360.12092	1
5172	C	86.15600	50.20880	114.52090	-427.06329	239.43245	-769.24642	1
5173	H	85.14000	50.56980	114.78890	-2914.04759	63.16303	-1184.29867	1
5174	H	86.84200	51.06980	114.37390	-874.83740	-2997.72464	382.79595	1
5175	H	86.58700	49.54880	115.30390	-2521.49096	-1567.58855	-1040.66119	1
5176	C	87.33200	47.86380	111.81290	737.98452	-530.38323	74.32013	1
5177	O	87.28100	47.98280	110.59890	396.32778	-502.71341	462.41837	1
5178	N	87.22900	46.69980	112.39890	-249.40738	613.04579	-524.06403	1
5179	H	87.31500	46.64780	113.38990	1722.25761	-1493.91079	-2168.01418	1
5180	C	87.00800	45.43480	111.73590	786.20236	-460.38551	37.17575	1
5181	H	87.60700	45.49580	110.83890	767.49152	2902.13019	-941.71299	1
5182	C	87.63800	44.22280	112.49690	-387.94917	-654.79188	502.18925	1
5183	H	87.57500	43.32580	111.84390	-1412.57714	-1579.46339	-2325.54240	1
5184	H	88.73700	44.38180	112.50190	-2510.80954	-1313.94657	1366.60385	1
5185	O	87.05400	43.98480	113.80390	453.46026	474.88097	438.73578	1
5186	H	87.22400	44.78680	114.30390	-843.74822	-2911.98385	-840.63382	1
5187	C	85.56100	45.12680	111.38790	-851.26790	-304.48452	-118.67241	1
5188	O	84.61300	45.60580	112.09190	45.16908	705.48613	-351.96066	1
5189	O	85.32200	44.42480	110.35290	-400.57190	247.81106	633.84467	1
5190	H	74.86860	109.09180	75.30230	1742.59588	-669.56566	2532.44302	2
5191	N	75.62660	108.42720	75.16160	-151.00642	-201.73376	-805.71263	2
5192	H	75.63660	108.35790	74.14620	-920.70512	-776.31231	-2906.52155	2
5193	C	76.86460	108.82700	75.72980	-799.31660	435.31761	55.15933	2
5194	H	76.52560	109.16850	76.73370	-1957.38869	-2461.41733	90.99702	2
5195	C	77.86460	107.55470	75.82210	-677.55133	465.66394	-394.37582	2
5196	H	78.24660	107.30710	74.80370	197.90251	3090.55316	554.56471	2
5197	H	78.76260	107.81150	76.43180	520.58710	3006.29156	-767.74107	2
5198	C	77.14260	106.37630	76.40660	652.02843	578.54495	267.57366	2
5199	H	76.23660	106.18410	75.78860	1582.05696	1150.60627	-2464.02663	2
5200	C	78.03160	105.13690	76.37440	82.41981	504.53742	755.04965	2
5201	H	77.49760	104.23490	76.77000	116.48044	2141.24475	-2302.11412	2
5202	H	78.36860	104.89460	75.33460	2538.03474	-1343.96595	1284.66394	2

5203	H	78.95160	105.27520	76.99780	2250.41064	-312.10107	2176.34352	2
5204	C	76.70060	106.63650	77.84230	548.11310	543.33650	-485.60115	2
5205	H	76.19360	105.74090	78.28550	1658.10582	811.60552	-2547.58862	2
5206	H	77.56960	106.88700	78.50280	-2218.26434	-137.62060	2226.78920	2
5207	H	75.97760	107.48890	77.90220	-2383.20577	-1944.91607	660.19539	2
5208	C	77.38660	110.03410	74.84170	354.49325	764.56738	-348.16986	2
5209	O	76.60960	110.92290	74.33670	620.93658	106.56319	-476.13997	2
5210	N	78.68160	110.06240	74.70270	-312.80742	450.53668	641.74801	2
5211	H	79.26760	109.37800	75.17470	2332.35712	1511.61220	1474.23370	2
5212	C	79.16560	111.34420	74.27250	361.58572	662.94307	-511.09026	2
5213	H	79.35660	111.87870	75.22520	99.61944	1005.80121	2979.37344	2
5214	C	80.48560	111.11930	73.45210	549.55947	-634.30105	-356.50746	2
5215	H	80.24560	110.50930	72.53820	1613.19275	2667.77888	422.83711	2
5216	O	81.54560	110.40320	74.13590	-153.23227	172.96956	755.13484	2
5217	H	81.66860	109.63480	73.55040	1709.74513	826.42634	-2508.38939	2
5218	C	80.81960	112.60110	73.02740	227.00171	146.66059	-870.86847	2
5219	H	81.68360	112.63970	72.32500	-1948.68275	-1888.40305	1592.10417	2
5220	H	79.95660	113.09410	72.51800	1525.80130	-542.05030	-2697.46883	2
5221	H	81.08460	113.22960	73.90860	-1991.39283	-1912.44732	-1508.35211	2
5222	C	77.91360	112.02210	73.34880	721.15823	20.30358	-557.64646	2
5223	O	77.80060	111.71130	72.15660	-399.76237	-233.50936	-639.75828	2
5224	N	77.76860	113.32190	73.81010	-142.68091	499.04832	665.78166	2
5225	C	76.91560	114.22870	73.15370	771.65402	164.11767	-457.23787	2
5226	H	76.16560	113.63750	72.57660	-1134.90288	-2769.56195	-969.40614	2
5227	C	76.36360	115.12590	74.36020	542.06811	572.61779	457.95418	2
5228	H	75.98260	116.11570	74.02520	-2294.95831	1989.42376	820.72266	2
5229	H	75.52760	114.62320	74.89560	82.22388	-3103.51788	-509.55102	2
5230	C	77.63560	115.21840	75.24760	734.20498	537.98103	-54.50195	2
5231	H	78.37460	115.93160	74.81220	-2156.52742	1852.81848	-1347.10036	2
5232	H	77.43660	115.55040	76.28980	1549.29061	246.53241	2727.11323	2
5233	C	78.15860	113.70780	75.14640	-730.54783	368.91385	402.06150	2
5234	H	79.26560	113.57840	75.24740	1506.28857	-1645.63157	2218.38177	2
5235	H	77.64160	112.98840	75.82870	-2149.98554	1131.36852	-1998.94814	2
5236	C	77.81960	115.24140	72.19930	735.66930	-537.27078	-39.77186	2
5237	O	78.84160	115.75540	72.58080	459.16318	-497.08963	-407.06056	2
5238	N	77.14460	115.43900	71.08000	432.28801	-392.32972	609.81699	2
5239	H	76.26460	114.94570	70.93140	-2048.94953	1114.38755	-2111.43848	2
5240	C	77.65360	116.34720	70.12070	-66.19096	779.29053	-468.80276	2
5241	H	78.58460	116.78320	70.55460	-2003.26241	-858.91823	-2268.79382	2
5242	C	77.89060	115.47230	68.79250	239.90206	-62.31579	877.50484	2
5243	H	76.94060	114.91150	68.57760	-1806.19495	2562.36747	264.87537	2
5244	O	78.92560	114.47910	68.88430	25.33343	-568.33858	547.70130	2
5245	H	78.39960	113.65440	68.85410	1839.34285	-1946.38300	1651.25326	2
5246	C	78.10260	116.56900	67.68720	399.73098	-179.83494	799.57835	2
5247	H	78.20760	116.11330	66.67500	-1588.10144	1412.10040	-2319.94235	2
5248	H	77.24660	117.27900	67.64220	95.01673	-1629.14356	-2689.81214	2
5249	H	79.02360	117.16810	67.87710	-2169.67168	1688.54881	1529.56006	2
5250	C	76.44360	117.40720	69.81500	475.42419	-734.33607	257.24187	2
5251	O	75.26860	117.01860	69.71290	661.09426	-50.97493	428.93258	2
5252	N	76.94160	118.60150	69.64300	502.67520	-560.97869	381.17299	2
5253	H	77.95460	118.59100	69.76160	1897.00604	629.71559	-2429.61984	2
5254	C	76.27460	119.76060	69.17360	838.53066	-1.52937	-358.21084	2
5255	H	77.13260	120.39750	68.85820	-129.66827	-3029.55963	838.55876	2
5256	C	75.30960	119.38920	67.94850	-810.78658	237.64049	-342.93311	2
5257	H	75.09560	120.32380	67.35720	2602.40595	427.72661	1715.44731	2
5258	H	75.90860	118.72020	67.27540	-181.86621	942.80005	-2996.04389	2
5259	O	74.03660	118.82210	68.26780	558.20959	-436.39202	-348.69943	2
5260	H	74.35660	118.02150	68.84150	62.39940	3017.43750	-888.48381	2
5261	C	75.37460	120.51430	70.28660	-715.05129	-363.89084	-433.28525	2
5262	O	74.94060	121.62970	70.02390	541.72122	390.24166	-421.75443	2
5263	N	75.26460	119.86870	71.47380	-412.30973	-48.66340	-735.05432	2
5264	H	75.66060	118.94700	71.26260	49.19352	-2580.28481	-1799.42672	2

5265	C	74.01060	120.05060	72.25810	585.54745	-663.97319	218.46003	2
5266	H	73.25960	120.21410	71.45150	-2284.83326	489.18851	-2106.76477	2
5267	C	73.77460	118.80050	73.06340	-438.37233	-653.99013	-459.97566	2
5268	H	74.71460	118.56730	73.61220	1045.95188	2908.31325	588.15386	2
5269	C	72.66060	118.97230	74.08410	-730.66560	-510.69212	191.76117	2
5270	H	72.46960	118.02330	74.65660	-2424.63274	-864.21332	1809.01012	2
5271	H	72.90960	119.77190	74.84070	2281.49829	2161.05042	151.17173	2
5272	H	71.69160	119.26580	73.59470	2243.22530	638.28286	2111.57796	2
5273	C	73.43260	117.60480	72.19080	-415.53920	-443.14887	-679.99798	2
5274	H	73.36960	116.65790	72.79230	-2172.72336	2048.86570	-989.77207	2
5275	H	72.43760	117.74000	71.68460	1769.95561	1910.25789	-1765.33231	2
5276	H	74.19860	117.43250	71.36920	-1252.68589	2389.69443	1618.13621	2
5277	C	74.22060	121.39310	73.17390	480.90611	651.73947	-418.82692	2
5278	O	74.29660	121.33300	74.37660	-587.38670	-347.83899	-397.00393	2
5279	N	74.19660	122.49100	72.42080	-425.55365	421.56962	594.85749	2
5280	H	74.22760	122.41860	71.37140	1549.04007	-1689.13521	2155.34761	2
5281	C	74.69360	123.67760	73.06350	556.86673	688.15405	218.61941	2
5282	H	74.24760	123.61880	74.08320	2429.98857	-1875.08555	690.96741	2
5283	C	76.27260	123.54020	73.08470	681.56567	-489.50379	-356.79865	2
5284	H	76.57160	122.61590	73.63050	-2224.74059	2027.84782	914.65226	2
5285	H	76.66360	123.42250	72.04840	-610.23472	1934.61197	-2404.81109	2
5286	C	76.86560	124.81330	73.76290	793.81854	189.70557	406.58937	2
5287	H	76.57060	125.72230	73.18830	-1934.14804	-1865.50657	-1636.20990	2
5288	H	76.40660	124.96560	74.76470	3047.95798	-244.31595	-740.59983	2
5289	C	78.43460	124.76860	73.90690	-653.52408	91.82360	629.22628	2
5290	O	79.01260	125.70800	74.39110	94.00375	412.92580	666.54543	2
5291	N	79.00060	123.62610	73.46250	-642.90477	537.81345	100.51090	2
5292	H	78.56660	122.79470	73.04350	-259.77013	-2132.17754	2298.81810	2
5293	H	80.00860	123.43850	73.49250	1277.59881	-1548.50601	2422.41546	2
5294	C	74.22960	124.94830	72.15610	168.68935	852.68998	-275.52622	2
5295	O	75.05660	125.51310	71.48890	543.79617	-1.54767	572.63475	2
5296	N	72.91760	125.21790	72.27400	531.04695	197.91591	-625.69219	2
5297	C	72.25660	126.05240	71.32270	586.14614	-405.64852	568.62376	2
5298	H	72.87460	126.02790	70.39480	-1536.70364	378.67561	-2719.07575	2
5299	C	70.83360	125.34730	71.22260	-210.38887	-238.66926	854.53175	2
5300	H	70.04860	126.01860	70.80870	-1514.35135	-2516.53520	1127.83722	2
5301	H	70.86860	124.45040	70.56430	-2000.57644	1842.75410	1581.19494	2
5302	C	70.58660	124.94740	72.70960	-377.06732	-707.81804	-433.89500	2
5303	H	70.26760	125.82480	73.31450	-1833.18359	1640.53436	1961.20146	2
5304	H	69.79860	124.17160	72.83630	1084.44534	2725.37649	1137.77306	2
5305	C	72.03160	124.44510	73.13740	2.88091	-436.99831	-800.29693	2
5306	H	72.31060	124.65330	74.19730	-2824.73571	-974.03327	-985.06526	2
5307	H	72.24060	123.37380	72.90690	-1269.96415	1182.42511	-2624.36433	2
5308	C	72.00660	127.57660	71.86420	-558.31608	-553.59803	-461.80449	2
5309	O	71.34860	128.33790	71.19490	-533.35334	504.46255	-290.99653	2
5310	N	72.53460	127.81180	73.06560	799.64648	-251.92381	98.85442	2
5311	H	73.08960	127.04460	73.44260	-2537.92425	-969.91895	1586.32403	2
5312	C	72.55260	129.16420	73.61210	586.84184	348.35174	-604.74683	2
5313	H	72.18260	129.81160	72.78000	1119.50725	687.70862	2858.66868	2
5314	C	71.66660	129.18750	74.84990	404.27139	-764.60365	288.78523	2
5315	H	72.02060	128.38390	75.53280	-648.10356	2447.63655	-1867.42158	2
5316	C	71.76460	130.51030	75.58530	528.23456	584.54411	-459.05057	2
5317	H	71.14160	130.51620	76.52260	-431.25259	-1426.81315	2770.64102	2
5318	H	72.82460	130.73820	75.88730	2932.01629	1135.39336	-111.30419	2
5319	H	71.41260	131.36630	74.94600	-2597.65530	-995.61545	-1469.40909	2
5320	C	70.22060	128.89130	74.50000	-737.30563	-529.19495	-88.22767	2
5321	H	69.56660	128.84940	75.41420	-1520.44829	-2457.09192	-1244.65356	2
5322	H	69.79260	129.67760	73.81710	-404.11480	2788.27601	1400.15511	2
5323	H	70.12160	127.90650	73.96590	-1126.24669	-1286.68001	2640.88038	2
5324	C	74.11260	129.46560	74.10020	-747.16071	-183.11628	489.56134	2
5325	O	74.78360	128.60910	74.62180	631.38231	-243.02764	407.33423	2
5326	N	74.39260	130.75070	73.93650	-465.38375	-510.23859	-485.53768	2

5327	H	73.68760	131.34990	73.51100	1645.14278	2060.84196	-1716.00170	2
5328	C	75.71360	131.18570	74.21520	413.25965	-507.30693	-635.06467	2
5329	H	76.25660	130.26660	74.54280	1557.24493	-2350.94366	1395.09081	2
5330	C	76.28060	131.85950	72.89420	583.53793	-74.86724	-696.65586	2
5331	H	76.10260	131.21240	72.00600	-222.87105	1172.87369	2910.82841	2
5332	H	75.75160	132.81530	72.68300	898.98467	2148.19688	2115.49119	2
5333	C	77.80860	132.09970	73.12190	-171.09162	860.67629	247.82047	2
5334	H	77.98660	132.64020	74.07960	1887.72926	-415.22665	2482.39628	2
5335	H	78.35360	131.13230	73.21020	-1651.59957	1685.31687	2080.90176	2
5336	C	78.35260	132.94790	71.90310	-452.70043	91.74043	786.19146	2
5337	H	78.18660	132.41640	70.93870	332.06243	2299.87388	2120.97640	2
5338	H	77.80460	133.91430	71.81500	-2259.23349	1342.20730	1729.90458	2
5339	C	79.86060	133.17890	72.15890	-465.08369	-692.38048	-368.45276	2
5340	H	80.10760	133.61020	73.15410	-878.67670	1891.69954	-2355.33996	2
5341	H	80.50160	132.29460	71.96960	127.46997	1027.00573	-2971.06662	2
5342	N	80.34360	134.26080	71.13650	-350.26981	497.98381	-584.80379	2
5343	H	81.37460	134.50170	71.20160	390.77252	-2657.82305	-1637.52854	2
5344	H	80.25260	134.02500	70.10470	2401.37657	-2031.45583	-69.31101	2
5345	H	79.90760	135.22820	71.18120	-724.67596	1778.49378	-2491.99335	2
5346	C	75.70360	132.41590	75.31230	295.55129	-669.13009	-544.39449	2
5347	O	75.02960	133.44420	75.21830	-500.52639	-526.65888	-309.40425	2
5348	N	76.67360	132.14370	76.14720	508.36918	498.77976	453.26793	2
5349	H	77.14960	131.26060	75.97600	930.34245	2310.01954	-1922.62812	2
5350	C	76.86660	132.84630	77.37890	-107.68176	736.26898	527.03286	2
5351	H	75.83660	133.03930	77.75410	1960.21260	1451.58084	-1987.13509	2
5352	C	77.72660	131.87570	78.28420	412.87398	-678.69640	-447.61287	2
5353	H	77.27560	130.85850	78.31430	1775.77808	-58.28991	2596.42846	2
5354	H	78.73460	131.73720	77.83240	1017.21119	-1328.44442	-2664.34665	2
5355	C	77.85860	132.46440	79.72790	726.03867	-11.65096	-551.52797	2
5356	H	78.18560	133.53540	79.68020	2474.11025	-1912.55496	-345.16401	2
5357	H	76.88060	132.45950	80.25890	-1693.09895	2317.38923	1288.93340	2
5358	C	78.93260	131.58850	80.49060	731.68366	-19.37851	-543.79638	2
5359	H	78.58260	130.53600	80.60310	98.63496	2211.84285	2235.22898	2
5360	H	79.87960	131.53020	79.90690	2240.01947	1404.61532	-1705.16709	2
5361	C	79.19160	132.23690	81.87000	735.82829	-538.52242	1.15350	2
5362	H	79.62260	133.25660	81.82520	-1312.20376	-1963.00299	2079.17455	2
5363	H	78.32360	132.22230	82.55900	-110.64244	1442.03704	2794.01390	2
5364	N	80.28860	131.38330	82.59220	-79.89147	688.60769	481.77702	2
5365	H	80.58160	131.73020	83.55150	-289.83434	-2120.17102	2306.31679	2
5366	H	80.05660	130.36870	82.79850	2325.16833	381.83078	-2084.71190	2
5367	H	81.22860	131.29890	82.10750	43.27301	-3040.06257	808.93339	2
5368	C	77.66160	134.23860	77.11520	-358.50456	838.39857	-3.65031	2
5369	O	78.27860	134.77030	78.01140	-509.59437	340.31223	498.12488	2
5370	N	77.52760	134.65780	75.85320	582.43016	441.52645	422.49473	2
5371	H	76.90260	134.12380	75.23760	-2445.18770	300.10025	1956.84010	2
5372	C	77.76560	136.05590	75.63920	-853.28349	142.84686	-288.01575	2
5373	H	78.57560	136.31800	76.35960	1476.23408	-2092.42639	-1827.76119	2
5374	C	78.20260	136.23260	74.10720	467.96664	-402.45250	-671.18568	2
5375	H	77.47360	135.68460	73.45240	-2190.13949	-946.25309	2050.88281	2
5376	O	79.50860	135.71170	73.80200	18.51639	-789.37942	-12.82603	2
5377	H	79.30260	135.07890	73.08700	2978.98666	-382.29707	-936.86374	2
5378	C	78.03460	137.77610	73.87160	-580.89247	701.63774	41.46600	2
5379	H	78.36060	138.07070	72.84690	2030.98393	-1362.32562	-1979.24213	2
5380	H	76.97060	138.10050	73.97790	-882.10862	2545.80242	-1624.50012	2
5381	H	78.63760	138.36820	74.59780	2875.12388	-443.04449	-1198.16547	2
5382	C	76.40260	136.87270	75.97540	-609.64388	655.18387	-174.69815	2
5383	O	76.52460	138.05570	76.21160	215.43762	53.08835	757.88884	2
5384	N	75.28060	136.16130	75.89680	-243.97042	213.69135	-779.41435	2
5385	H	75.24660	135.13550	75.68270	-356.06659	-2443.05621	-1950.10748	2
5386	C	74.08860	136.95140	75.91490	310.92696	75.03547	-853.89994	2
5387	H	74.48460	137.97630	76.14130	-1134.58106	-2432.66746	-1641.06096	2
5388	C	73.40760	136.86310	74.46410	423.00707	276.42367	-759.01645	2

5389	H	73.22660	135.80150	74.17920	1935.88283	1329.06185	2093.84299	2
5390	H	72.42160	137.38410	74.47590	-224.74671	-3136.74864	-92.32069	2
5391	C	74.33660	137.54680	73.45210	-436.84911	38.07751	-799.47730	2
5392	C	74.38660	138.97390	73.41980	884.88412	19.94487	219.16501	2
5393	H	73.76460	139.57710	74.10540	2031.41062	1443.06442	-1920.71919	2
5394	C	75.14860	136.77110	72.57140	-372.57036	-778.83894	-293.34662	2
5395	H	75.11860	135.66710	72.60460	-1784.08392	2567.40981	-351.67833	2
5396	C	75.24260	139.58890	72.50810	699.20162	312.46857	494.90553	2
5397	H	75.28460	140.69250	72.48410	2295.68572	136.57999	2146.95115	2
5398	C	75.98460	137.43570	71.67030	234.66799	-157.10225	867.00682	2
5399	H	76.60860	136.82880	70.99240	2197.57369	-228.08814	2239.83747	2
5400	C	76.06560	138.85770	71.60330	-634.94668	-80.13830	-649.51642	2
5401	O	76.92460	139.54190	70.70390	341.80309	-482.26454	523.65904	2
5402	H	77.29760	138.77200	70.21310	-2639.78092	-1068.99156	1336.80213	2
5403	C	73.12560	136.39880	77.09980	-873.74337	-8.22918	260.68334	2
5404	O	73.54060	136.36310	78.25660	-653.65831	-59.34966	-439.13057	2
5405	N	71.92560	136.12810	76.64190	180.22179	592.26801	573.94338	2
5406	H	71.77560	136.24600	75.64020	-313.02754	2914.20788	1143.51757	2
5407	C	70.97260	135.36630	77.38340	-761.77781	474.30402	161.80624	2
5408	H	70.24860	135.03040	76.60690	-2452.67380	-651.20783	-1859.71659	2
5409	C	71.77560	134.16870	78.05460	899.87403	-85.58999	119.80020	2
5410	H	72.44760	133.68950	77.30640	1945.29243	-2053.54524	-1377.32187	2
5411	H	72.45160	134.54880	78.85680	1486.26182	-1318.32270	2439.52399	2
5412	C	70.75860	133.14160	78.63370	-560.46807	-394.51030	601.40516	2
5413	H	70.10960	133.61190	79.40580	-2119.39474	-942.74720	-2125.46933	2
5414	H	70.06960	132.76520	77.84610	1842.43010	-195.59170	2542.71930	2
5415	C	71.64160	131.95860	79.24950	560.40431	391.88200	-603.18033	2
5416	H	72.25860	131.38120	78.51460	1577.73754	1931.59019	1917.79295	2
5417	H	72.30860	132.24890	80.10100	-933.15033	-2059.56773	2187.60999	2
5418	N	70.65160	131.10300	79.75270	158.60937	772.85389	-300.35349	2
5419	H	69.69560	131.40480	79.64470	334.84213	-2988.70533	-923.98455	2
5420	C	70.87860	129.99370	80.33210	544.75846	662.58563	-309.30488	2
5421	N	72.21160	129.59430	80.47370	302.46105	-747.07235	251.14242	2
5422	H	73.06360	130.06510	80.17230	-2032.62033	2314.15084	-641.39433	2
5423	H	72.51760	128.72720	80.91800	2216.72692	-1842.47658	1260.80452	2
5424	N	69.67860	129.38220	80.72230	593.21766	157.66047	579.57594	2
5425	H	68.71060	129.68690	80.62490	2532.12213	-1734.94003	-690.33822	2
5426	H	69.64060	128.48900	81.21380	-1423.18318	-441.02402	-2770.96981	2
5427	C	70.25260	136.30880	78.49570	-38.09106	-11.97720	910.96467	2
5428	O	69.04360	136.41840	78.47830	-735.11374	288.35227	9.37988	2
5429	N	71.10960	136.82050	79.36500	493.85710	565.34291	-386.21866	2
5430	H	72.14060	136.66750	79.22850	-1051.92943	-2944.04701	-352.50235	2
5431	C	70.59760	137.69220	80.43290	-63.48870	-728.28016	545.00293	2
5432	H	69.66460	137.15500	80.72660	-37.65542	-2957.73065	-1071.74516	2
5433	C	71.63760	137.81950	81.52940	-337.75935	434.43445	-727.07382	2
5434	H	72.56160	138.24270	81.07300	-1621.67197	1770.14962	-2033.46418	2
5435	C	71.17760	138.76840	82.62020	-670.46698	455.11399	418.08646	2
5436	H	71.95460	138.88810	83.42570	-906.37480	-1539.84701	2589.51388	2
5437	H	70.96360	139.79530	82.20760	372.38762	-837.28730	-3009.73482	2
5438	H	70.23560	138.40610	83.11670	-2295.00627	-1359.54838	1668.17285	2
5439	C	71.99660	136.47410	82.13420	-775.46996	429.03228	214.54287	2
5440	H	72.79560	136.57090	82.91930	-2281.30448	2102.00299	524.84238	2
5441	H	71.10560	135.99160	82.62240	-27.72195	-2975.56894	1021.49262	2
5442	H	72.37560	135.75770	81.35380	-221.52985	-2442.11852	-1971.09307	2
5443	C	70.25460	139.16130	79.74630	-696.95975	-176.83973	-560.73686	2
5444	O	70.95760	140.12030	79.94480	-475.49938	-38.25694	629.33614	2
5445	N	69.14860	139.07910	79.02670	-63.30393	195.19886	818.87869	2
5446	H	68.67460	138.16470	78.87410	-1874.75856	1800.53060	1772.45483	2
5447	C	68.69060	140.28260	78.42350	-155.21733	893.34934	-96.36147	2
5448	H	69.07560	141.09200	79.08600	1950.78607	1868.32601	1613.07714	2
5449	C	69.31960	140.39390	76.93560	517.95490	445.31590	604.04261	2
5450	H	69.12260	139.44540	76.38190	-2463.29718	-1651.20360	-1050.67592	2

5451	H	68.81160	141.20150	76.35550	313.88956	2742.99591	-1508.53340	2	
5452	C	70.79560	140.65870	77.02600	528.83897	532.44922	-517.95576	2	
5453	H	71.25360	139.88630	77.69020	-2112.43083	-770.50209	-2200.49739	2	
5454	C	71.43860	140.56890	75.64760	-690.20847	-395.67516	-445.53838	2	
5455	H	72.54160	140.75800	75.69450	2034.40660	2333.14030	-562.02523	2	
5456	H	71.29260	139.55860	75.18710	2248.94519	1961.22634	997.02710	2	
5457	H	71.00260	141.32170	74.94120	-1653.09412	-128.81697	-2673.74498	2	
5458	C	71.08160	142.02660	77.63160	570.24062	-573.92057	-420.58508	2	
5459	H	72.16560	142.29710	77.54740	1757.74695	-1540.64070	2105.93877	2	
5460	H	70.49560	142.83850	77.12800	751.83258	-183.54370	3049.47302	2	
5461	H	70.82460	142.04870	78.72440	1622.11417	-2533.02760	-922.35730	2	
5462	C	67.08960	140.21570	78.30330	-144.31220	732.67894	-523.26529	2	
5463	O	66.43260	139.26310	78.63070	-509.60359	492.38969	348.54525	2	
5464	O	66.46360	141.36840	77.76290	574.46196	539.67837	48.66154	2	
5465	H	67.27060	141.93960	77.64490	2831.71317	-407.24322	-1309.11410	2	
5466	5463								
5467		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	50.0000	200000
		0.2500	400.00	0.00	0.00	-25963.4904	0.2194	400.0000	
5468	N	59.32925	94.60114	60.17705	271.35006	-592.96075	106.19491	1	
5469	H	59.45444	94.48318	61.21740	1945.44748	55.50556	653.44217	1	
5470	H	59.96964	95.36992	60.02052	-827.26400	1277.59156	2850.84393	1	
5471	H	56.18374	97.62321	56.25805	-377.28197	-74.00573	-1322.78841	1	
5472	C	59.54298	93.40518	59.47197	-21.08611	281.75011	29.15743	1	
5473	H	60.23468	92.80201	60.15496	2306.08717	590.25168	-1466.72256	1	
5474	C	58.12407	92.68044	59.32990	-638.42110	-112.10884	-474.30528	1	
5475	H	58.32782	91.64076	58.91158	1027.37746	-535.75796	-156.17767	1	
5476	H	57.46840	93.14445	58.60516	391.30278	-2195.60374	1695.57201	1	
5477	C	57.57380	92.83528	60.79101	-319.46084	-594.93744	-193.23657	1	
5478	H	57.62634	93.95293	60.99037	491.53102	-1422.18652	1093.39794	1	
5479	H	58.24268	92.48654	61.62316	-534.59506	-565.44274	-714.33892	1	
5480	S	55.95330	91.93372	60.73313	-276.72994	-278.48295	59.42670	1	
5481	C	54.98879	92.84946	61.98185	-561.72265	-587.70720	508.63893	1	
5482	H	54.55786	93.84318	61.70403	-914.87520	1647.62000	-1211.07718	1	
5483	H	54.12394	92.32817	62.39693	-202.45800	43.39419	-2680.50820	1	
5484	H	55.52626	93.33882	62.87380	-556.34510	992.93955	965.80848	1	
5485	C	60.27188	93.43057	58.03160	294.01850	-543.10689	-7.80390	1	
5486	O	60.13723	92.53253	57.23616	-494.52661	-317.58210	-130.42765	1	
5487	N	60.94828	94.60005	57.84207	-221.94050	-660.16152	110.41625	1	
5488	H	60.98009	95.27902	58.66875	-3089.77970	408.72416	686.07439	1	
5489	C	60.88810	95.20855	56.53657	256.54620	486.44270	259.28406	1	
5490	H	61.10027	94.27884	55.97006	-176.46707	-69.72563	-170.30418	1	
5491	C	59.53346	96.04642	56.43582	-556.43475	1054.86722	180.35087	1	
5492	H	59.68578	96.95544	57.09911	1789.31693	456.76486	-1832.78754	1	
5493	H	59.34252	96.46785	55.41925	224.57071	2155.94628	-1218.02608	1	
5494	C	58.33817	95.16581	56.84036	548.67175	-63.95644	-487.19200	1	
5495	H	58.57741	94.61605	57.74068	2537.13495	523.27357	-2980.79175	1	
5496	H	58.09546	94.45355	55.98038	-342.38674	1763.57803	-1889.47812	1	
5497	C	57.21427	96.24706	57.11820	167.09655	-254.03887	-185.71994	1	
5498	O	57.13629	96.81661	58.17480	612.70846	254.66907	-469.39090	1	
5499	O	56.59923	96.73392	55.93335	408.27598	52.21467	31.89802	1	
5500	C	62.19801	96.18343	56.68810	-457.95056	1318.63898	406.32007	1	
5501	O	62.15052	97.11055	57.49042	274.07598	-913.07829	-28.74658	1	
5502	N	63.14815	96.03557	55.69734	-43.61819	-551.90268	-616.35502	1	
5503	H	62.97931	95.08775	55.32352	2713.01166	-1228.95309	-90.80713	1	
5504	C	64.37880	96.60809	56.23154	90.44152	104.11505	-267.71328	1	
5505	H	64.01676	97.58216	56.64142	645.64017	1029.59248	1769.53233	1	
5506	H	65.06867	96.74607	55.33358	-1732.13063	94.24752	3247.72997	1	
5507	C	65.05796	95.64263	57.33839	389.40382	187.12259	1392.67155	1	
5508	O	65.46297	94.54585	57.11387	59.16685	278.77221	-330.24761	1	
5509	N	65.48482	96.48477	58.31734	-358.39856	-223.48690	290.00179	1	
5510	H	65.01283	97.38877	58.26927	1103.43442	-1254.65042	4093.24517	1	
5511	C	66.15499	96.03457	59.54693	110.03861	-792.45961	-600.28691	1	

5512	H	66.76536	95.23235	59.03991	3881.73884	-3246.48529	-1713.23894	1
5513	C	66.86292	97.24311	60.13028	52.08378	-63.61845	-148.20308	1
5514	H	67.33189	97.87399	59.34886	-884.03102	646.23456	-3087.81658	1
5515	C	65.88710	98.15465	60.82359	718.48539	-2022.10708	805.87632	1
5516	H	65.20514	98.63532	60.05887	895.31732	1686.03186	-444.65291	1
5517	H	66.42826	99.04779	61.28863	690.24942	2073.65902	49.83573	1
5518	H	65.29110	97.63567	61.56247	712.84460	-410.47752	1975.22241	1
5519	C	67.91992	96.74089	61.12998	-516.99123	165.41361	0.52115	1
5520	H	67.67292	95.85373	61.75908	-4240.08894	2619.55492	-79.90132	1
5521	H	68.24434	97.56800	61.81029	-1663.34688	-1221.87864	-909.86082	1
5522	C	69.19349	96.38098	60.29166	-483.27781	-701.69206	-447.21025	1
5523	H	70.05618	96.15120	60.99200	2139.68355	-210.18795	-2581.86122	1
5524	H	69.52009	97.16482	59.57236	-3039.11316	923.36106	1150.44268	1
5525	H	69.14960	95.51538	59.62565	1946.66276	132.09554	1460.33304	1
5526	C	65.13741	95.27173	60.60791	891.83152	-671.48702	552.87713	1
5527	O	65.59917	94.54091	61.45986	-209.21340	-631.06791	70.71439	1
5528	N	63.79863	95.53916	60.41326	-315.45965	-334.43737	89.93755	1
5529	H	63.68019	96.07082	59.53924	520.56012	594.69913	-925.42302	1
5530	C	63.17443	96.11190	61.62459	364.55265	-302.73529	-1271.76631	1
5531	H	64.06677	96.39402	62.20518	-1278.82200	1071.06573	-2767.04637	1
5532	C	62.22480	97.24161	61.15371	-1032.23587	775.96994	-740.22741	1
5533	H	61.70797	97.74917	61.96845	1869.34245	-839.10498	1084.29825	1
5534	H	62.77055	97.98559	60.55459	1512.85121	-2229.80572	2436.59716	1
5535	O	61.00467	96.74528	60.18003	-196.82662	297.68478	77.01953	1
5536	H	61.51877	96.80085	59.34875	104.26440	-1297.24387	-3150.99267	1
5537	C	62.37532	94.92994	62.39599	-91.09533	258.41843	-212.37998	1
5538	O	61.93308	95.28370	63.49328	-537.22125	-420.46274	-814.90440	1
5539	N	62.18252	93.81704	61.75142	-758.45566	166.38333	-992.43112	1
5540	H	62.64574	93.77649	60.82954	780.29074	1327.64348	-57.06099	1
5541	C	62.04416	92.48391	62.30149	28.81129	873.17671	435.81495	1
5542	H	62.22571	91.79343	61.49499	763.58041	1314.05362	1439.89031	1
5543	C	63.05085	92.38014	63.43330	139.27596	-1318.36300	764.20323	1
5544	H	62.88467	93.23041	64.19772	-679.62479	579.17937	-2534.08637	1
5545	C	62.70585	91.16084	64.30894	-1250.11297	771.64091	-23.04158	1
5546	H	63.40612	91.13804	65.16861	494.15987	-113.40211	-311.36992	1
5547	H	61.64021	91.36551	64.74677	-561.27292	-1666.38761	-1021.35239	1
5548	H	62.74257	90.23191	63.66121	3316.31731	-385.28006	895.45141	1
5549	C	64.44671	92.38095	62.93691	132.72633	523.39349	-157.29239	1
5550	H	64.50015	93.30740	62.24877	-2133.18391	-982.57768	-1380.68346	1
5551	H	64.64877	91.43161	62.32678	894.15604	2191.70205	962.66558	1
5552	C	65.47055	92.56865	64.14147	215.10070	317.60265	-237.91986	1
5553	H	66.43385	92.02413	63.96196	-562.50423	449.29084	676.16245	1
5554	H	65.77546	93.65866	64.29749	3783.28305	1.13035	-722.13108	1
5555	H	65.10935	92.09428	65.09958	1535.61186	-831.32642	202.37370	1
5556	C	60.46384	92.21919	62.85855	1278.28757	-362.13292	-676.06600	1
5557	O	59.89687	91.16033	62.60312	-1111.57679	93.36246	249.66018	1
5558	N	60.10633	93.17396	63.70146	263.57567	-327.00968	-305.89760	1
5559	H	60.77530	93.99198	63.78300	-2528.73668	243.86984	-553.23964	1
5560	C	58.76008	93.35746	64.08138	-11.93960	-199.57436	-263.99158	1
5561	H	58.14161	92.40197	63.82198	-476.53435	-1653.21494	2313.34811	1
5562	C	58.87048	93.49787	65.63106	-76.47412	-943.76637	6.68314	1
5563	H	59.28193	94.47708	65.90794	1306.92943	-817.53450	-3734.63506	1
5564	H	59.62290	92.74627	66.02501	-481.60695	-207.35339	-576.79214	1
5565	C	57.53775	93.15891	66.28590	388.42732	-78.00393	250.65470	1
5566	C	57.31655	91.74944	66.47768	-459.88665	-450.58771	147.63204	1
5567	H	58.09531	91.12175	66.10450	-704.73805	-129.60006	1623.38794	1
5568	C	56.16933	91.33385	67.18878	359.19146	286.04745	-1388.17363	1
5569	H	56.29566	90.25852	67.47581	-411.27872	758.09926	-1526.45592	1
5570	C	55.13672	92.27473	67.50985	244.42923	252.52822	137.22366	1
5571	O	53.90785	91.85681	68.05315	-208.05076	-114.34113	70.86236	1
5572	H	53.98120	90.83138	67.84134	-2385.74346	-65.12607	-2376.04346	1
5573	C	56.55835	94.16116	66.65667	-766.66768	-1410.11230	-623.15769	1

5574	H	56.70894	95.20640	66.39477	2874.10504	-521.05779	2288.94830	1
5575	C	55.38491	93.63767	67.20120	166.12471	-238.90747	724.01036	1
5576	H	54.48665	94.25875	67.34514	-2838.42778	636.50105	-1360.40139	1
5577	C	58.02844	94.78608	63.58571	18.88269	-1002.23445	-115.83540	1
5578	O	56.83820	94.94922	63.79305	-20.78638	-557.77763	43.55451	1
5579	N	58.92097	95.54075	63.03451	-235.66913	-80.93540	169.89330	1
5580	H	59.80466	95.12294	62.80379	-2269.24845	890.06337	-913.23298	1
5581	C	58.64985	96.96680	62.95067	-212.25111	-672.29738	-414.64313	1
5582	H	59.56273	97.10705	62.28319	-1251.40072	1233.27351	3062.55179	1
5583	C	57.28449	97.21757	62.17124	267.67838	167.25811	9.16839	1
5584	H	57.17788	98.32498	61.77882	-1095.31795	-3757.01095	971.30828	1
5585	O	56.03880	97.20731	62.82015	-373.59760	-682.26895	476.69085	1
5586	H	56.11086	96.25407	63.35985	-351.94935	2586.56492	2328.56655	1
5587	C	57.17710	96.53210	60.71677	184.46610	543.07556	32.37531	1
5588	H	58.13288	96.71022	60.15341	149.45783	1040.30843	60.78155	1
5589	H	57.07818	95.44201	60.81772	981.82110	236.45923	-237.55639	1
5590	H	56.24589	96.84961	60.17927	2052.90811	-1823.04692	-1442.93830	1
5591	C	58.90415	97.62533	64.38763	178.71805	10.66583	720.33979	1
5592	O	58.81257	97.17321	65.54256	180.41407	-70.28064	-775.35859	1
5593	N	59.09288	98.90896	64.03881	-452.87481	259.65035	201.64218	1
5594	H	59.27371	99.09640	63.04811	-4253.94708	-1292.17833	-1065.16666	1
5595	C	58.85315	99.90142	65.05673	10.22087	-429.64363	248.57024	1
5596	H	57.81174	99.69592	65.31101	-1458.39872	-182.07176	-314.84649	1
5597	C	59.80504	99.76346	66.36974	138.09117	-391.38804	-746.88640	1
5598	H	59.45514	100.50846	67.16315	1238.49289	988.07306	-461.19209	1
5599	H	59.43658	98.78150	66.78808	641.33275	-757.87063	475.48523	1
5600	O	61.19793	99.87738	66.13620	215.33689	-533.86049	178.45068	1
5601	H	61.37505	100.79136	66.30702	904.13280	1216.13298	-1307.19825	1
5602	C	59.10876	101.37255	64.48920	417.42146	-240.25463	-128.50613	1
5603	O	59.56906	101.73828	63.39067	129.77349	66.53313	997.45764	1
5604	N	58.79354	102.21799	65.50531	328.51064	-576.51570	-238.87236	1
5605	H	58.37521	101.91819	66.40867	-1518.00667	-158.24277	1424.92745	1
5606	C	58.31621	103.54027	65.08366	513.39895	-280.71622	640.90798	1
5607	H	57.63052	103.32384	64.18880	-20.63138	-734.58123	933.73767	1
5608	C	57.64593	104.25977	66.28290	47.16549	984.87471	-322.23667	1
5609	H	56.69734	104.80280	65.97552	2392.19196	-448.06798	1335.33691	1
5610	H	58.29792	105.09920	66.76208	1906.43067	580.96617	1844.27438	1
5611	C	56.97969	103.29596	67.54322	-323.11192	-327.42646	-732.81034	1
5612	O	57.36161	102.15820	67.76695	416.02310	407.67660	340.06965	1
5613	O	56.26901	103.97478	68.25975	591.72482	-487.49016	324.73034	1
5614	C	59.57722	104.42531	64.64818	-421.99918	-311.65626	1166.58460	1
5615	O	59.46408	105.45947	64.05180	-178.90778	181.01323	775.77010	1
5616	N	60.77347	103.87589	64.99555	419.57978	-107.79759	-550.12963	1
5617	H	60.86296	103.04173	65.58217	217.44791	-1276.05322	-1543.28155	1
5618	C	61.92682	104.70323	64.84971	785.64442	434.13444	-200.71106	1
5619	H	61.58673	105.72985	64.46319	3524.82552	1015.71317	98.29262	1
5620	C	62.63310	104.68518	66.30449	231.55685	530.48471	269.63988	1
5621	H	62.05952	105.42380	66.94158	1256.98169	-1193.71174	-800.46771	1
5622	H	63.62414	105.10301	66.12345	256.38718	734.71587	2450.81465	1
5623	C	62.70069	103.37065	67.09992	222.24728	540.98992	-706.30479	1
5624	O	61.93275	102.39730	66.91270	-525.06589	816.86258	-144.65027	1
5625	N	63.74067	103.44970	67.93422	-385.04663	41.44348	-21.15067	1
5626	H	64.12829	102.64543	68.46751	-610.53517	-1074.44827	2359.85132	1
5627	H	64.37485	104.30985	67.87040	648.97581	-1099.57142	-526.42847	1
5628	C	62.80557	103.97703	63.74140	897.17759	399.36739	-500.30324	1
5629	O	63.82173	104.58356	63.36172	-561.19186	430.14220	-289.22591	1
5630	N	62.34746	102.90186	63.10757	-561.56343	-238.72721	-548.98397	1
5631	H	61.33938	102.61120	63.35224	-698.31290	-2438.17187	-512.48076	1
5632	C	63.20926	101.80631	62.74732	282.87244	783.60812	-491.46277	1
5633	H	64.13713	102.31174	62.54446	321.42304	1781.00806	-656.36736	1
5634	C	63.44920	101.03820	64.12979	-338.52665	622.12284	1064.91222	1
5635	H	64.00317	101.72956	64.81250	-1107.83008	368.34581	-1048.46905	1

5636	H	62.51833	100.87777	64.74812	-3253.32490	-2101.97912	-285.30762	1
5637	C	64.22788	99.72653	64.03719	916.61086	721.76460	-131.92515	1
5638	C	65.61901	99.63041	63.91383	148.02830	-152.51061	254.39478	1
5639	H	66.22031	100.53751	63.85898	1204.52054	-2562.29742	-704.85918	1
5640	C	66.33390	98.40398	64.02334	645.49228	582.32706	270.43895	1
5641	H	67.44236	98.45840	63.94745	-1945.01911	2805.85088	-2270.40583	1
5642	C	65.60669	97.16980	64.13188	251.64540	-176.61959	-170.60553	1
5643	O	66.20019	95.87444	64.12230	162.19395	631.12489	403.23842	1
5644	H	65.74370	95.53417	63.31849	-498.05509	-2119.91763	1832.68412	1
5645	C	63.47933	98.52235	64.24275	212.89899	-744.76234	-537.05323	1
5646	H	62.31498	98.51037	64.44292	-276.57417	1451.41024	990.07450	1
5647	C	64.17410	97.34146	64.25327	318.00939	-627.62900	-3.61953	1
5648	H	63.41339	96.48126	64.34834	-1287.06219	482.38733	-2042.54975	1
5649	C	62.71630	100.82849	61.52038	683.81416	-110.75992	-801.90748	1
5650	O	63.57012	100.40744	60.79521	263.35995	790.59860	694.17459	1
5651	N	61.37884	100.68261	61.52773	-393.51794	-195.82231	293.92597	1
5652	H	60.85068	101.03348	62.40620	-878.21579	-1712.30502	1977.46918	1
5653	C	60.90032	100.56057	60.15506	-81.87596	-84.25322	506.35658	1
5654	H	61.77189	100.13741	59.64128	259.73210	3831.76100	2519.44935	1
5655	C	59.49264	99.77687	60.00298	-334.44644	232.13541	1099.21620	1
5656	H	58.69078	100.57836	60.27051	-1023.74857	52.34937	-951.28216	1
5657	O	59.18577	98.68645	60.85404	61.13960	-233.33669	-1158.27761	1
5658	H	59.59802	97.93752	60.23291	-1620.18296	-2346.39410	-319.42597	1
5659	C	59.54944	99.36128	58.47773	-909.65997	238.34370	89.00647	1
5660	H	58.79591	98.57949	58.23656	-1182.32980	808.26481	610.19040	1
5661	H	60.51220	98.88734	58.24533	4107.91675	796.26093	-899.46669	1
5662	H	59.39489	100.19576	57.81979	1035.85745	-512.22001	2120.15758	1
5663	C	60.67905	102.03137	59.55278	-1029.31749	-895.67673	435.00554	1
5664	O	59.86923	102.20159	58.64380	-154.01858	-491.79537	-181.45257	1
5665	N	61.44910	102.95473	60.15758	-618.87611	-118.94189	-227.16164	1
5666	H	61.89296	102.53194	60.90870	219.98502	-3357.60193	329.73072	1
5667	C	61.07240	104.33395	60.03998	399.53718	-422.42073	-568.86482	1
5668	H	60.48454	104.28283	59.08097	1083.22859	-2401.46340	-164.47079	1
5669	C	60.41697	104.72480	61.44120	362.14719	411.07401	220.30699	1
5670	H	60.57366	103.97692	62.23245	4935.53072	3405.57608	1216.17565	1
5671	H	60.83691	105.61094	61.97303	-1281.84473	285.86280	-45.74877	1
5672	C	58.88153	104.88769	61.15315	-152.38714	227.02785	520.36199	1
5673	H	58.49790	103.95824	60.71856	-1588.40319	863.05557	784.92045	1
5674	H	58.33786	105.02104	62.10376	875.95562	1924.26752	2365.40401	1
5675	C	58.72266	106.12575	60.05347	-262.85418	549.90937	-408.91926	1
5676	O	57.65628	106.13524	59.45144	-354.06783	108.94323	483.74634	1
5677	O	59.59895	106.99878	59.92113	-538.81824	-411.20164	169.59860	1
5678	C	62.46718	105.15389	59.85562	535.08620	126.13437	-408.58553	1
5679	O	63.47583	104.63194	59.44655	-323.08839	162.16037	480.85768	1
5680	N	62.21087	106.44215	60.16547	455.61472	-466.61767	-479.24893	1
5681	H	61.28041	106.84671	60.45498	410.15238	-1734.89461	1149.44398	1
5682	C	63.39419	107.25653	60.26036	-117.63826	91.37175	-338.74557	1
5683	H	64.19373	106.68074	59.67645	-1182.61014	-1348.42261	872.45746	1
5684	C	63.00247	108.64612	59.61959	-287.63891	-456.97052	-323.52491	1
5685	H	63.83520	109.37534	59.70671	1112.95205	543.33647	1171.80086	1
5686	H	62.07222	109.19682	60.00704	3152.74912	-1281.24404	-1270.02242	1
5687	C	62.82217	108.18017	58.15061	622.71615	-326.99246	-176.06769	1
5688	H	62.13004	107.34835	58.03502	500.66215	2438.88661	-661.79518	1
5689	H	62.26654	108.89826	57.56812	2986.95695	-511.56316	-902.05824	1
5690	C	64.29349	107.90104	57.43192	-982.73719	1254.41729	-486.40214	1
5691	O	64.22427	107.85843	56.20197	121.16131	-338.54097	-335.58652	1
5692	O	65.29548	107.81830	58.16380	5.22858	-111.02898	67.70412	1
5693	C	63.76144	107.53452	61.83749	512.08054	326.23910	90.92611	1
5694	O	62.96940	107.52358	62.75735	-41.40323	-326.28600	333.69335	1
5695	N	65.07007	107.85344	61.88305	68.39287	232.85459	386.53416	1
5696	H	65.34966	107.85034	60.87987	1933.80526	-141.95290	1291.79395	1
5697	C	65.96830	107.01919	62.67963	-735.16522	-199.07711	-216.25938	1

5698	H	65.45203	107.07823	63.72703	654.64083	-691.47543	1754.50174	1
5699	C	65.92851	105.58181	62.02034	84.89714	30.66284	-105.52066	1
5700	H	66.27552	104.72547	62.60698	-1462.55851	1376.85975	-2031.11071	1
5701	H	64.86868	105.22897	61.70675	-644.33858	1718.22079	1218.73074	1
5702	C	66.81462	105.58810	60.77744	686.67673	122.61879	-13.27330	1
5703	H	67.88954	105.86132	61.03879	2094.97390	1004.81356	-263.73462	1
5704	H	66.33730	106.26982	60.01012	-510.33931	-195.80673	1054.34381	1
5705	S	66.83581	103.73084	60.17211	25.83463	570.39914	386.47383	1
5706	C	66.15706	103.87953	58.42414	25.05472	-12.72296	626.86136	1
5707	H	66.59621	104.62769	57.75640	-1339.03361	-2386.91770	-839.67647	1
5708	H	65.14872	104.39583	58.45798	475.75006	-638.99744	1936.31223	1
5709	H	65.99556	102.93518	57.82257	795.91667	-1349.11094	-1230.47953	1
5710	C	67.51212	107.45476	62.69908	263.92856	-412.06866	318.44053	1
5711	O	68.16954	107.92620	61.78299	619.64612	-192.28713	189.24632	1
5712	N	67.97935	106.80634	63.78315	836.72358	379.58567	-103.15496	1
5713	H	67.36405	106.28586	64.45006	-1912.37806	-2400.68694	319.42816	1
5714	C	69.32111	107.20826	64.09420	-635.18175	316.28688	647.41069	1
5715	H	69.52840	108.24480	63.64785	1655.54340	1815.01743	2144.74577	1
5716	H	69.39710	107.17683	65.25456	422.18176	-1432.79473	1853.91825	1
5717	C	70.29769	106.14871	63.43906	-66.82379	775.27844	515.01269	1
5718	O	70.85271	105.33921	64.17278	-393.52836	-508.09512	-1290.72721	1
5719	N	70.32124	106.31266	62.09648	329.57484	342.24172	401.58901	1
5720	H	69.59525	106.90726	61.64047	1378.51241	1142.75280	-1266.55282	1
5721	C	70.77096	105.10812	61.39344	-245.71672	-547.47360	11.89277	1
5722	H	70.45960	104.26271	62.02383	53.60239	-2245.48160	-89.58537	1
5723	C	70.18021	105.16082	59.94716	310.60388	183.54096	-293.71701	1
5724	H	69.49837	106.02399	59.92059	603.09415	1647.76992	-1083.25428	1
5725	H	71.11663	105.36310	59.32627	-143.65081	870.10565	-1511.90856	1
5726	O	69.82155	103.88355	59.35315	-87.83103	-294.93183	222.37899	1
5727	H	68.76068	103.89547	59.56669	210.42322	720.61030	1947.49693	1
5728	C	72.40295	105.20667	61.33804	758.87815	48.77599	-137.64008	1
5729	O	72.97628	105.65480	60.37481	-185.81857	523.09581	-375.50609	1
5730	N	72.88691	104.69759	62.46036	-105.39106	297.22773	-159.32419	1
5731	H	72.13841	104.54692	63.18661	195.19942	-53.91046	-181.56448	1
5732	C	73.67084	103.44609	62.17848	119.63870	-261.56061	106.73309	1
5733	H	73.10141	102.67336	61.54315	884.70516	647.91511	-2404.17292	1
5734	H	74.53334	103.87390	61.62672	-952.84663	-7.55389	-2684.62205	1
5735	C	74.04694	102.83092	63.55741	-166.65126	-1098.17052	52.85335	1
5736	O	74.12232	101.62738	63.73091	16.91798	-22.74627	640.17447	1
5737	N	74.28400	103.86213	64.53040	102.35910	23.16833	-348.20464	1
5738	H	74.48146	104.83845	64.19513	-1602.72630	-2165.89004	-586.69221	1
5739	C	74.87233	103.42637	65.74634	59.45663	-1088.44427	57.42303	1
5740	H	74.65058	102.33639	65.88121	-947.23759	1898.09265	-1816.17653	1
5741	C	76.41574	103.59764	65.76762	4.77489	294.75976	122.58672	1
5742	H	76.69546	104.65833	66.22293	-3997.84102	-68.52324	2537.60590	1
5743	H	76.88208	103.70505	64.79008	-431.90552	415.98774	2035.35406	1
5744	C	77.19301	102.36961	66.64822	608.10050	-138.99138	316.64360	1
5745	O	78.39027	102.63374	66.93555	395.95784	-18.54771	-40.15370	1
5746	O	76.63126	101.28633	66.71023	-844.99768	-384.19340	392.01039	1
5747	C	74.13933	104.23055	67.01691	1624.63902	80.16128	1142.94337	1
5748	O	74.48415	103.99777	68.15947	135.50600	-265.09012	657.24685	1
5749	N	73.09690	104.95988	66.67280	-13.51113	460.72806	203.74646	1
5750	H	72.76880	105.02792	65.72546	-2727.98440	637.55657	2703.53600	1
5751	C	72.66568	106.13297	67.35736	-26.51060	-666.67152	366.93695	1
5752	H	73.20552	105.91445	68.32568	226.28846	-449.44046	159.28564	1
5753	C	73.06221	107.44295	66.54983	607.70265	349.74508	-827.13554	1
5754	H	72.31320	108.24008	66.80676	2792.39588	809.17654	-97.27744	1
5755	H	72.90645	107.27054	65.48592	-1763.67263	1069.84555	-2357.18600	1
5756	C	74.45670	108.07969	66.73553	-124.57004	1484.99036	207.71208	1
5757	C	75.51782	107.15326	66.83717	-778.79517	-749.33582	-254.60816	1
5758	H	75.30250	106.12510	66.47596	540.46623	1117.67336	-59.39611	1
5759	C	76.79382	107.54001	67.23769	-396.46245	377.64462	495.53614	1

5760	H	77.64069	106.77709	67.22798	1844.72415	-1146.44328	-774.52500	1
5761	C	77.09419	108.93042	67.56768	57.29144	1037.77290	-1022.22283	1
5762	O	78.38319	109.41610	67.97072	-218.90375	136.72260	-729.56528	1
5763	H	78.41670	109.20019	68.88873	579.55969	1477.89535	-2665.80394	1
5764	C	74.66525	109.45545	67.09794	463.91968	26.68614	-491.15193	1
5765	H	73.82875	110.13114	67.22269	-902.02360	-1092.28540	-1502.87093	1
5766	C	75.95793	109.77298	67.50301	707.53164	-134.15265	356.02770	1
5767	H	76.22712	110.80293	67.89965	2070.65500	-3569.57077	1349.55047	1
5768	C	71.02110	106.20845	67.47184	331.33914	227.12618	17.00695	1
5769	O	70.29273	107.16887	67.39349	-314.86178	299.95864	-709.38602	1
5770	N	70.66769	104.94793	67.94985	-778.59963	-95.72665	529.08036	1
5771	H	71.32018	104.25346	67.61656	520.40985	4395.38229	1636.24987	1
5772	C	69.17735	104.82347	68.07005	-113.89387	-541.05417	650.25433	1
5773	H	68.86095	105.74046	68.66844	-2027.79807	-811.59929	-2040.76765	1
5774	C	68.53656	104.91918	66.68667	-248.97560	53.14426	230.07401	1
5775	H	68.95210	105.80474	66.13829	1703.07967	-472.73987	-469.10022	1
5776	H	68.82605	104.10199	66.05737	-769.75638	-1088.34137	-201.73763	1
5777	C	66.96643	105.19096	66.65475	-337.57828	1181.17341	-758.13953	1
5778	O	66.36810	105.76405	65.74197	-596.57655	280.70298	455.31619	1
5779	O	66.41392	104.75194	67.70527	8.79251	-237.02661	-127.92842	1
5780	C	68.90992	103.41856	68.78844	269.59986	-539.69133	-881.65961	1
5781	O	69.67060	102.46115	68.84695	322.17109	-184.66964	651.64863	1
5782	N	67.69289	103.43959	69.35082	-395.75443	-1262.50075	79.35250	1
5783	H	67.04949	104.24955	69.19573	1916.04273	-775.61810	-3567.22030	1
5784	C	67.38554	102.32912	70.23750	548.11555	-24.02341	-560.42429	1
5785	H	68.35434	101.91173	70.56429	-3236.92396	-2366.68997	-3654.37142	1
5786	C	66.43320	102.98848	71.28865	252.72848	-177.49701	46.29289	1
5787	H	65.70550	102.19296	71.68980	-76.62924	2357.73548	-3815.95293	1
5788	H	65.81857	103.85823	70.84649	-2073.98472	1256.27632	-425.10834	1
5789	O	67.22699	103.86570	72.19655	-28.35827	-631.04393	382.38833	1
5790	H	67.28888	103.19225	72.94710	-124.62220	-2261.39465	1134.98166	1
5791	C	66.68349	101.24770	69.23389	-79.38564	144.29958	-75.27612	1
5792	O	65.48828	101.15884	69.11163	232.37471	728.92186	-490.94988	1
5793	N	67.72598	100.65951	68.58241	-784.80969	200.85660	313.24847	1
5794	H	68.72375	101.00805	68.45247	-1377.96813	416.81646	514.38278	1
5795	C	67.21858	100.00842	67.35428	23.64880	-352.79232	-480.09362	1
5796	H	66.40453	99.36952	67.74217	-1294.58978	573.57742	1577.38728	1
5797	C	66.72327	101.07805	66.29247	-474.18533	753.27951	204.76787	1
5798	H	66.01408	100.41955	65.74066	2678.27183	2188.10460	-5149.74334	1
5799	H	66.13367	101.88887	66.82799	2529.90202	1061.06314	508.00667	1
5800	C	67.90945	101.62483	65.39958	152.19329	-600.80825	-434.86320	1
5801	H	68.90500	101.85444	65.97524	-1928.16587	1886.93325	-2909.31792	1
5802	H	68.35522	100.79907	64.66365	2519.57866	-864.05388	-22.67159	1
5803	S	67.05802	102.91430	64.49102	-393.30781	-120.22204	-290.84598	1
5804	C	68.34604	103.44011	63.31155	334.82130	-182.77250	-324.11720	1
5805	H	68.20757	104.44445	62.74908	-729.88924	-780.97621	-573.46446	1
5806	H	69.36209	103.42649	63.68428	-549.56034	1514.68650	-2376.88287	1
5807	H	68.62077	102.59126	62.69164	-518.50998	2756.88625	950.37589	1
5808	C	68.40709	99.12621	66.78055	63.65582	89.32021	-305.56498	1
5809	O	69.55776	99.56114	66.82952	-804.35664	143.32171	-749.21497	1
5810	N	68.05053	97.90921	66.33697	576.01068	517.28769	195.98129	1
5811	H	67.08049	97.58268	66.28169	2263.08206	-1775.38944	1195.06253	1
5812	C	69.12118	96.98689	66.18345	218.31634	500.64921	-169.19653	1
5813	H	69.80180	97.19396	67.10773	2866.32723	-6.86992	-1154.51632	1
5814	C	68.64381	95.47197	66.16257	-135.26143	-385.47725	-718.45969	1
5815	H	68.02999	95.23698	65.23811	1186.10522	-1670.12440	-3661.24541	1
5816	H	69.52547	94.76477	66.18538	-1465.42999	-1634.15221	3676.09937	1
5817	C	67.84554	95.21592	67.49134	-333.04777	-303.70143	-522.04989	1
5818	H	66.84958	95.72271	67.52706	-2009.86783	-2154.54215	-939.11352	1
5819	H	68.51889	95.69651	68.21194	-3001.91081	-148.41211	2795.73437	1
5820	C	67.70769	93.69896	67.82515	674.78888	-522.42570	-980.80073	1
5821	H	68.63294	93.17484	67.57073	1599.01468	2394.21117	-784.93366	1

5822	H	66.87088	93.27891	67.13066	545.45154	-789.90977	-1134.56609	1
5823	C	67.47381	93.51983	69.34696	-516.57556	-262.13995	-560.28201	1
5824	H	67.70193	92.54497	69.74269	564.33834	637.97314	579.09182	1
5825	H	66.52711	93.88891	69.73624	3815.42437	424.27227	872.89564	1
5826	N	68.51234	94.45145	70.06337	473.69948	864.27780	-231.11256	1
5827	H	68.62716	94.20851	71.11426	603.53439	-1174.73157	1059.17044	1
5828	H	69.58584	94.48516	69.61545	-1249.91901	-242.12226	198.39343	1
5829	H	68.31898	95.56318	70.08024	-361.81758	-1413.00125	2279.50983	1
5830	C	69.96250	97.22449	64.80571	-259.21920	-333.98989	589.01190	1
5831	O	69.89890	96.49327	63.84300	185.84654	206.43251	614.01045	1
5832	N	70.75935	98.28313	64.99702	-478.26769	-453.04486	153.54548	1
5833	H	70.65487	98.75731	65.90333	-1884.26061	-1701.89537	1070.51088	1
5834	C	72.06488	98.13875	64.35923	-377.06335	-265.63095	526.91144	1
5835	H	71.97302	97.08950	63.99152	1304.98748	-1111.63069	5357.12276	1
5836	C	72.29962	99.17192	63.18804	-705.43259	-493.66404	-169.59928	1
5837	H	72.54435	100.14853	63.69311	2683.15426	1128.18106	3543.35469	1
5838	H	73.18348	98.88516	62.55805	-588.94202	1453.35019	-256.32346	1
5839	C	70.95207	99.29422	62.38796	-919.78019	-132.77436	394.63787	1
5840	H	70.37365	98.33713	62.40838	1828.84721	-524.79994	24.62374	1
5841	H	71.18592	99.46241	61.34356	-1573.59723	-1517.82706	636.37616	1
5842	C	69.99443	100.41837	63.05131	267.22849	-599.37610	-1144.31832	1
5843	O	68.77863	100.05570	63.10358	436.89200	230.35808	998.94321	1
5844	O	70.36740	101.48515	63.48645	-51.42190	983.75326	-327.92978	1
5845	C	73.21020	98.30600	65.46589	125.96594	466.77883	118.43234	1
5846	O	74.26628	97.63247	65.39826	-329.90494	-811.35976	52.09558	1
5847	N	72.93537	99.39080	66.22055	947.85110	-59.30312	3.26807	1
5848	C	72.11428	100.52321	65.79321	-494.10971	640.98289	685.15215	1
5849	H	71.12606	100.31918	65.22450	-466.31350	1053.42888	3249.48394	1
5850	H	72.66483	101.27171	65.20985	-91.05200	1447.47192	1674.51387	1
5851	C	73.65677	99.65506	67.40139	889.15705	483.92845	-1034.96239	1
5852	H	74.67112	99.72740	66.94726	-1804.02745	1218.64174	-1125.88821	1
5853	C	73.10223	101.03314	67.97812	1031.86505	-330.28378	761.33645	1
5854	H	73.85822	101.84724	67.79653	-2716.51113	-2429.22873	-21.15631	1
5855	H	72.80162	101.03773	69.02199	-884.83627	-3738.85657	-1604.68701	1
5856	C	71.78973	101.29554	67.16096	-696.52078	273.97301	235.91309	1
5857	H	71.46568	102.32628	66.93769	-601.25499	-1433.31243	-1085.97711	1
5858	H	70.95396	100.87283	67.76170	397.65221	705.84149	2989.15343	1
5859	C	73.57241	98.42722	68.49470	1292.65115	-454.60886	312.13612	1
5860	O	72.96154	98.65221	69.53533	659.93816	-95.33243	936.58969	1
5861	N	74.33358	97.42121	68.07465	798.04592	158.88052	689.68394	1
5862	H	74.81503	97.54850	67.18708	2935.80575	1431.91494	1351.57039	1
5863	C	74.08407	96.05811	68.47431	-250.45814	-542.79729	624.12135	1
5864	H	73.32914	96.12821	69.28992	1609.41603	-1234.74519	1194.97490	1
5865	C	73.55377	95.36420	67.18064	-682.70623	604.33204	101.89780	1
5866	H	73.95841	95.89786	66.30898	465.35140	1209.76695	-30.95690	1
5867	H	74.05234	94.38041	67.08426	-1645.20764	146.94405	1475.84807	1
5868	S	71.73668	95.36599	67.36723	-105.13143	-222.63977	-142.85913	1
5869	C	75.52394	95.27564	68.86451	424.35973	-280.96251	-208.06361	1
5870	O	75.57688	94.04373	68.93346	-347.30789	-289.58206	819.15627	1
5871	N	76.60623	96.06978	68.85047	399.86689	92.24995	-127.25726	1
5872	H	76.22638	97.01320	68.81804	2211.55122	1040.26023	680.90680	1
5873	C	77.82485	95.52927	69.40064	569.98495	-596.74084	-1102.81532	1
5874	H	77.86679	94.60935	68.80950	1197.66245	1918.19719	1505.02562	1
5875	C	79.06575	96.49201	69.20717	-141.85137	547.94396	242.68460	1
5876	H	79.88113	96.14541	69.84449	-1418.14399	1746.59955	-1860.59569	1
5877	H	78.63743	97.44285	69.67058	4675.54747	-470.92879	-661.28973	1
5878	C	79.35348	96.79823	67.72603	-1028.87636	-285.26869	-541.15691	1
5879	C	80.31923	95.88608	67.20556	-655.95971	-478.44912	831.48569	1
5880	H	80.81615	95.06326	67.79697	2411.96211	217.21909	2660.36816	1
5881	C	80.58078	95.97967	65.84504	1211.24663	-127.44722	-243.46366	1
5882	H	81.38859	95.35471	65.45618	-126.47631	1001.17130	1538.30689	1
5883	C	79.92022	96.90235	65.00371	882.22123	28.30219	-797.77945	1

5884	H	80.08228	96.98416	63.92336	1652.84822	797.44099	165.87788	1
5885	C	78.73597	97.78477	66.96472	1095.54944	-134.24031	229.94298	1
5886	H	78.00337	98.44681	67.42570	2639.88234	-1998.79844	3388.87602	1
5887	C	79.02009	97.81999	65.57268	-293.19916	-990.33281	96.47109	1
5888	H	78.61415	98.68568	65.01327	458.90938	-2359.37944	1961.53787	1
5889	C	77.68091	95.37626	71.00727	-564.94689	-48.09105	130.53855	1
5890	O	77.95793	96.27392	71.75526	-230.40194	-573.97396	96.16315	1
5891	N	77.56607	94.03459	71.34027	-393.93417	41.04051	-766.81876	1
5892	H	77.17035	93.61591	70.48740	2109.64424	355.79782	1272.12849	1
5893	C	76.71436	93.73527	72.53683	-146.21219	576.80902	-717.06452	1
5894	H	75.94492	94.53044	72.45628	-528.49827	-975.19542	716.88378	1
5895	C	76.21677	92.27482	72.22865	225.05408	356.49097	352.56466	1
5896	H	76.42829	91.62647	73.09968	-2665.98755	2509.10792	587.33001	1
5897	H	76.75148	91.85292	71.36958	34.68398	477.26256	82.26591	1
5898	C	74.64989	92.23427	72.09563	-314.00710	629.13452	-299.62580	1
5899	H	74.22646	93.14756	71.62094	1195.59510	4125.86177	1674.46631	1
5900	H	74.33157	91.41141	71.38888	1476.93194	883.69646	534.07621	1
5901	C	73.93703	92.25803	73.52282	338.04031	481.51272	-98.13528	1
5902	H	74.28553	93.16344	74.13948	1421.57559	391.70407	-2387.73933	1
5903	H	74.07767	91.33663	74.06707	623.99891	-1884.01765	-1300.06026	1
5904	N	72.65858	92.62426	73.20314	-181.20165	549.01519	76.73510	1
5905	H	72.44283	93.62441	73.05510	2172.68209	-117.64222	-668.68774	1
5906	C	71.62066	91.83148	73.30299	82.67211	-1142.65430	37.38534	1
5907	N	71.94637	90.50793	73.55154	-915.25704	-442.64419	-1421.05716	1
5908	H	72.88253	89.98894	73.71279	-267.37036	-421.60857	1580.33636	1
5909	H	71.18809	89.79247	73.59258	2780.64002	-2336.70064	-2248.26524	1
5910	N	70.37635	92.43538	73.15326	234.69999	226.26186	-514.14808	1
5911	H	70.13914	93.44073	72.86192	-649.90463	1972.24960	286.10204	1
5912	H	69.48784	91.89623	73.02005	-2419.05396	-1350.53273	1572.56076	1
5913	C	77.44910	93.93595	73.93837	-386.66480	-664.03931	-62.90695	1
5914	O	76.71551	94.15946	74.88454	-281.81477	-1254.48423	407.15511	1
5915	N	78.76404	94.01743	73.71069	-197.04348	30.61047	-328.52838	1
5916	H	79.07766	93.79975	72.76533	2637.28561	420.95810	-1166.57848	1
5917	C	79.58856	94.58825	74.71696	-105.27177	498.14880	204.11360	1
5918	H	80.45557	94.88541	74.02211	119.77631	556.71388	-394.07944	1
5919	C	78.96026	95.84296	75.48374	497.09344	60.71221	395.37154	1
5920	H	77.88610	95.79991	75.90033	-1157.06690	-72.82216	-1292.19679	1
5921	H	79.66362	96.14484	76.30866	-507.84837	-1694.08716	-101.04488	1
5922	C	79.08797	97.03737	74.47943	173.91130	-111.16371	365.99740	1
5923	H	78.53870	97.93727	74.80321	-398.56310	-1766.11597	-616.57612	1
5924	H	78.58549	96.74851	73.55982	-3447.80274	-496.44666	4415.52102	1
5925	C	80.68196	97.44784	74.25008	390.21692	885.45633	-296.55860	1
5926	O	81.13321	98.56390	74.52652	341.51178	-574.71504	530.95380	1
5927	O	81.34893	96.50129	73.83241	-29.13091	-736.09269	1147.62719	1
5928	C	79.88525	93.49178	75.87218	-337.43213	480.34834	-206.17163	1
5929	O	79.15054	92.59109	76.21656	-119.71986	729.20937	124.45381	1
5930	N	81.11704	93.78519	76.34284	-1167.84892	-670.31657	-357.81685	1
5931	H	81.62274	94.59557	76.07746	-109.27097	2699.38799	-3994.59109	1
5932	C	81.68321	93.48289	77.67723	978.63478	916.03327	344.56130	1
5933	H	81.30285	92.48910	78.01729	3184.41350	-2203.76608	-592.45596	1
5934	C	83.25183	93.50781	77.45867	-493.98243	-40.65460	1110.16988	1
5935	H	83.71604	94.19991	78.22020	-1331.40427	-1717.62917	1794.56360	1
5936	H	83.61721	94.05308	76.47541	-517.63282	-403.65356	4841.03506	1
5937	C	83.74836	92.04068	77.55677	-53.21184	-281.64923	-146.35726	1
5938	H	84.86094	91.93084	77.35903	-2704.54614	5913.93390	-2028.56221	1
5939	H	83.21722	91.40564	76.80954	-890.41431	1902.13963	2217.53632	1
5940	C	83.37906	91.71490	79.06963	-246.00958	-175.92686	353.86029	1
5941	O	84.01676	92.14019	80.05134	-1106.51722	-309.15336	87.55300	1
5942	O	82.31665	91.07112	79.23134	-253.23075	-1382.40508	213.37710	1
5943	C	81.19160	94.64247	78.66421	648.35828	317.29876	210.76422	1
5944	O	80.43206	95.49674	78.33628	-1081.99470	-421.77337	500.60741	1
5945	N	81.94842	94.51466	79.80952	29.20648	-534.22111	-385.87615	1

5946	H	82.61395	93.69509	79.95882	-364.88906	401.52370	-717.32243	1
5947	C	81.30454	95.07840	81.00582	-77.03539	1663.74196	392.96848	1
5948	H	81.11574	96.14028	80.76068	-2249.67891	562.83651	-1438.44534	1
5949	C	79.89232	94.32701	81.06098	356.39356	-542.80460	114.18590	1
5950	H	80.23785	93.31521	80.88290	1299.54085	-2356.36650	-776.89073	1
5951	H	79.23436	94.65751	80.32975	1420.52369	-1994.44430	-1584.88091	1
5952	C	79.16365	94.56529	82.40651	-155.78247	662.54231	361.14958	1
5953	O	79.78325	94.53839	83.48021	-561.94934	-690.75060	-61.78901	1
5954	N	77.83240	94.63893	82.27839	-327.84866	510.55842	-109.89109	1
5955	H	77.38348	94.59613	81.33342	3003.31989	1696.68621	-4146.68887	1
5956	H	77.13747	94.74763	83.06580	-1113.92296	-94.72718	1501.93143	1
5957	C	82.32088	94.89911	82.19320	-500.88814	51.86795	294.03856	1
5958	O	82.66481	93.74048	82.38747	-203.85888	-352.25966	-109.32439	1
5959	N	82.79186	95.95946	82.85632	-301.49112	571.76537	985.24423	1
5960	H	82.40746	96.93395	82.77819	2110.98072	-1197.84309	821.39250	1
5961	C	83.55586	95.69358	84.02355	-67.42740	426.37345	386.73298	1
5962	H	83.86042	94.61600	83.97160	-2724.80835	3185.27184	-791.71955	1
5963	C	84.87232	96.64255	84.10817	169.86861	601.13483	109.41896	1
5964	H	85.63729	96.27000	84.79037	1573.01302	1239.72160	1562.88838	1
5965	H	85.31928	96.81404	83.05119	1981.68885	644.12815	-495.63830	1
5966	H	84.63111	97.58967	84.61177	584.38206	-3620.99960	-1193.88259	1
5967	C	82.65981	95.80685	85.37093	-110.65648	-170.29690	-244.18410	1
5968	O	83.20701	95.66341	86.44019	103.69839	-803.14485	-139.51476	1
5969	N	81.33235	96.11442	85.22829	-87.37035	201.10098	761.58044	1
5970	H	80.94996	96.00784	84.31102	3069.59022	-968.22078	-1781.86382	1
5971	C	80.61321	95.99851	86.41131	-944.55037	26.46837	-406.73644	1
5972	H	81.41156	96.19969	87.23295	-633.74889	456.25891	-495.75305	1
5973	C	79.41043	96.98773	86.46092	-577.71038	724.19143	539.97545	1
5974	H	79.73620	97.98138	86.08748	1618.02457	-418.20756	245.47571	1
5975	H	79.14771	97.23228	87.59041	1667.22438	-70.80923	1715.65362	1
5976	C	78.06036	96.51679	85.71306	-260.68523	-21.89333	-374.72080	1
5977	O	77.82961	96.70074	84.52887	703.13254	-383.11140	-536.49548	1
5978	N	77.26234	96.06935	86.65053	473.16798	-796.36334	-244.24758	1
5979	H	77.67774	95.89292	87.57802	704.75892	2938.15464	3344.87535	1
5980	H	76.35044	95.57358	86.48988	-324.42801	546.81768	-1612.98295	1
5981	C	80.19543	94.45792	87.05534	-97.09281	305.05699	-628.10548	1
5982	O	80.12761	94.25799	88.22115	170.23047	188.29577	712.61475	1
5983	N	79.85683	93.65920	86.06854	206.64827	-5.51085	-787.88883	1
5984	H	79.70394	94.04964	85.07835	1875.58209	-979.31731	-2797.81850	1
5985	C	79.21943	92.39433	86.25558	-93.09614	408.75825	368.37474	1
5986	H	78.83353	92.28401	87.29589	2457.26628	1375.36293	1668.13490	1
5987	C	78.12031	92.57460	85.10356	722.66590	-379.67307	322.76012	1
5988	H	78.42545	92.30782	84.12242	1155.70126	2021.94341	-1555.34029	1
5989	H	77.85592	93.63918	85.10495	1642.11238	1209.05768	-643.82433	1
5990	C	76.88195	91.77109	85.51676	-206.04052	-401.43531	153.59485	1
5991	C	76.44260	90.73409	84.64309	172.10357	-529.87747	-407.25106	1
5992	H	77.12565	90.40917	83.86653	-577.26427	388.56021	1097.11479	1
5993	C	75.13156	90.17362	84.88262	880.69363	494.14229	-260.36559	1
5994	H	74.77280	89.42522	84.15183	-2280.52760	-1353.54538	2199.34519	1
5995	C	74.35811	90.50139	85.95261	-98.32525	-80.23271	253.82595	1
5996	H	73.30306	90.07334	86.13889	-4642.16767	965.79701	-1279.06888	1
5997	C	76.11736	92.05587	86.67544	275.58188	-206.22292	-306.43985	1
5998	H	76.36014	92.86418	87.31572	-2616.65884	-879.14558	2440.31161	1
5999	C	74.88474	91.45313	86.90868	251.10121	374.45460	-695.41971	1
6000	H	74.26133	91.75223	87.75867	1026.79527	3611.24665	1380.79672	1
6001	C	80.13038	91.14020	85.82485	180.59794	78.46451	-416.82933	1
6002	O	79.81832	90.02207	86.13483	83.42419	115.21175	76.64581	1
6003	N	81.30116	91.49166	85.13159	668.42870	732.76666	216.06736	1
6004	H	81.16796	92.48817	84.95384	356.52486	435.90525	1870.49997	1
6005	C	81.56031	90.70268	84.00404	15.65891	514.13574	-683.84199	1
6006	H	80.97281	89.73120	84.13730	2377.00354	3449.40651	1.95238	1
6007	C	81.19406	91.48413	82.70199	355.63573	-345.72267	310.86674	1

6008	H	82.00646	91.67398	81.94547	-1730.37177	-1483.13337	-51.08260	1
6009	H	80.81896	92.53302	82.98745	401.88645	-563.36263	256.24078	1
6010	C	79.93866	90.74599	81.98960	1313.69628	-199.51679	-198.15791	1
6011	O	78.88957	90.78159	82.56909	-74.45044	339.78767	334.01540	1
6012	N	80.31075	90.10378	80.87067	663.99376	-126.80829	21.00542	1
6013	H	81.18697	90.30521	80.32464	324.20137	249.14764	2602.45172	1
6014	H	79.67495	89.42015	80.42020	615.24176	-348.55431	-2485.02102	1
6015	C	83.15674	90.44560	83.98979	128.03674	-762.19614	36.87888	1
6016	O	83.58961	89.41425	84.42236	681.35487	911.15759	643.90234	1
6017	N	83.74782	91.66823	83.91692	113.53139	307.10552	-132.72075	1
6018	H	83.23172	92.42738	83.33727	-307.71971	2373.91495	356.71090	1
6019	C	85.22569	91.69227	84.06148	-722.22465	143.67955	260.73506	1
6020	H	85.46475	90.86618	83.38915	282.63086	-1032.04389	203.05581	1
6021	C	85.99136	92.94775	83.56661	-1.20362	-266.40099	783.24480	1
6022	H	86.96294	93.15561	83.98715	652.91269	722.14849	1143.93072	1
6023	H	85.43729	93.71301	84.06278	-1817.66045	-1397.23831	-1378.17357	1
6024	C	85.76434	93.22015	82.00802	3.72312	364.42900	175.66243	1
6025	H	84.72935	93.62863	81.90481	-1918.99719	426.36303	1778.26648	1
6026	H	85.79599	92.26870	81.51225	-804.12721	-2196.59276	144.58777	1
6027	C	86.81168	94.24320	81.46865	-679.78944	256.88530	193.78475	1
6028	H	87.52037	94.27249	82.35374	839.83106	-3277.18156	-1665.35444	1
6029	H	86.43368	95.31539	81.45741	1679.91413	-1011.41695	-1041.31195	1
6030	C	87.41662	93.99268	80.01579	-149.59301	-670.81511	908.29559	1
6031	H	87.87227	94.88370	79.51386	1997.77354	-403.49353	-2982.64676	1
6032	H	88.14280	93.17663	80.01169	-1378.12431	-1019.12704	-669.64396	1
6033	N	86.41167	93.59230	79.03292	-486.36376	-147.83683	605.25144	1
6034	H	86.69268	92.79890	78.34041	-939.58921	-835.71039	-1205.48016	1
6035	H	85.50084	93.27164	79.41554	1849.04475	-1170.97660	-4297.51083	1
6036	H	85.95430	94.64743	78.42758	1327.23110	2392.20591	-5109.60291	1
6037	C	85.78477	91.34634	85.58739	-154.66708	850.27292	388.66302	1
6038	O	86.89949	91.76795	85.79254	-15.98820	411.43312	-23.31171	1
6039	N	84.97017	90.69687	86.38243	159.67061	565.65743	6.41454	1
6040	H	84.06659	90.38909	85.97303	1745.49619	1669.78271	-232.90092	1
6041	C	85.25854	90.54798	87.80570	871.02788	847.71735	226.78319	1
6042	H	86.41331	90.68678	87.74736	-964.47372	1978.30550	-1712.90453	1
6043	C	84.54039	91.72022	88.54888	-219.68524	-888.08085	424.30531	1
6044	H	84.52855	91.56892	89.64808	-1001.42408	1141.94271	1034.77161	1
6045	C	85.33627	93.05329	88.25849	324.13451	-370.03471	-783.61239	1
6046	H	85.13030	93.83851	89.00838	912.29624	262.01917	131.88523	1
6047	H	85.07430	93.49814	87.20268	-2645.13370	-1468.91348	283.95704	1
6048	H	86.43361	92.92322	88.30231	-3535.98263	389.03232	586.63796	1
6049	C	83.06327	92.07985	87.91856	185.65929	-349.44446	209.50432	1
6050	H	83.09701	93.14234	87.59101	314.87939	-921.42440	-1339.27498	1
6051	H	83.00199	91.61580	86.90741	-3288.48551	-35.77931	-337.92286	1
6052	C	81.91221	91.66931	88.87786	1121.33849	-195.08636	-85.58919	1
6053	H	82.18733	90.60910	89.11046	-934.24037	1778.66325	2573.97256	1
6054	H	81.77544	92.27802	89.81073	127.98549	-2970.81856	2982.51588	1
6055	H	80.87550	91.51582	88.46250	1068.05780	-51.00578	2541.40483	1
6056	C	84.90005	89.02375	88.28921	10.14182	-322.86752	989.86339	1
6057	O	85.57822	88.48706	89.13151	-331.35427	799.99705	250.75470	1
6058	N	83.74720	88.64633	87.69794	-201.73296	-340.51873	1017.78118	1
6059	H	83.23527	89.37299	87.22973	-537.88252	-1791.06782	1691.36410	1
6060	C	83.13739	87.42861	88.07554	-630.17044	-312.55225	243.17244	1
6061	H	83.50603	87.09686	89.07857	2502.90647	-3292.17144	-1364.00461	1
6062	C	81.58671	87.70700	88.19816	488.63521	818.30371	464.10621	1
6063	H	81.14347	88.12814	87.26317	412.26417	248.74084	682.34648	1
6064	H	81.36958	88.45767	88.97161	2811.71682	-3325.37620	-101.53152	1
6065	C	80.89754	86.33227	88.56805	1002.10345	229.57903	-575.14241	1
6066	C	80.11743	85.53122	87.69363	-223.22178	-385.79029	432.22098	1
6067	H	80.13123	85.95574	86.67279	1390.27616	229.13966	-2146.60278	1
6068	C	79.40000	84.34180	88.00890	148.59986	-886.08935	-155.61086	1
6069	H	78.84100	83.76780	87.28590	-323.95670	-2958.00140	1021.52142	1

6070	C	79.47800	83.93480	89.35490	-638.99266	453.47035	-466.37326	1
6071	H	78.96900	83.02580	89.64090	-632.11128	-440.06841	3050.41003	1
6072	C	80.95579	85.86274	89.92279	-556.98980	226.95203	120.44259	1
6073	H	81.52731	86.47861	90.63842	-2030.25273	519.71676	-2661.25873	1
6074	C	80.30600	84.65280	90.26790	24.69251	-623.90608	-664.51674	1
6075	H	80.48200	84.28180	91.26690	-2373.94869	-1191.52542	-1686.07859	1
6076	C	83.53550	86.31397	86.89626	170.44797	-583.94564	421.91148	1
6077	O	83.61434	85.11657	87.18615	-265.64630	-380.93254	554.72669	1
6078	N	83.44595	86.87726	85.71747	-222.00228	923.52404	-877.34227	1
6079	H	83.27233	87.85890	85.57075	3070.78027	2073.24620	7.02372	1
6080	C	83.47659	86.02814	84.56843	771.46604	-178.22123	579.47013	1
6081	H	82.77290	85.27092	84.85372	-2185.73405	-1499.74307	-2030.60992	1
6082	C	82.91934	86.76034	83.23476	-51.84808	993.78003	-380.94003	1
6083	H	83.20458	86.00850	82.40903	4583.47503	213.80021	391.19547	1
6084	H	83.40566	87.74135	83.00003	-1551.73947	-2431.97050	-1665.22144	1
6085	C	81.43786	86.90832	83.46713	855.30987	-30.45636	-520.43797	1
6086	H	81.24799	87.43179	84.41488	3473.89613	2942.63986	1394.68163	1
6087	C	80.64053	87.41091	82.28641	473.70309	-322.50998	651.47338	1
6088	H	79.54127	87.62078	82.52041	2922.66457	2479.62272	2334.00683	1
6089	H	80.75860	86.76049	81.34627	499.23618	2670.24261	-517.49449	1
6090	H	81.00142	88.45999	82.00768	2436.69360	930.45168	-1335.36152	1
6091	C	80.87944	85.50104	83.79171	204.33035	-22.05488	687.56012	1
6092	H	79.80000	85.44042	83.70078	-1474.17147	2648.96370	-783.40077	1
6093	H	81.24225	85.04656	84.76351	-169.86480	3151.81665	-29.15865	1
6094	H	81.25712	84.74850	83.03717	1237.85729	-320.29542	519.23379	1
6095	C	84.93968	85.38295	84.28894	271.42409	189.78324	-471.46435	1
6096	O	84.87300	84.21580	83.92590	489.99464	-232.86132	573.85372	1
6097	N	86.02649	86.12889	84.43236	512.44442	-31.39339	1445.28796	1
6098	C	86.03185	87.56577	84.57719	-112.84683	-566.50545	-199.12504	1
6099	H	85.44523	87.74352	85.54455	2396.31468	-592.59393	1242.80837	1
6100	H	85.50553	88.08498	83.71775	3140.70656	-124.78226	-2973.85249	1
6101	C	87.32047	85.53230	84.21725	-349.27475	-1146.87057	190.59339	1
6102	H	87.36000	84.75980	83.39390	-1951.11782	-1726.41590	-1763.76122	1
6103	C	88.36487	86.70913	84.18311	-135.26797	-117.57355	326.29888	1
6104	H	88.64425	87.07707	83.14022	-2170.74555	759.39917	-2257.35839	1
6105	H	89.36311	86.43897	84.63469	1640.72733	-935.82324	-1905.02887	1
6106	C	87.57783	87.93676	84.79748	502.21110	-175.33828	-327.25893	1
6107	H	87.83550	88.14316	85.88591	735.45434	-2106.16865	829.53051	1
6108	H	87.88174	88.89326	84.39667	214.03785	-1157.08849	3619.55944	1
6109	C	87.49300	84.44880	85.47990	485.99674	-771.15644	-23.99827	1
6110	O	88.17500	83.43780	85.31690	667.02038	338.23839	-253.58595	1
6111	N	86.94800	84.79480	86.61690	-351.21097	360.46375	-677.78243	1
6112	H	86.46484	85.70031	86.58833	-1357.09294	-2310.47533	-3579.10238	1
6113	C	86.99100	84.05980	87.81290	752.58343	418.51104	-299.86278	1
6114	H	88.04200	83.90580	88.00490	-1282.28310	1354.76212	-2533.49480	1
6115	C	86.54200	84.90880	89.03390	422.30738	559.35235	-583.29447	1
6116	H	85.57586	85.44111	88.83249	-752.78403	-2332.78598	-3668.41649	1
6117	O	87.41220	86.27432	89.25132	207.62375	424.65633	318.47157	1
6118	H	86.72891	86.98116	89.09417	2252.03960	907.28915	-1062.52164	1
6119	C	86.58800	84.13880	90.31390	-280.22500	861.65118	102.38256	1
6120	H	86.42200	84.88380	91.12190	-1792.57882	1437.36362	2149.15640	1
6121	H	87.58000	83.65880	90.45790	-432.47922	1218.71390	2868.08723	1
6122	H	85.87300	83.28880	90.33790	850.54544	-2923.52327	792.34485	1
6123	C	86.28000	82.71080	87.71290	352.70556	-609.86529	-578.89043	1
6124	O	86.82200	81.66680	88.07090	491.28648	-367.68551	-497.06357	1
6125	N	85.01900	82.70380	87.12790	152.03866	116.75225	-822.14685	1
6126	H	84.59100	83.60380	87.13890	-2670.47446	1533.40975	-644.55172	1
6127	C	84.34600	81.49680	86.73990	-169.54950	895.80157	-15.60477	1
6128	H	84.30700	80.75780	87.52590	2630.13013	725.45100	-1566.64054	1
6129	C	82.88500	81.78680	86.44690	476.61807	489.67358	603.74332	1
6130	H	82.91900	82.67580	85.78090	-1563.19923	-1396.76035	2345.99551	1
6131	C	82.17700	80.62380	85.67890	-681.83180	-555.91392	-239.82518	1

6132	H	81.07800	80.71880	85.54690	602.73017	-2089.52721	-2273.50360	1
6133	H	82.70400	80.35880	84.73790	465.57596	2498.61775	-1854.28546	1
6134	H	82.32100	79.72080	86.31090	1408.56024	-2171.16793	1788.91422	1
6135	C	82.07000	82.12980	87.72690	833.83245	-259.28105	262.57912	1
6136	H	81.10200	82.37580	87.23990	2009.33983	-1845.03907	-1567.35782	1
6137	H	82.53400	83.06080	88.11890	2001.44440	-772.01096	2301.40079	1
6138	C	81.94500	81.05480	88.81990	-711.29367	296.77117	-487.27733	1
6139	H	82.88100	80.59980	89.20790	-587.70429	3052.00527	-487.94852	1
6140	H	81.31400	80.20680	88.47790	2819.11105	-507.83191	1301.13253	1
6141	H	81.40000	81.55980	89.64590	-694.54622	-1642.16649	2592.12673	1
6142	C	85.05200	80.71580	85.59890	-4.22895	117.73405	-904.19678	1
6143	O	85.24900	79.52680	85.71490	33.01373	785.75877	71.55753	1
6144	N	85.49400	81.43280	84.53190	-389.96503	-638.06614	-391.75397	1
6145	H	85.40200	82.42480	84.48490	-912.91230	-3006.00745	-169.51857	1
6146	C	86.03100	80.79380	83.32290	-680.12736	-510.63371	328.83277	1
6147	H	85.31500	80.12480	82.86790	2092.89870	-1750.34149	1566.62246	1
6148	C	86.55300	81.83280	82.24690	-280.07891	679.12645	-540.17967	1
6149	H	87.16500	81.34780	81.45690	-401.43550	1247.37788	2860.26646	1
6150	H	87.19100	82.46680	82.89890	-1414.90619	-2747.45996	589.68677	1
6151	C	85.50700	82.73980	81.58390	-381.73017	-518.08598	-646.00309	1
6152	C	84.15500	82.39380	81.53690	13.98738	736.61994	537.25824	1
6153	H	83.79200	81.55280	82.10890	-1971.37046	-504.49935	-2399.45934	1
6154	C	83.21100	83.32080	80.93390	-807.86256	349.76018	-237.64869	1
6155	H	82.15600	83.09880	80.98090	2041.51106	1767.43141	-1614.51077	1
6156	C	83.64600	84.52480	80.37890	778.54054	-29.86410	473.74442	1
6157	O	82.64628	85.35683	79.58630	-1251.13342	-225.13891	660.57574	1
6158	H	81.83700	84.81180	79.82390	-1073.70180	-2324.00967	1828.76181	1
6159	C	85.92600	83.94280	80.96390	12.02304	-905.25558	-108.71426	1
6160	H	86.96400	84.21780	81.07890	2835.24504	-600.94536	-1224.12273	1
6161	C	84.98800	84.82180	80.36790	-671.76561	494.51852	-368.28440	1
6162	H	85.28319	85.79739	80.01434	196.41368	1965.47873	-272.27716	1
6163	C	87.28100	79.90080	83.70090	-597.77310	657.57265	-204.24626	1
6164	O	87.52500	78.85780	83.08590	-544.70164	560.35624	113.70242	1
6165	N	88.11400	80.46780	84.61090	647.50288	512.31416	-175.91620	1
6166	H	87.81200	81.38580	84.85490	559.06666	2850.33201	1208.83337	1
6167	C	89.22100	79.75680	85.24590	-797.62956	436.77539	66.82327	1
6168	H	89.95300	79.50280	84.49390	-1460.06880	-2547.55562	1129.77241	1
6169	C	89.96200	80.65580	86.28690	-454.18283	-344.00928	711.91753	1
6170	H	90.83200	80.05380	86.62590	2287.01729	-336.87369	-2134.07926	1
6171	H	89.32800	80.96580	87.14490	935.25630	2256.94615	-1982.35111	1
6172	O	90.43900	81.84080	85.66990	614.75734	91.34602	487.19252	1
6173	H	89.67500	82.42080	85.62090	2373.53990	-1179.91475	1694.79668	1
6174	C	88.73400	78.47380	85.93690	-905.12227	101.27148	44.14489	1
6175	O	89.25800	77.41880	85.68690	455.97762	479.88502	430.60655	1
6176	N	87.62200	78.53080	86.72490	-698.23013	282.60942	-381.15468	1
6177	H	87.11900	79.38180	86.85290	1749.77418	2397.46164	-1043.40512	1
6178	C	87.01300	77.34680	87.36090	-109.87209	694.32003	580.77433	1
6179	H	87.78600	76.78980	87.87090	2154.73553	2267.17444	339.50120	1
6180	C	85.83700	77.64780	88.31690	-570.15198	-362.84637	-612.14396	1
6181	H	85.15200	78.26580	87.69790	2173.88273	954.33054	2064.39176	1
6182	C	85.23200	76.35180	88.91690	-581.57871	629.52021	-311.32219	1
6183	H	84.85900	75.70780	88.09290	1916.25287	867.57994	-2339.55257	1
6184	H	85.99500	75.79680	89.50290	-1845.52259	-1492.04024	2065.45117	1
6185	H	84.35600	76.61180	89.54990	-672.14676	3070.81391	128.63473	1
6186	C	86.39100	78.49780	89.48490	356.99775	773.14505	-325.96063	1
6187	H	87.06500	79.27980	89.07290	1431.02713	-2197.52367	-1738.18218	1
6188	H	87.08200	77.89680	90.11390	-988.36040	-1147.52745	2757.63498	1
6189	C	85.32100	79.24980	90.26490	550.97854	-644.36010	-335.66904	1
6190	H	85.66100	79.80480	91.16590	-1836.89018	-1093.54418	2308.29413	1
6191	H	84.50800	78.55480	90.56390	2591.63684	369.16478	-1745.09658	1
6192	H	84.81600	79.99880	89.61990	946.08171	-1654.16507	-2503.37643	1
6193	C	86.59100	76.33380	86.29590	40.75260	705.04492	-576.80317	1

6194	O	86.87600	75.13580	86.32990	266.79178	-247.24634	-700.94124	1
6195	N	85.94400	76.86980	85.20790	-711.83126	-4.55967	453.81467	1
6196	H	85.63800	77.81680	85.14890	842.37471	1784.07581	-2450.65391	1
6197	C	85.54400	75.97380	84.09090	-585.75515	55.87593	-696.57719	1
6198	H	84.97100	75.16780	84.52390	-586.97010	-2292.83159	-2072.82793	1
6199	C	84.70500	76.68680	83.02590	816.47427	-154.59043	-375.39655	1
6200	H	85.34800	77.43880	82.51990	-2027.81144	-1170.43123	-2101.49893	1
6201	C	84.27500	75.71480	81.91990	390.62822	-9.12547	823.87943	1
6202	H	85.09700	75.06980	81.54390	-1043.18891	1845.65843	-2324.54901	1
6203	H	83.47900	75.04880	82.31590	-1130.74826	2166.20224	1981.71705	1
6204	H	83.83700	76.40380	81.16690	-1216.70776	-1778.85079	-2292.05984	1
6205	C	83.45000	77.48980	83.55590	419.46463	384.39946	712.55700	1
6206	H	82.97200	77.88180	82.63290	2756.57425	499.32282	1431.85241	1
6207	H	83.89400	78.25780	84.22490	-2550.79173	-1013.73960	-1537.53692	1
6208	C	82.33100	76.72480	84.30590	-569.19555	-645.58374	-301.14624	1
6209	H	81.47300	77.36780	84.59690	625.84537	408.42952	3056.09704	1
6210	H	82.01000	75.87880	83.66190	-2554.73294	-333.43172	1805.65477	1
6211	H	82.78500	76.35380	85.24990	1986.33564	2424.54117	-272.57487	1
6212	C	86.82000	75.33080	83.39190	637.84342	6.19652	651.58912	1
6213	O	86.93000	74.10180	83.14490	-599.14387	513.65301	28.53841	1
6214	N	87.87300	76.12580	83.05390	-663.86913	290.65683	-432.97653	1
6215	H	87.78700	77.10580	83.21590	969.26659	2388.87271	1803.34014	1
6216	C	89.14600	75.69580	82.51290	630.94474	149.00597	-641.21522	1
6217	H	88.77200	75.17380	81.64490	1623.04462	-2062.26052	-1735.23311	1
6218	C	89.90200	76.92480	82.03590	429.36837	562.65273	-574.90495	1
6219	H	89.27500	77.50780	81.32890	-1806.21469	1033.38445	2359.64643	1
6220	H	90.24800	77.70980	82.74190	968.87177	-2107.61869	2125.43106	1
6221	C	91.23100	76.59480	81.38190	335.66772	-777.81997	337.30443	1
6222	C	91.21500	76.27080	80.01490	-23.36967	907.47043	86.03647	1
6223	H	90.34000	76.17680	79.38890	-467.53920	-1960.65393	-2415.67164	1
6224	C	92.38300	75.83580	79.33690	124.29451	103.54849	897.37372	1
6225	H	92.23500	75.47680	78.32890	1781.61946	-2563.46973	-390.74451	1
6226	C	93.59700	75.74780	79.99190	629.41964	-214.97680	-623.75227	1
6227	H	94.46100	75.44580	79.41890	-281.46604	2946.36560	1066.73935	1
6228	C	92.48600	76.63880	82.03490	851.84921	315.37290	-79.64839	1
6229	H	92.45700	76.91580	83.07890	1218.97345	-2335.50035	1719.81629	1
6230	C	93.65300	76.24480	81.37190	120.85959	619.33722	658.22896	1
6231	H	94.58100	76.33180	81.91690	2968.31632	-683.86815	787.17776	1
6232	C	89.91100	74.63880	83.25790	-899.20530	-97.73742	115.44797	1
6233	O	90.31700	73.58680	82.77890	113.37404	592.87936	-509.18329	1
6234	N	90.07200	74.84380	84.60690	-64.86282	763.94033	-353.35574	1
6235	H	89.75100	75.72580	84.94490	-1902.98710	2503.37145	99.98835	1
6236	C	90.99200	74.14780	85.47890	176.20601	833.55186	324.95190	1
6237	H	91.87600	73.95580	84.88990	-1938.84985	1230.85296	2150.36938	1
6238	C	91.44100	74.96580	86.68890	173.02299	894.91988	-25.14875	1
6239	H	90.54900	75.39680	87.18990	1719.42224	-1244.72462	-2322.17011	1
6240	H	91.98500	74.47680	87.52490	-140.95733	3113.86396	-426.85887	1
6241	C	92.29500	76.20180	86.29890	-749.23088	-254.34103	453.22702	1
6242	H	91.81200	76.81980	85.51190	2493.22330	789.70012	-1748.83891	1
6243	C	92.49600	77.08680	87.49090	615.93485	-41.19508	671.10225	1
6244	H	93.34000	76.67480	88.08490	-644.39557	2184.95975	-2170.00725	1
6245	H	92.75900	78.11980	87.17690	-2280.25586	-592.01586	-2085.22821	1
6246	H	91.62000	77.10680	88.17290	-2013.59702	1687.69269	1730.70698	1
6247	C	93.63900	75.80880	85.71290	-662.53911	-597.98125	186.84578	1
6248	H	94.39500	76.62280	85.73390	2425.53471	-1273.93938	-1546.63701	1
6249	H	94.08800	74.94380	86.24590	218.14437	-1964.51532	2447.71706	1
6250	H	93.51200	75.52980	84.64590	2280.59240	1358.96732	-1688.29274	1
6251	C	90.49500	72.83780	85.92890	-810.95123	-84.95218	408.15712	1
6252	O	91.27500	71.96380	86.38890	-129.50298	-269.20414	731.01665	1
6253	N	89.19100	72.60280	85.69690	-251.93515	121.47951	796.51974	1
6254	H	88.59100	73.30280	85.31790	43.31501	-3145.28314	-59.53133	1
6255	C	88.45900	71.35680	85.94490	726.48390	-372.36520	406.22199	1

6256	H	89.12800	70.64180	86.40090	2333.32560	-2080.92148	351.54472	1
6257	C	87.22600	71.64880	86.78490	631.74897	106.00902	648.92706	1
6258	H	86.71000	70.67580	86.92890	-1829.54859	1647.60973	1958.66290	1
6259	O	86.29500	72.52080	86.19690	722.07675	-294.97409	123.38023	1
6260	H	86.60700	73.42780	86.23990	272.75475	493.84464	-3095.14920	1
6261	C	87.61600	72.22880	88.17090	-735.97154	-495.50351	-210.41188	1
6262	H	86.73200	72.42180	88.81590	-1085.15946	2935.96839	317.40318	1
6263	H	88.12700	73.21380	88.10690	-35.06783	-1908.79420	2500.70014	1
6264	H	88.25200	71.51380	88.73390	1027.51984	2137.29586	-2067.46115	1
6265	C	88.17800	70.69480	84.65590	-47.19641	571.30404	-709.10874	1
6266	O	88.41700	69.53780	84.41390	235.50712	-361.22663	-661.57309	1
6267	N	87.69700	71.45480	83.66790	-641.78769	345.94488	-425.56196	1
6268	H	87.49600	72.42580	83.77290	2623.53799	492.24444	1665.22373	1
6269	C	87.33000	70.99180	82.32790	-514.93006	-529.73946	-534.48494	1
6270	H	86.87200	71.79880	81.77690	-1048.08217	-1588.60383	2505.21214	1
6271	H	86.53900	70.25880	82.39390	3137.72187	-193.95131	123.73591	1
6272	C	88.38800	70.38780	81.46990	-130.35224	-889.90919	-150.06972	1
6273	O	88.07800	69.34780	80.89690	-369.07184	-568.54953	405.17236	1
6274	N	89.50700	71.10180	81.21690	-378.33265	-574.17396	489.75602	1
6275	H	89.71200	71.85980	81.82990	-620.69684	-1577.17562	2650.56197	1
6276	C	90.54000	70.62380	80.30890	-321.64006	682.06396	512.62797	1
6277	H	90.04700	70.37080	79.38190	2550.62627	-1531.66824	1022.99769	1
6278	C	91.49700	71.77680	80.00190	-684.88866	-170.05872	577.45871	1
6279	H	90.87200	72.69580	80.01990	-275.26504	2904.80995	-1176.66246	1
6280	C	92.63800	71.97780	81.09890	362.06379	824.28792	144.60375	1
6281	H	93.11400	72.96780	80.93290	-1446.05167	-651.16070	2717.19534	1
6282	H	93.41500	71.18380	81.09390	-1775.22326	-144.94800	-2593.41448	1
6283	H	92.18000	72.00080	82.11090	2936.47914	-377.82875	1064.21893	1
6284	C	92.06200	71.74980	78.55590	282.82799	-290.71302	816.66717	1
6285	H	91.23500	71.68480	77.81690	-1767.79188	2090.98319	1549.49263	1
6286	H	92.43600	72.79180	78.45790	-1695.32947	2126.98507	1581.14475	1
6287	C	93.19900	70.75380	78.20890	626.50407	-561.61670	-351.46882	1
6288	H	94.09500	70.93880	78.83990	-2524.82516	385.19354	-1837.14727	1
6289	H	93.64100	70.73480	77.18990	902.56296	-2279.38943	1971.79871	1
6290	H	92.87200	69.72480	78.47090	-2537.52079	633.89517	1748.53978	1
6291	C	91.19200	69.33780	80.85890	-845.85400	40.75214	338.11430	1
6292	O	91.46200	68.34780	80.13890	-212.93731	675.59238	-349.08432	1
6293	N	91.48600	69.32480	82.18790	-413.14054	594.69609	-433.96284	1
6294	H	91.23100	70.17480	82.64090	2768.65843	-1191.23536	902.06154	1
6295	C	91.91500	68.12480	82.90290	674.76662	-4.89852	-613.28380	1
6296	H	92.79300	67.74880	82.39990	1137.05328	2474.96393	1574.76652	1
6297	C	92.25100	68.54980	84.34890	-623.70194	-217.42377	628.62850	1
6298	H	91.36300	68.83680	84.95190	2031.03728	-2134.16384	-1103.83808	1
6299	C	92.93000	67.35280	85.13090	-38.21424	545.58213	729.61004	1
6300	H	93.39500	67.66780	86.08990	2816.88312	785.42742	-1160.38765	1
6301	H	93.59900	66.86780	84.38790	683.50592	2165.82641	2177.20965	1
6302	H	92.08600	66.72380	85.48590	-1297.42712	-2085.69786	-1965.90273	1
6303	C	93.12200	69.81780	84.36490	-82.64499	-713.48418	-561.74829	1
6304	H	92.59100	70.79080	84.28690	418.05189	-1824.98671	-2528.41499	1
6305	H	93.47800	69.79780	85.41690	-1799.71518	611.07834	-2507.15671	1
6306	H	93.92400	69.74080	83.59990	-2110.06411	-1558.22569	-1737.17828	1
6307	C	90.88500	67.01480	82.85490	-556.90750	641.70428	-330.93904	1
6308	O	91.19100	65.97680	82.31990	578.50465	275.09237	-461.82658	1
6309	N	89.59800	67.27880	83.21290	527.47058	507.40287	420.70109	1
6310	H	89.33800	68.17280	83.56890	-3101.06471	-449.88638	281.47141	1
6311	C	88.50800	66.28280	83.31090	-543.31176	554.50542	478.31693	1
6312	H	87.63400	66.81180	83.66190	-1058.56279	-2935.79372	398.47993	1
6313	H	88.77800	65.52880	84.03490	13.31072	2345.67527	2096.62981	1
6314	C	88.13700	65.55880	82.06790	314.14467	-561.63813	-646.00831	1
6315	O	88.04400	64.34280	82.03790	301.13903	-577.45636	446.63929	1
6316	N	87.94300	66.29480	80.94490	-133.31966	640.18901	-533.90653	1
6317	H	88.08700	67.28080	80.99990	-2812.65001	978.91141	-1014.37598	1

6318	C	87.72000	65.63780	79.67190	413.69976	-526.35060	-619.07879	1
6319	H	87.02600	64.82080	79.79990	1059.06714	206.50054	2955.32748	1
6320	C	86.96700	66.60780	78.71390	-92.17659	171.75748	-890.76026	1
6321	H	87.46400	67.58080	78.50890	3104.91925	80.66297	501.19475	1
6322	H	86.78100	66.01880	77.79090	2249.29314	359.21715	-2170.22340	1
6323	C	85.61000	66.79680	79.39290	257.20112	777.19145	-401.58690	1
6324	O	84.83300	65.81480	79.48890	41.48806	742.67780	265.20870	1
6325	N	85.34400	67.99780	79.87490	293.16062	776.53241	154.03428	1
6326	H	86.08300	68.66580	79.96190	-2086.18902	-1479.44611	1832.28840	1
6327	H	84.39500	68.15680	80.14790	-3074.19845	130.00965	656.22221	1
6328	C	88.89800	64.98780	79.03490	729.59863	376.10731	-397.08957	1
6329	O	88.72200	64.04280	78.34190	-693.58536	354.52459	-129.91881	1
6330	N	90.14400	65.40080	79.46790	210.13862	-791.79120	-203.91357	1
6331	H	90.25700	66.25580	79.96790	-1062.04363	2020.92879	-2164.74858	1
6332	C	91.31700	64.73480	79.05890	97.70485	515.88956	745.49495	1
6333	H	91.30700	64.62180	77.98490	-2927.03199	1151.10278	-75.31504	1
6334	H	92.21500	65.29480	79.27790	1062.09970	-1925.40192	2250.11064	1
6335	C	91.40100	63.43180	79.75790	310.82975	-796.83060	-316.06465	1
6336	O	91.82500	62.42080	79.26990	-577.07887	332.13922	424.60658	1
6337	N	91.02800	63.38680	81.05790	661.05041	154.45958	-501.82356	1
6338	H	90.80500	64.21680	81.56290	-2517.52490	1601.70543	-997.41382	1
6339	C	90.91800	62.15580	81.79590	275.37986	-734.86526	-464.31669	1
6340	H	91.86200	61.64080	81.70190	-1066.15996	2389.99152	1746.27308	1
6341	C	90.82800	62.40680	83.27890	331.56885	-794.75202	299.80382	1
6342	H	90.54300	61.55180	83.92790	1677.69666	2644.70176	298.51762	1
6343	H	89.92600	63.04680	83.38890	-2285.97755	-1673.79653	1367.82238	1
6344	C	92.01900	63.17780	83.96190	-507.29365	-341.32403	-676.46291	1
6345	H	92.39400	64.07880	83.43090	2371.87763	457.82649	2015.64324	1
6346	C	91.67700	63.61180	85.38990	-427.74577	655.48410	467.78751	1
6347	H	91.21000	62.80180	85.98990	-2952.71904	-361.96864	-1024.03866	1
6348	H	92.58900	63.86880	85.96890	1883.89389	-747.97171	-2406.18128	1
6349	H	90.99500	64.48680	85.45990	-1863.27798	1324.56257	-2161.47065	1
6350	C	93.24800	62.26580	83.90690	395.64209	142.65578	809.05356	1
6351	H	93.04800	61.32980	84.47190	2319.96381	-1501.10801	1504.21703	1
6352	H	94.12500	62.84280	84.26990	-1438.91126	1875.01864	-2076.55140	1
6353	H	93.55700	61.98580	82.87690	1529.33518	1892.55504	1994.39103	1
6354	C	89.83700	61.22880	81.39190	-670.64914	389.97123	-479.16926	1
6355	O	90.05200	60.01880	81.38790	781.35197	-104.16432	47.60376	1
6356	N	88.67800	61.73480	81.04490	330.59139	-215.15975	746.38322	1
6357	H	88.46700	62.70780	81.09490	-1221.30094	-2124.56655	1973.03503	1
6358	C	87.67100	60.85880	80.39390	540.49009	460.58516	571.99894	1
6359	H	87.32000	60.08580	81.06090	-2109.82119	420.31282	-2295.69552	1
6360	C	86.36900	61.62080	80.15290	437.16704	378.29483	705.14467	1
6361	H	86.66700	62.53680	79.59990	-931.64399	-1905.93439	2323.29073	1
6362	C	85.41000	60.79180	79.24990	-40.18690	139.68571	-900.17994	1
6363	H	85.78800	60.71980	78.20790	-337.71721	2233.51169	2189.88558	1
6364	H	84.42100	61.27980	79.11590	-2232.42026	1456.66377	1671.12438	1
6365	H	85.21300	59.82180	79.75490	-1555.71342	-964.44593	-2558.87202	1
6366	C	85.66900	62.05280	81.46790	59.94967	164.68914	894.83771	1
6367	H	84.86800	62.78280	81.22090	2288.98316	-975.36532	-1925.47262	1
6368	H	85.26400	61.20280	82.05790	1418.49257	-211.68327	-2800.23128	1
6369	H	86.41700	62.61580	82.06690	1686.79616	1795.69322	-1956.63763	1
6370	C	88.14800	60.21080	79.10090	-460.61643	407.85428	673.00698	1
6371	O	87.98300	59.02080	78.84890	-678.66037	361.86766	-179.16229	1
6372	N	88.93200	60.97080	78.26790	603.21865	-484.47884	-337.75701	1
6373	H	88.88200	61.95180	78.43890	950.00296	-2010.56634	-2225.61084	1
6374	C	89.63900	60.42180	77.09990	725.26411	366.18609	413.94532	1
6375	H	88.99200	59.82980	76.46890	-2637.04200	-778.25505	-1529.23341	1
6376	C	90.13200	61.55680	76.21090	-245.39354	328.56694	-814.41806	1
6377	H	90.77500	62.20780	76.84090	2388.04920	1975.44820	-541.34249	1
6378	C	91.04800	61.07380	75.04890	-454.31315	-405.65078	-678.60004	1
6379	H	91.94600	60.50580	75.37390	-1639.17125	-2672.23587	265.51703	1

6380	H	91.50200	61.91580	74.48490	2378.32481	2035.61491	313.16012	1
6381	H	90.55600	60.35680	74.35590	-884.49316	-328.70926	-3001.30776	1
6382	C	89.00800	62.48180	75.66090	7.02713	567.02539	714.06151	1
6383	H	88.47400	61.93980	74.85190	2612.78447	-1684.72838	-482.98432	1
6384	H	88.14100	62.60780	76.34490	-2631.13738	-1490.45271	-868.27012	1
6385	C	89.53000	63.78780	75.11390	-553.20240	-415.10246	594.22895	1
6386	H	90.19400	63.52080	74.26490	942.90686	-3000.78915	66.46305	1
6387	H	88.68400	64.35180	74.66590	-2106.33165	2266.34950	-570.30969	1
6388	H	89.97900	64.42080	75.90890	-2572.36207	1655.35637	-735.50996	1
6389	C	90.77300	59.45680	77.46190	332.79423	-609.46388	-590.97613	1
6390	O	90.96700	58.38780	76.89490	-33.13991	738.45028	277.88517	1
6391	N	91.47500	59.73380	78.58890	-205.99053	-461.63039	676.11949	1
6392	H	91.42900	60.64380	78.99590	1676.62045	1711.55738	2039.05405	1
6393	C	92.46700	58.82380	79.17890	-724.88543	-475.55518	-282.55864	1
6394	H	93.13400	58.59180	78.36190	-2154.49200	2198.57070	-650.13636	1
6395	C	93.39400	59.54580	80.25190	-727.45292	-66.62977	545.73229	1
6396	H	93.67500	58.93680	81.13790	-477.43093	1900.27554	2461.55211	1
6397	H	92.68800	60.32980	80.60090	-1885.56164	2439.64756	-625.30258	1
6398	C	94.60100	60.20980	79.64990	0.07779	136.16699	-901.61497	1
6399	H	94.23900	60.46180	78.62990	-1494.27344	2209.19348	-1668.78317	1
6400	C	95.06300	61.43480	80.47190	181.28753	817.11273	-361.81848	1
6401	H	95.28300	61.04180	81.48790	-1711.81780	-2403.28153	1091.85344	1
6402	H	94.26400	62.20680	80.47790	-1638.91079	-1988.92275	-1804.54535	1
6403	H	96.00300	61.82780	80.02690	789.63194	-1754.67722	2489.13951	1
6404	C	95.76500	59.20580	79.52190	-723.88704	514.99269	205.47768	1
6405	H	96.08900	58.91780	80.54590	-2579.66576	1679.81506	649.43986	1
6406	H	95.53700	58.21280	79.07790	1397.94009	-2453.65391	1386.92906	1
6407	H	96.53300	59.68580	78.87890	591.89494	-2907.09292	1047.23319	1
6408	C	91.86500	57.57880	79.69390	-582.56779	-303.19306	-632.56600	1
6409	O	92.42900	56.49880	79.48290	535.77260	-24.90168	-579.61613	1
6410	N	90.65400	57.56080	80.28190	-381.42184	-696.43704	286.64460	1
6411	H	90.21300	58.42780	80.50190	-2074.13190	2027.32988	-1219.07205	1
6412	C	89.92200	56.39580	80.60690	-269.30077	-32.73197	-870.54966	1
6413	H	90.56100	55.73180	81.16890	2609.90647	-683.93234	-1618.28644	1
6414	C	88.72200	56.64380	81.52490	-255.95642	818.20196	-310.61692	1
6415	H	88.11700	57.51680	81.19890	-2200.53987	-872.08249	2072.51602	1
6416	C	87.81900	55.37180	81.65790	-270.06871	308.71118	-814.37786	1
6417	H	87.24900	55.30580	80.70590	-1679.32935	2605.55697	537.72862	1
6418	H	88.39100	54.44580	81.87890	2325.06348	1309.71624	-1666.41814	1
6419	H	87.10100	55.43280	82.50390	1541.58712	-1896.34312	-1981.31727	1
6420	C	89.30500	57.08480	82.90890	-335.17659	787.08053	-315.61352	1
6421	H	89.91800	58.00280	82.78290	2332.24242	609.63530	-2021.68651	1
6422	H	89.92900	56.23680	83.26390	-1968.73005	1708.57905	1761.55779	1
6423	H	88.39800	57.27180	83.52290	-1980.23295	-1726.76671	-1730.65895	1
6424	C	89.44700	55.63980	79.32990	-359.27848	576.33568	608.44652	1
6425	O	89.89800	54.49180	79.18290	-449.67866	648.30608	33.39991	1
6426	N	88.71500	56.24380	78.37590	-687.55598	361.92186	-330.07821	1
6427	H	88.39800	57.18380	78.48190	-1682.32476	-210.17816	-2650.25183	1
6428	C	88.13600	55.43780	77.35890	481.60797	-515.20904	-577.98305	1
6429	H	87.98700	54.42380	77.69790	2167.44450	1544.81508	-1677.48530	1
6430	C	86.80000	55.99480	76.89190	518.43415	-69.51995	746.88955	1
6431	H	86.79700	57.04880	76.53890	-1143.95498	2795.22945	-881.07069	1
6432	H	86.30400	55.48680	76.03690	1254.94298	2533.45344	-1380.20217	1
6433	C	85.67600	55.90280	77.97190	-484.48634	-150.54762	757.66708	1
6434	H	86.01400	56.61080	78.75890	1871.95387	1227.76250	2210.56875	1
6435	H	85.62800	54.90080	78.44890	-2218.83620	1002.44526	1992.50988	1
6436	S	83.95900	56.24880	77.57990	-404.97605	-144.73323	355.32703	1
6437	C	84.12800	58.00880	77.20090	-197.22130	-509.73989	-729.87671	1
6438	H	83.24300	58.67880	77.24590	-414.07682	-2980.23816	919.21005	1
6439	H	84.54900	58.20380	76.19090	411.47298	2082.84638	-2321.78103	1
6440	H	84.85200	58.45580	77.91490	2087.45348	1033.17280	-2115.02202	1
6441	C	89.02800	55.25480	76.12090	452.00509	-403.62784	-681.34204	1

6442	O	88.67300	54.33880	75.34490	-482.40885	216.79530	-586.43732	1
6443	N	90.17100	55.99680	75.92590	-667.46038	-222.59038	466.50022	1
6444	H	90.45000	56.78180	76.47390	1347.87838	2726.98930	-803.10612	1
6445	C	91.03600	55.84080	74.74190	-889.83329	191.54029	-54.40627	1
6446	H	91.33000	56.77180	74.28090	-1586.87762	296.94965	-2700.34564	1
6447	H	90.59400	55.18780	74.00390	-572.29216	2941.77648	957.42313	1
6448	C	92.32500	55.26980	75.05690	636.94938	-640.72478	123.36225	1
6449	O	92.92800	54.78180	74.07790	-199.28590	-698.80068	309.17628	1
6450	N	92.85900	55.28180	76.31390	-420.26493	-726.64527	89.64558	1
6451	H	92.39700	55.80080	77.02990	-2179.54868	-321.32446	2246.00632	1
6452	C	94.18600	54.76780	76.54990	-516.28029	736.80378	-148.41107	1
6453	H	94.42000	54.19980	75.66190	2046.46465	2181.63635	-975.02384	1
6454	C	95.24000	55.87480	76.84190	-403.38982	768.94288	-278.30649	1
6455	H	96.23400	55.39980	76.97990	1643.87484	994.04106	-2491.54252	1
6456	H	94.96800	56.43880	77.75990	1807.35693	-538.28990	-2518.31911	1
6457	C	95.32500	56.83880	75.67490	658.83343	599.46334	-195.02109	1
6458	C	94.57400	58.04680	75.56990	735.77653	-405.26549	354.74468	1
6459	H	93.81100	58.35680	76.26890	1625.72964	-2631.85930	573.18932	1
6460	C	94.76300	58.89280	74.47790	-420.74497	-268.55247	-763.08862	1
6461	H	94.19800	59.78980	74.27190	-2210.21796	872.57426	2061.98374	1
6462	C	95.64700	58.60780	73.44990	417.26536	581.36110	565.11937	1
6463	O	95.87200	59.44180	72.41690	-555.02119	-364.40461	427.53712	1
6464	H	96.32200	59.00280	71.69190	1960.54608	-1695.32460	1783.35632	1
6465	C	96.26800	56.58880	74.66090	-707.17336	-527.74710	-229.86917	1
6466	H	96.92000	55.72780	74.64290	-1392.07536	228.65270	-2812.12915	1
6467	C	96.40200	57.42980	73.55890	243.88306	-863.32614	-163.21773	1
6468	H	97.07000	57.15380	72.75690	1815.36562	1085.64151	-2328.96037	1
6469	C	94.25100	53.70880	77.63690	517.31090	682.10256	-313.96900	1
6470	O	94.75800	52.60880	77.40090	-416.13956	-623.25887	-249.00497	1
6471	N	93.66100	53.96080	78.80590	256.79754	-672.06997	441.64383	1
6472	H	93.27600	54.86780	78.95390	-1234.01676	-2604.29812	1262.16487	1
6473	C	93.44100	53.00680	79.89090	-599.56266	600.82935	-333.13618	1
6474	H	94.35700	52.47780	80.10790	1827.87857	1575.23439	2018.84194	1
6475	C	92.94400	53.62880	81.25290	445.77242	-396.55549	-689.55181	1
6476	H	92.05600	54.20480	80.91490	1528.57417	1902.28294	1985.70059	1
6477	H	92.64800	52.84180	81.97990	1217.80572	896.89466	2758.75976	1
6478	C	93.94700	54.46080	82.04690	-393.38206	815.68796	106.55845	1
6479	H	94.47900	55.07880	81.29190	-1516.57166	-2750.17328	186.50351	1
6480	H	94.64500	53.84780	82.65590	2442.85213	-1927.82729	462.79762	1
6481	C	93.27700	55.39580	83.02990	-567.21803	42.86215	712.65528	1
6482	O	92.47900	54.97380	83.85390	278.53089	-654.64459	342.76557	1
6483	N	93.52300	56.72180	82.88790	-587.28231	-86.24744	600.27756	1
6484	H	94.41900	57.02380	82.56290	-2097.16996	45.48301	-2344.78905	1
6485	H	92.86000	57.35880	83.28190	1729.79074	364.51200	-2602.53362	1
6486	C	92.57700	51.86780	79.50590	309.23997	595.98626	616.94572	1
6487	O	92.78500	50.65780	79.79990	-586.64018	395.11844	-351.22919	1
6488	N	91.47300	52.18080	78.75590	361.09023	362.27129	671.59932	1
6489	H	91.20800	53.14080	78.70990	2028.97080	263.32461	2390.01337	1
6490	C	90.61600	51.17280	78.07990	625.30084	-488.83724	448.87417	1
6491	H	90.80800	50.23680	78.58390	-2144.40996	-1361.23221	-1856.55030	1
6492	C	89.08300	51.53180	78.20090	477.40451	-650.07167	425.37367	1
6493	H	88.90900	52.51580	77.71390	-2984.13350	-814.07351	574.85456	1
6494	H	88.49600	50.75480	77.66490	387.63192	2809.97985	1360.87507	1
6495	C	88.66600	51.54680	79.65090	-16.46731	727.72636	549.17591	1
6496	H	89.15400	52.39480	80.17690	1412.95289	2456.78161	-1366.02141	1
6497	H	89.07300	50.61780	80.10390	2470.71274	-1055.01199	-1637.30098	1
6498	C	87.13900	51.48180	79.68990	-432.57797	-796.00644	-103.44587	1
6499	H	86.76700	52.34880	79.10290	822.00885	-1659.18601	2543.54663	1
6500	H	86.88900	50.48680	79.26190	-2959.95700	805.02226	699.15660	1
6501	C	86.57500	51.74980	81.08890	626.28866	582.54457	-315.99896	1
6502	H	86.92000	52.73180	81.47690	-1470.60068	2538.39473	-1136.71109	1
6503	H	86.98500	50.92780	81.71390	428.27849	-2564.59065	-1771.34937	1

6504	N	85.12500	51.68880	81.07790	-325.89062	634.10551	-452.08162	1
6505	H	84.77400	50.75480	80.78390	2061.34753	2252.62626	-758.12104	1
6506	H	84.69900	52.02580	81.96490	-2254.09242	-2171.37274	-320.05317	1
6507	H	84.83800	52.34680	80.32490	2702.72499	846.95956	-1369.73113	1
6508	C	90.95300	50.94980	76.60790	-791.95575	415.04482	178.87113	1
6509	O	90.98900	51.89480	75.82090	-477.04654	-343.75641	-527.14833	1
6510	N	91.05100	49.72080	76.17790	-649.59839	398.10287	363.60462	1
6511	H	90.96200	48.97080	76.82890	1458.14370	2348.37727	-1502.38722	1
6512	C	91.29900	49.34780	74.85290	-196.54250	852.49423	257.05181	1
6513	H	91.82800	50.10280	74.28990	810.25378	-484.59869	-3001.14631	1
6514	C	92.38200	48.18380	74.82990	-232.57955	668.07899	-575.35052	1
6515	H	92.07000	47.34480	75.48790	1997.64510	893.54082	2260.35950	1
6516	H	92.30400	47.74580	73.81190	-1462.04695	-2629.60319	919.69126	1
6517	C	93.85500	48.62380	74.83190	-424.38912	617.07221	520.16032	1
6518	H	94.07900	49.05780	73.83490	-1533.42661	-1555.59845	-2264.27527	1
6519	H	94.46100	47.69280	74.87390	-1012.94100	-909.17038	-2836.47422	1
6520	C	94.33100	49.57380	75.99790	-123.48169	749.27765	504.76358	1
6521	H	93.81300	50.55380	75.93290	2516.78984	1864.77128	294.31821	1
6522	H	94.18600	49.06480	76.97490	-1086.76355	2939.52485	-276.34191	1
6523	C	95.82100	49.84980	75.84490	662.05657	334.81084	530.12621	1
6524	H	96.00100	50.55280	75.00390	1609.52510	-840.60521	2569.24854	1
6525	H	96.33200	48.90480	75.56290	-1866.05211	2255.16258	1153.39391	1
6526	N	96.36400	50.35680	77.12790	83.85254	-840.00723	-5.37561	1
6527	H	95.93900	49.92380	77.97290	366.75803	-1847.68540	-2519.87568	1
6528	H	96.24700	51.38080	77.26290	-212.69305	-2418.09462	-2001.45105	1
6529	H	97.39300	50.20580	77.11590	2220.86465	1037.98853	1971.94479	1
6530	C	90.00100	49.00580	74.10290	-646.14395	-433.52289	475.40183	1
6531	O	90.08300	48.49180	72.98190	-109.13754	630.33862	463.02208	1
6532	N	88.81000	49.29580	74.67490	645.30425	-291.62975	459.57241	1
6533	H	88.70200	49.78880	75.53390	-1336.66204	-690.57977	2763.08892	1
6534	C	87.55400	48.97680	74.08890	810.69662	332.42387	252.42102	1
6535	H	87.68600	49.00780	73.01690	1261.16373	-2809.95431	641.75465	1
6536	C	87.15200	47.53380	74.50490	195.68149	-372.14895	-809.11366	1
6537	H	87.00100	47.55280	75.60590	627.64980	-2730.86972	1430.60566	1
6538	H	88.03400	46.90580	74.25790	-294.96673	1838.16130	2536.21448	1
6539	C	85.88800	46.98380	73.78190	-514.60994	-676.19537	-330.73772	1
6540	H	85.04600	47.70380	73.87690	2159.55539	2127.79094	840.86413	1
6541	C	86.19700	46.73680	72.27590	513.37198	-390.36037	644.60763	1
6542	H	86.97300	45.94380	72.21590	757.55728	1552.81916	-2629.27478	1
6543	H	86.79000	47.58380	71.86990	-2370.02827	2.51577	2069.10268	1
6544	H	85.32100	46.35980	71.70490	1419.99629	2200.09975	-1743.96039	1
6545	C	85.44900	45.69380	74.43390	-572.82536	-688.13157	172.61823	1
6546	H	86.17400	44.86080	74.31090	-2596.52346	1295.27064	1215.96304	1
6547	H	84.50200	45.40480	73.93090	-2898.30672	-262.72757	-1195.41566	1
6548	H	85.30700	45.81980	75.52790	-2858.06058	-603.19043	1168.70751	1
6549	C	86.58300	49.95080	74.48290	470.41433	35.85679	780.30485	1
6550	O	86.54200	50.31480	75.64190	-588.56167	469.27101	-238.76160	1
6551	N	85.76300	50.38280	73.53390	74.47277	-813.32802	213.59687	1
6552	H	85.97600	50.05580	72.61690	1805.71083	1545.11727	2061.61278	1
6553	C	84.62100	51.21080	73.67290	-165.33727	-443.14724	-779.57367	1
6554	H	84.52300	51.36680	74.73690	-1667.06575	2602.13103	-589.94247	1
6555	C	84.88700	52.61880	73.07790	871.12257	223.68728	-150.20145	1
6556	H	83.94100	53.16780	72.88390	1370.99310	582.96801	2771.05620	1
6557	H	85.25400	52.43280	72.04590	-1938.95471	-86.65666	-2476.12025	1
6558	C	85.88700	53.42880	73.88690	645.13091	-641.00778	66.07680	1
6559	H	86.80800	52.87480	74.16590	-292.94778	2772.15421	-1458.61881	1
6560	H	85.38700	53.70380	74.83990	-220.80937	2915.27530	-1162.17013	1
6561	C	86.28500	54.67180	73.14490	-46.40004	-652.09192	-635.66828	1
6562	H	85.41500	55.31380	72.88890	972.19535	2320.72695	-1888.72678	1
6563	H	86.96800	55.30180	73.75390	1566.75036	2000.37395	1855.26914	1
6564	N	87.02500	54.16280	71.89790	-608.96999	352.30617	466.59212	1
6565	H	86.52100	54.27380	71.04090	2255.82456	2188.50576	-141.15364	1

6566	C	88.26400	53.66480	71.80990	-569.81877	363.39144	-612.13090	1
6567	N	89.10000	53.50980	72.82190	577.68006	610.17971	-81.47856	1
6568	H	88.79100	53.70980	73.75190	-327.84551	2636.03825	1685.83686	1
6569	H	90.04200	53.23980	72.62390	2824.26856	630.69254	1234.48785	1
6570	N	88.74400	53.35480	70.59690	243.88392	-464.76129	661.20335	1
6571	H	88.15000	53.32880	69.79290	593.76744	-1077.70321	-2895.55215	1
6572	H	89.71700	53.20780	70.42090	1555.41710	2697.84599	447.80674	1
6573	C	83.32200	50.61480	73.20590	-627.51682	-478.99942	-456.32576	1
6574	O	83.24600	50.07780	72.10590	158.13124	76.39803	769.92537	1
6575	N	82.30300	50.67980	74.02090	288.65807	-357.90700	-707.99109	1
6576	H	82.47000	51.01780	74.94390	-1317.19795	2080.32748	1958.43135	1
6577	C	80.90500	50.41080	73.69990	213.65388	861.83773	207.45781	1
6578	H	80.90700	49.61780	72.96590	2621.91957	1226.50582	1232.65870	1
6579	C	80.09800	49.91280	74.88890	891.07230	99.44429	165.98792	1
6580	H	80.65700	49.07480	75.35590	-610.32980	2738.34949	-1423.78574	1
6581	H	79.13500	49.50380	74.51390	-1334.15046	-2455.18096	-1445.80609	1
6582	O	79.93000	50.94380	75.84990	404.99634	677.47108	25.26136	1
6583	H	80.78600	51.10580	76.25190	2045.17830	-1934.17400	1405.14871	1
6584	C	80.20200	51.63780	73.09290	-290.77136	460.76193	731.16446	1
6585	O	80.82500	52.67380	72.89290	6.22925	-670.23758	417.57636	1
6586	N	78.90600	51.49280	72.63190	804.15742	-245.13745	76.88145	1
6587	H	78.46200	50.61780	72.45690	1966.48604	2031.87133	1379.36862	1
6588	C	78.10900	52.61380	72.12490	-38.80295	-523.18019	-745.80683	1
6589	H	78.62900	53.02480	71.27190	571.29205	3037.68164	586.80650	1
6590	C	76.74700	52.13880	71.62190	-1.64929	686.49319	600.14613	1
6591	H	76.16900	52.99880	71.21990	960.73814	-1454.63825	2619.01432	1
6592	H	76.18700	51.79780	72.51890	-1762.84482	-2491.16498	-764.65771	1
6593	C	76.84800	51.01580	70.56590	-675.82134	331.44193	514.64820	1
6594	H	75.93000	51.16180	69.95690	965.02650	1592.22819	2536.09138	1
6595	H	77.66100	51.23680	69.84290	2357.70359	464.66706	2030.65126	1
6596	S	76.94200	49.31380	71.19890	341.30531	408.22216	167.55883	1
6597	C	75.79700	48.59480	69.95690	827.16267	245.02624	295.32196	1
6598	H	75.35400	47.67380	70.39290	2064.85392	-2370.72865	-119.37418	1
6599	H	76.40800	48.33680	69.06590	-360.06608	-2325.14734	2088.60443	1
6600	H	75.08300	49.32480	69.51890	1737.04504	1346.82353	-2250.99248	1
6601	C	77.92300	53.80080	73.01490	-216.78428	637.19466	615.17358	1
6602	O	78.11000	54.94380	72.61990	511.66076	-576.12974	-172.93066	1
6603	N	77.71000	53.58280	74.34390	116.26666	-800.05617	243.03183	1
6604	H	77.59800	52.67680	74.74290	-1357.08445	-1232.82351	2556.69596	1
6605	C	77.68700	54.67680	75.33990	-678.35284	-109.41542	-599.43031	1
6606	H	76.94800	55.38980	75.00390	-1206.66008	2905.34747	33.96701	1
6607	C	77.20500	54.32980	76.79390	472.54445	10.69847	-779.76810	1
6608	H	77.72800	53.41580	77.14590	2373.67726	-1298.61513	-1605.45359	1
6609	O	75.76300	54.21780	76.78490	249.98320	-474.61047	-579.55201	1
6610	H	75.63300	53.42280	76.26290	3029.87441	-803.06926	-270.49405	1
6611	C	77.39900	55.42680	77.81890	-565.84948	425.25063	574.82803	1
6612	H	76.81700	55.15480	78.72490	2380.54261	2038.40372	275.95904	1
6613	H	78.42900	55.46880	78.23490	223.84325	3107.75120	-435.89326	1
6614	H	77.11100	56.36280	77.29590	-8.05197	-3029.05317	850.29306	1
6615	C	78.99300	55.41280	75.48290	701.70330	-576.93621	-78.79146	1
6616	O	79.01200	56.64380	75.52890	-59.21911	-775.59247	-136.29617	1
6617	N	80.04200	54.60680	75.54790	-398.63876	510.83580	-541.11571	1
6618	H	79.91100	53.62580	75.42390	-2349.11562	2066.51292	330.76636	1
6619	C	81.45000	55.05880	75.60490	206.95057	637.15206	-618.59495	1
6620	H	81.54600	55.60980	76.52890	632.20188	-642.48221	-3014.26004	1
6621	C	82.49400	53.85080	75.62690	598.64805	397.00326	-561.65820	1
6622	H	83.54200	54.17680	75.80090	-2232.34802	-1661.32334	-1467.94186	1
6623	H	82.40300	53.30880	74.66190	676.89204	2401.68197	-1916.23775	1
6624	C	82.13700	52.85880	76.75290	-370.00610	37.83435	-832.53531	1
6625	O	82.51800	51.66580	76.56390	-351.41515	21.40122	706.87807	1
6626	O	81.53100	53.20380	77.76190	286.97340	74.62546	731.91840	1
6627	C	81.81100	55.96680	74.36290	205.71236	700.87909	-545.80393	1

6628	O	82.31600	57.09180	74.51690	411.41298	417.00731	529.59560	1
6629	N	81.46000	55.58180	73.12090	230.67136	-741.50725	-331.10424	1
6630	H	80.97900	54.71980	72.97790	2577.54806	1047.01609	1469.09140	1
6631	C	81.68400	56.29980	71.95890	389.38357	-169.83255	-806.83848	1
6632	H	82.73300	56.54780	72.03390	-1969.42367	1749.85328	-1719.77037	1
6633	C	81.30300	55.39580	70.72990	-581.59895	323.43404	-623.36513	1
6634	H	81.29600	56.08680	69.85890	-2342.50797	-2032.69013	528.25512	1
6635	H	80.24900	55.09180	70.90490	-2701.29281	1283.89242	976.14733	1
6636	C	82.34400	54.32980	70.40590	45.24449	-679.72194	606.12047	1
6637	H	82.91800	54.03380	71.31090	-1064.36985	1985.27929	2196.36272	1
6638	H	83.11200	54.74680	69.71990	-611.85400	-2639.79983	1598.53612	1
6639	C	81.85800	53.05580	69.67590	660.61407	-567.71870	269.69526	1
6640	H	81.45300	53.35580	68.68590	-2517.02422	-608.94234	1786.61818	1
6641	H	81.02700	52.73880	70.34090	-286.32125	-1820.26254	-2550.07660	1
6642	C	82.96900	51.98280	69.53090	-514.95006	-516.07252	547.67380	1
6643	H	83.51800	51.86480	70.48990	1856.94857	1393.62275	2123.15423	1
6644	H	83.71600	52.20480	68.73890	1301.85931	-1533.97425	2418.74173	1
6645	N	82.51400	50.65680	69.16890	535.25158	528.00295	383.91525	1
6646	H	82.10400	50.74380	68.21690	-169.33332	2201.55980	-2241.13518	1
6647	H	83.32800	50.00980	69.15490	-692.77952	2016.47948	2313.45916	1
6648	H	81.81100	50.26080	69.82490	-1891.10716	-2335.74071	930.72835	1
6649	C	80.96500	57.63780	71.82890	831.35342	-336.52414	164.48099	1
6650	O	81.52700	58.63680	71.43890	528.41780	45.66680	-585.07812	1
6651	N	79.66900	57.69580	72.21290	67.36990	405.06377	-737.60215	1
6652	H	79.23700	56.80280	72.31390	1052.74506	-1323.30612	2653.07651	1
6653	C	78.91900	58.95380	72.34290	673.98104	4.29476	614.15154	1
6654	H	79.04000	59.54580	71.44790	-1796.10232	2269.58137	1233.38685	1
6655	C	77.45800	58.71880	72.77690	817.18460	-349.45788	-203.81249	1
6656	H	76.82600	59.62580	72.87990	-1459.46663	-662.24447	2707.32629	1
6657	H	77.44500	58.21880	73.76890	-2750.54998	1059.53428	1100.04007	1
6658	C	76.64300	57.82380	71.87090	570.71445	-85.92804	705.94079	1
6659	C	76.58300	58.10480	70.48090	196.61060	-845.10815	-280.33459	1
6660	H	77.12200	58.96280	70.10690	-2022.26458	1442.80133	-1930.54307	1
6661	C	75.81100	57.35880	69.59390	-620.67473	-144.62225	652.14898	1
6662	H	75.76500	57.60680	68.54390	-1774.85020	-1785.31973	-1886.99933	1
6663	C	75.22600	56.17080	70.00690	507.99053	-715.82818	246.95473	1
6664	O	74.53900	55.28780	69.16190	636.89690	24.24144	466.26378	1
6665	H	74.41500	54.44180	69.59890	-1229.13574	-2728.82755	-970.02668	1
6666	C	75.90500	56.70580	72.30390	-438.06824	-219.52237	768.99750	1
6667	H	75.83900	56.41280	73.34090	-1389.16845	2304.19206	1630.68580	1
6668	C	75.30900	55.81680	71.36490	-138.47807	486.79549	-758.48862	1
6669	H	74.94300	54.87280	71.74090	1875.29069	1905.15049	-1658.88899	1
6670	C	79.49600	59.91880	73.36590	314.93220	-626.23050	583.18443	1
6671	O	79.75100	61.08780	73.13790	166.40047	34.09026	-771.21720	1
6672	N	79.82100	59.45580	74.55290	-641.07289	-340.81376	-430.74798	1
6673	H	79.68400	58.49580	74.78390	2770.00984	-1453.88336	-333.90849	1
6674	C	80.44200	60.30880	75.56290	-729.93127	358.94081	-412.08353	1
6675	H	79.90500	61.24580	75.55490	-2787.83190	-900.98633	-1146.49167	1
6676	C	80.24100	59.73180	76.98690	332.98027	551.74550	-645.09848	1
6677	H	80.77400	60.48080	77.61190	2466.17135	124.53770	1949.54237	1
6678	H	80.74600	58.75980	77.17490	-1127.69053	2483.20785	-1568.50855	1
6679	C	78.72500	59.53680	77.40490	-655.38688	470.08820	-425.36587	1
6680	H	78.16700	60.42180	77.03090	2662.62756	1561.17670	-609.39974	1
6681	H	78.24300	58.62080	77.00190	-2099.73270	-1947.48585	1302.55430	1
6682	C	78.50600	59.36680	78.91590	31.97752	198.73558	889.34392	1
6683	H	78.94700	58.43680	79.33590	-74.44478	2293.05552	2152.80760	1
6684	H	77.42800	59.16480	79.09190	-1970.42781	-1072.69218	2205.66815	1
6685	N	79.05000	60.55680	79.71390	-229.64616	496.03660	643.33710	1
6686	H	79.41200	61.35180	79.22890	833.13704	-2924.64675	-806.56697	1
6687	C	79.10800	60.62180	81.05290	124.60381	-647.79417	-629.51379	1
6688	N	78.65600	59.79180	81.93890	-677.75721	-278.89576	418.96851	1
6689	H	78.00100	59.08680	81.66790	-1755.95806	-2224.39321	1366.35001	1

6690	H	78.68000	60.11080	82.88590	-1983.36234	-1569.63800	-1871.02555	1
6691	N	79.61200	61.72080	81.54490	-334.65245	-585.25440	-508.09184	1
6692	H	79.92100	62.44280	80.92490	-1562.22485	1491.63732	2287.50909	1
6693	H	79.73600	61.78780	82.53490	-1795.71036	1793.17424	-1859.61734	1
6694	C	81.91100	60.65180	75.26890	616.82672	440.14893	-507.19298	1
6695	O	82.34700	61.74380	75.64890	408.96491	673.97556	-46.17215	1
6696	N	82.63500	59.80580	74.56990	-190.24542	70.08760	-819.49173	1
6697	H	82.35300	58.85480	74.46790	-2529.63481	1462.88648	1165.82036	1
6698	C	83.96700	60.27580	74.06590	580.48783	-682.68440	168.60276	1
6699	H	84.51900	60.58080	74.94290	-2015.52347	-270.18547	2400.60225	1
6700	C	84.76500	59.15580	73.29790	807.44994	-162.97781	-391.04198	1
6701	H	84.27400	58.99080	72.31490	-1304.61225	1425.38317	-2482.84029	1
6702	H	84.62400	58.26080	73.94190	-1610.06251	2701.87052	76.29298	1
6703	C	86.25700	59.33680	73.14890	-736.82847	197.47386	499.53867	1
6704	H	86.42000	60.38280	72.81090	2282.69942	-2080.27261	-599.97954	1
6705	C	86.99400	59.10380	74.43890	-132.79600	758.65012	-488.12522	1
6706	H	88.03400	59.42780	74.21690	2316.28189	2059.60012	539.54772	1
6707	H	86.66200	59.73080	75.29390	1764.69691	-1722.13532	1954.05245	1
6708	H	86.94000	58.03480	74.73590	1618.11774	1947.21808	1867.68921	1
6709	C	86.78800	58.36680	72.08090	-33.05601	290.32281	863.75400	1
6710	H	86.63600	57.36080	72.52590	-1363.19630	2394.79000	-1518.19067	1
6711	H	87.88400	58.53880	72.02790	-262.56333	2650.23136	1674.98074	1
6712	H	86.34700	58.51580	71.07190	-2542.66483	1742.60188	629.61931	1
6713	C	83.83400	61.42680	73.15390	-349.49611	-412.57976	-734.22164	1
6714	O	84.63000	62.37580	73.26490	653.38230	407.13363	-175.95740	1
6715	N	82.85300	61.48880	72.22890	-696.62291	-443.72975	-174.62165	1
6716	H	82.23800	60.70680	72.16490	2557.02351	1717.87314	-639.35033	1
6717	C	82.51100	62.67080	71.40490	-174.66495	893.03350	-58.60317	1
6718	H	83.43700	63.02080	70.97290	2742.09203	936.70899	1225.45248	1
6719	C	81.45100	62.39580	70.30990	654.62704	631.74434	61.75378	1
6720	H	80.52300	61.97280	70.74890	-1124.67376	1215.25919	2675.15986	1
6721	H	81.11100	63.34480	69.84290	-1237.27166	-1033.78453	2701.60593	1
6722	N	83.07400	62.04880	68.49190	-65.61244	-824.28130	170.08128	1
6723	C	81.94000	61.60380	69.18490	553.72523	-722.80060	48.97612	1
6724	C	83.07900	61.30880	67.38090	-156.05578	800.76146	-407.28207	1
6725	H	83.93400	61.31080	66.70590	2707.28651	1600.97032	75.63083	1
6726	N	82.06700	60.43080	67.32990	27.73325	691.53841	-483.40230	1
6727	H	81.96900	59.68080	66.67590	2123.25559	2320.04986	-85.91020	1
6728	C	81.28500	60.67180	68.46190	751.95162	343.93963	-384.35049	1
6729	H	80.30900	60.21780	68.57990	2039.24247	190.54477	2388.18112	1
6730	C	81.99700	63.82580	72.29390	-160.21988	-892.31250	-97.77014	1
6731	O	82.45800	64.95180	72.13090	-742.17490	52.02864	-264.75775	1
6732	N	81.10700	63.58780	73.24290	-506.89933	-356.14508	573.48587	1
6733	H	80.64000	62.70880	73.29990	2261.43733	582.87510	-2108.17079	1
6734	C	80.62600	64.63480	74.15290	540.92378	420.08690	601.97962	1
6735	H	80.25900	65.41980	73.50690	1104.64224	2675.80596	-1232.09343	1
6736	C	79.51400	64.01580	75.02690	487.40404	679.16621	364.17243	1
6737	H	78.93200	63.32680	74.37890	1781.37923	-1451.21758	2149.15839	1
6738	H	80.05900	63.34980	75.72990	2047.54260	2138.23628	-1064.77281	1
6739	C	78.65200	64.92580	75.86790	150.99140	893.23266	-103.86534	1
6740	H	79.32500	65.43280	76.59190	1577.40469	-164.99908	-2717.13010	1
6741	C	77.84300	65.91680	75.11090	402.88510	394.90242	-716.37049	1
6742	H	78.40300	66.58380	74.41990	-2081.17384	-2130.37170	-1014.12924	1
6743	H	77.04300	65.37980	74.55790	1427.12257	-2280.78150	1630.82284	1
6744	H	77.34800	66.57180	75.85890	474.44067	676.84145	-3035.62480	1
6745	C	77.73700	63.96780	76.62590	178.26637	-636.12688	-628.50194	1
6746	H	78.25600	63.31880	77.36390	-2268.84858	-1446.41660	1630.46968	1
6747	H	77.23500	63.24180	75.95090	-2030.35526	-471.07066	-2356.68754	1
6748	H	77.01400	64.60180	77.18190	1036.87980	2968.51869	-104.89656	1
6749	C	81.76100	65.29180	74.99290	343.66896	299.69006	789.63822	1
6750	O	81.80900	66.50180	75.10190	447.19691	528.48600	379.92722	1
6751	N	82.73700	64.49880	75.49490	-433.79278	387.28297	-611.97060	1

6752	H	82.74800	63.51180	75.35190	2667.48998	-1434.27704	-851.80562	1
6753	C	84.02000	64.94880	76.06590	574.89745	-680.42524	194.84716	1
6754	H	83.77900	65.63080	76.86790	-1563.71622	1465.41777	2303.38199	1
6755	C	84.77200	63.73480	76.76590	595.79640	-682.68278	-102.08756	1
6756	H	85.81700	64.05580	76.96690	-1289.96943	2325.87140	1680.63301	1
6757	H	84.71000	62.84780	76.09990	2126.61121	2034.22205	-1112.51591	1
6758	O	84.15300	63.55380	78.01490	486.11575	-42.96009	-620.86483	1
6759	H	84.37800	64.25280	78.63390	-1787.26086	2063.96930	1563.31558	1
6760	C	84.93100	65.67980	75.13190	-663.49168	-288.52248	554.96358	1
6761	O	85.56500	66.64980	75.53790	-588.04176	-513.33378	-119.67683	1
6762	N	85.05100	65.29680	73.86190	-259.51888	742.08221	307.63002	1
6763	H	84.70800	64.42780	73.51290	-2106.68035	-139.62095	2332.51583	1
6764	C	85.69500	66.04380	72.82190	573.02431	366.65430	-607.17277	1
6765	H	86.70800	66.33380	73.05990	2764.78709	-1501.37226	-7.74138	1
6766	C	85.74100	65.15480	71.54090	-133.05896	-869.20207	-241.31740	1
6767	H	84.87900	64.46080	71.44990	148.62272	2088.94663	-2347.85849	1
6768	C	85.79600	65.94080	70.19390	454.61833	-363.57527	701.84486	1
6769	H	84.86900	66.50480	69.95490	2551.92878	-1366.56206	1232.23125	1
6770	H	85.96200	65.21880	69.36590	-1476.37308	-34.90144	-2778.00840	1
6771	H	86.63500	66.66980	70.17690	-1292.00135	2545.19150	1323.23807	1
6772	C	87.01400	64.26180	71.59490	-392.54470	622.82292	538.00676	1
6773	H	86.82200	63.39980	72.26990	-891.72079	-2485.89783	1709.78719	1
6774	H	87.92700	64.84480	71.84190	315.63313	-2973.12995	979.33663	1
6775	H	87.23900	63.84180	70.59090	-3023.59537	-818.79082	292.70952	1
6776	C	84.98600	67.39680	72.55390	-382.12363	-807.35395	-183.33613	1
6777	O	85.69000	68.41580	72.40690	210.25598	-515.88228	559.71879	1
6778	N	83.64700	67.48780	72.47490	216.00212	-314.44842	-753.08536	1
6779	H	83.09500	66.66380	72.57690	1593.33848	328.35976	2692.89409	1
6780	C	82.92000	68.76280	72.32790	-515.80784	257.10074	-706.60632	1
6781	H	83.22900	69.31680	71.45390	2024.47698	1690.93538	-1714.77600	1
6782	C	81.43200	68.40580	72.15790	648.50536	-302.09253	565.35997	1
6783	H	80.91900	69.33580	71.83390	-1725.51672	1315.79795	-2278.04610	1
6784	H	80.92200	68.18880	73.12090	-1757.06882	-1744.11894	1941.38727	1
6785	H	81.28100	67.60480	71.40290	-737.82683	1519.08542	2654.47119	1
6786	C	83.14400	69.72080	73.44490	-395.42291	812.29268	123.58130	1
6787	O	83.43900	70.90080	73.25090	539.79206	559.36134	-139.16412	1
6788	N	83.00700	69.24380	74.69190	-34.22935	573.50717	-618.53873	1
6789	H	82.62000	68.33680	74.84090	2966.83186	973.23497	385.93867	1
6790	C	83.27700	70.00580	75.90190	873.70478	24.39264	259.79983	1
6791	H	82.61000	70.85480	75.90990	-2612.51722	-285.31065	1729.61782	1
6792	C	83.12800	69.09680	77.13590	-189.12856	-631.34043	630.15130	1
6793	H	83.48300	69.52780	78.09690	-429.88148	1737.22478	2587.56221	1
6794	H	83.61800	68.12180	76.92790	552.37381	-3048.72003	-546.27430	1
6795	C	81.58900	68.79880	77.42290	506.34032	746.12677	-135.51871	1
6796	O	80.75700	69.59680	76.91990	634.58558	468.81093	33.83312	1
6797	O	81.33500	67.81580	78.15690	-681.02272	-129.27330	-378.31692	1
6798	C	84.71100	70.58080	75.95190	717.95488	52.30739	559.69253	1
6799	O	84.86800	71.75680	76.30490	-392.94383	-427.35786	535.33880	1
6800	N	85.74100	69.79480	75.67590	-415.04889	265.39372	-685.54568	1
6801	H	85.60700	68.83480	75.43990	2137.04559	-2200.43123	699.54610	1
6802	C	87.13300	70.09780	75.63590	-188.65217	-889.33474	-70.32133	1
6803	H	87.32400	70.52680	76.60790	1091.87028	-2116.68285	2055.65056	1
6804	C	87.91400	68.77880	75.41390	489.60820	-592.84580	490.17207	1
6805	H	87.59900	68.21680	74.50790	700.09827	2650.52625	1543.63184	1
6806	H	87.63200	68.11480	76.25890	-2482.03662	1382.94635	1350.99216	1
6807	C	89.44000	68.82480	75.48290	692.80416	570.40126	-161.60383	1
6808	H	89.72900	69.58180	74.72290	298.18466	-1746.60285	2599.74818	1
6809	C	89.94100	69.29480	76.88690	181.95516	681.49958	577.84223	1
6810	H	89.75800	68.53080	77.67190	2543.27422	1849.91670	-88.26466	1
6811	H	91.05200	69.32680	76.88190	1546.58761	710.38340	2646.06281	1
6812	H	89.44900	70.26980	77.09490	2913.61036	807.48848	870.09380	1
6813	C	89.95100	67.43480	75.03090	-434.95320	-440.02011	669.81267	1

6814	H	89.65900	67.25180	73.97490	-2229.65148	-1205.77526	1863.59505	1
6815	H	91.05800	67.51580	75.08490	-2346.62516	2037.49304	-490.10068	1
6816	H	89.58900	66.62280	75.69590	2317.98498	2115.13878	226.62696	1
6817	C	87.46200	71.14180	74.60090	243.29597	-515.30183	711.84416	1
6818	O	88.19800	72.07180	74.83790	242.16191	-373.73155	652.15762	1
6819	N	86.84400	71.04980	73.39090	-206.19084	-790.70397	212.00203	1
6820	H	86.17000	70.32580	73.26190	-2329.37301	-1645.87292	1327.91187	1
6821	C	87.01800	71.85880	72.20590	-797.26164	-385.05976	-218.06846	1
6822	H	88.03400	71.65880	71.90090	-1368.50983	-1180.41086	-2575.27421	1
6823	C	86.05600	71.26180	71.07990	-544.54715	-641.45881	351.35453	1
6824	H	85.03600	71.30180	71.51890	1898.93754	-2218.42496	1170.83439	1
6825	H	86.42000	70.23180	70.88090	-1156.17871	-2079.34627	2058.59080	1
6826	C	86.06000	71.96180	69.68690	-557.49996	616.60391	-374.75914	1
6827	H	85.52600	72.93580	69.71790	1897.10684	-331.51851	2487.83186	1
6828	C	87.48200	72.28980	69.17990	222.43514	-630.28591	-620.25259	1
6829	H	88.21400	71.45680	69.22790	757.91180	3044.92607	228.51948	1
6830	H	87.92000	73.10780	69.79090	-673.91154	2373.74099	-1951.77436	1
6831	H	87.44600	72.71180	68.15290	1938.39703	1427.72827	2025.44691	1
6832	C	85.20100	71.16880	68.59090	73.40772	-590.80600	690.65952	1
6833	H	85.60800	70.14180	68.47390	358.89761	-2861.34974	1257.81414	1
6834	H	84.15200	71.20580	68.95590	-2358.21230	2029.33669	-467.81789	1
6835	H	85.20300	71.73380	67.63390	1743.93046	-27.50855	-2618.43007	1
6836	C	86.64900	73.30080	72.42790	172.18240	-757.68989	477.18996	1
6837	O	87.45100	74.21280	72.17190	122.55922	-369.80880	-686.91187	1
6838	N	85.50800	73.52580	73.11090	162.34887	-288.33841	-776.64412	1
6839	H	84.97100	72.71180	73.31890	2621.72506	-1513.35586	-857.05191	1
6840	C	85.11500	74.80280	73.59690	627.09744	-477.05513	458.93159	1
6841	H	85.32400	75.60080	72.90090	1530.70822	1534.00608	-2280.78581	1
6842	C	83.55300	74.85180	73.84290	675.88439	204.91434	576.75073	1
6843	H	83.38800	74.05380	74.59790	-1785.28981	-1117.81202	2336.97728	1
6844	H	83.04800	74.70080	72.86490	-1449.53844	-2337.75312	1527.08051	1
6845	C	83.06600	76.20680	74.31390	-316.55822	790.68701	325.66234	1
6846	C	83.49400	77.39480	73.61290	-683.51343	354.64960	488.34830	1
6847	H	84.09300	77.25680	72.72490	-727.13514	2292.88436	-2027.85158	1
6848	C	83.02700	78.64780	74.04590	593.16071	-653.76433	-228.48102	1
6849	H	83.34500	79.53480	73.51790	2491.16766	408.28340	1877.66200	1
6850	C	82.11700	78.73280	75.12690	-66.97421	795.26514	-441.04288	1
6851	H	81.80600	79.73380	75.39090	-2023.60898	283.96525	2392.19495	1
6852	C	82.25700	76.31380	75.36790	516.22629	691.61670	-294.32595	1
6853	H	81.88900	75.42480	75.85690	-283.41445	3128.62409	-172.08652	1
6854	C	81.80600	77.52180	75.83390	161.00809	-648.26628	-620.70785	1
6855	H	81.02300	77.59480	76.57490	1616.68512	1950.46833	1865.53712	1
6856	C	85.85600	75.28680	74.89890	558.42224	-319.32804	646.25476	1
6857	O	86.21200	76.46780	74.94090	-617.03132	-329.65839	366.36720	1
6858	N	86.17100	74.39980	75.83690	365.84895	181.75465	738.77743	1
6859	H	86.02200	73.41680	75.76590	-963.78762	622.65670	2929.44334	1
6860	C	86.82000	74.75980	77.14490	92.88478	-707.91608	567.16686	1
6861	H	86.15300	75.48880	77.57990	-2690.93431	370.99464	1587.28125	1
6862	C	86.94000	73.58780	78.11590	410.88764	701.60620	-412.76033	1
6863	H	87.14500	72.68280	77.50590	2428.38666	1806.31783	859.29061	1
6864	C	88.11000	73.73880	79.17790	432.87521	-784.56392	-168.90679	1
6865	H	89.11200	73.50380	78.75790	-2802.28668	8.86839	-1430.15277	1
6866	H	87.89000	73.00680	79.98390	1689.26299	-2020.98145	1720.53793	1
6867	H	88.01200	74.79180	79.51590	-2365.18424	1456.71194	-1477.20008	1
6868	C	85.60400	73.41880	78.88190	489.21410	391.20761	662.62898	1
6869	H	85.67200	72.50580	79.51190	2305.33576	1919.54368	-948.15892	1
6870	H	85.36200	74.27280	79.54890	1150.20989	-2924.23098	-155.29525	1
6871	H	84.74200	73.40480	78.18090	848.83691	-2268.82709	2007.51732	1
6872	C	88.17300	75.40380	76.92690	269.85313	-698.95484	-519.70416	1
6873	O	88.54300	76.32780	77.61390	222.86699	-474.16548	-590.86769	1
6874	N	88.89700	74.85580	75.91890	-237.45874	-514.82712	-625.49074	1
6875	H	88.53000	74.08180	75.40890	-401.06002	2256.45471	2155.40930	1

6876	C	90.29200	75.32580	75.66290	-228.46060	-244.74551	848.14880	1
6877	H	90.89600	75.29980	76.55790	2246.14420	1860.68591	-1179.36865	1
6878	C	90.95300	74.41080	74.56690	341.32691	764.75637	360.68634	1
6879	H	90.23300	74.14880	73.76190	2554.11733	1652.47885	802.51140	1
6880	C	92.24400	75.00980	73.95790	-637.87628	639.76897	123.53346	1
6881	H	92.97600	75.11480	74.78690	-1452.19126	1638.97488	2259.01043	1
6882	H	92.67300	74.27880	73.23890	1802.54928	-2168.26235	1395.59331	1
6883	H	91.99400	75.90680	73.35290	2254.70122	-2192.03053	-97.72796	1
6884	C	91.30800	73.01580	75.20290	580.51474	-213.05230	-670.12115	1
6885	H	90.39500	72.66380	75.72790	-1253.55495	2442.55631	1536.47157	1
6886	H	92.16300	73.06880	75.90890	-2566.35490	-1170.15823	-1393.83589	1
6887	C	91.58000	71.93880	74.11790	-544.80879	723.46474	105.98658	1
6888	H	92.58900	72.13780	73.69690	-1849.55825	1926.39631	1663.23713	1
6889	H	90.83500	71.82580	73.30090	3081.44701	557.50540	303.47698	1
6890	H	91.68900	70.94580	74.60390	1172.41242	2849.92965	-633.70050	1
6891	C	90.27000	76.76580	75.16090	43.99705	529.99175	-740.69157	1
6892	O	91.26100	77.50980	75.35290	-669.29467	-418.02486	-30.44806	1
6893	N	89.15800	77.21180	74.50990	-185.76579	-545.19233	-617.19420	1
6894	H	88.43600	76.60280	74.19090	1200.96570	1543.34285	2464.54873	1
6895	C	89.12800	78.59280	74.10490	384.61821	503.00683	656.12801	1
6896	H	90.03400	78.84180	73.57190	1476.59375	-1263.13412	-2474.34624	1
6897	C	87.93400	78.86780	73.12990	-21.66292	-737.14628	536.28078	1
6898	H	88.03500	79.86580	72.65290	882.49886	-2368.00120	-1874.03103	1
6899	O	86.60800	78.75480	73.78290	501.75101	-525.68570	309.07555	1
6900	H	86.49900	77.90180	74.21090	3140.14368	27.99916	192.19760	1
6901	C	87.97000	77.75680	72.01390	-713.52948	-542.73673	-166.62390	1
6902	H	87.68400	76.74380	72.36890	1938.00761	2469.06701	-214.61793	1
6903	H	87.16200	78.06680	71.31790	1565.64258	-1314.16470	-2391.64393	1
6904	H	88.96600	77.83780	71.52890	202.51630	-1564.01020	2722.33089	1
6905	C	88.96700	79.58880	75.24390	-546.08792	-598.26994	-418.70284	1
6906	O	89.33600	80.75080	75.13190	-473.21638	-515.99724	-365.29486	1
6907	N	88.46200	79.15180	76.40990	-43.52075	-816.92906	-208.33901	1
6908	H	88.27300	78.17780	76.50590	-1752.13224	-1467.47552	-2162.12267	1
6909	C	88.07500	80.00680	77.54090	-22.34412	188.91236	891.77568	1
6910	H	87.30100	80.66680	77.17790	2302.06814	330.51885	-2118.83595	1
6911	C	87.30500	79.28680	78.65090	-594.77166	183.24338	-666.42294	1
6912	H	87.05400	79.85480	79.57290	-1998.90857	1716.74723	-1719.11887	1
6913	H	87.98500	78.45680	78.93890	48.26060	-2588.39189	1787.77084	1
6914	C	85.94700	78.73980	78.20890	-391.05240	313.85106	761.59473	1
6915	H	86.02600	78.13580	77.27990	-2803.23397	1413.33989	-206.33925	1
6916	C	85.44800	77.83980	79.37790	-895.95207	-10.76464	-169.13015	1
6917	H	86.11200	76.94880	79.37190	227.33190	-2794.30265	-1427.73216	1
6918	H	85.48900	78.35180	80.36290	-2610.76036	1750.12024	-138.69293	1
6919	H	84.39600	77.56880	79.14390	-3046.09747	-127.33998	776.72450	1
6920	C	84.96300	79.87180	77.92290	-896.33437	84.57238	144.51028	1
6921	H	85.05400	80.27480	76.89190	2459.16703	1961.86027	42.75521	1
6922	H	85.04300	80.76780	78.57490	-1997.82917	-1897.36799	-1518.84809	1
6923	H	83.95600	79.43980	78.10290	832.03319	-1456.25588	-2661.81626	1
6924	C	89.17800	80.94580	78.08890	-711.38404	491.58397	289.35955	1
6925	O	88.80600	82.04980	78.42590	650.20613	447.96805	13.55916	1
6926	N	90.47200	80.68380	78.13390	-569.16004	-19.26878	623.18364	1
6927	C	90.96500	79.30680	78.36890	-409.24103	-448.61170	-680.23550	1
6928	H	91.18800	78.92780	77.34790	-1619.60431	1655.05126	2129.76839	1
6929	H	90.26700	78.62680	78.90290	-1439.77459	-1857.19598	-2091.91263	1
6930	C	91.54100	81.64680	78.45690	-29.16890	-449.96339	-792.54850	1
6931	H	91.23900	81.98780	79.43590	1756.31519	-1808.82317	-1881.95163	1
6932	C	92.73700	80.82480	78.49790	-842.40104	144.23372	-317.81774	1
6933	H	93.63600	81.30280	78.94390	415.84241	-1809.51773	2539.87143	1
6934	H	93.12400	80.48380	77.51490	16.29837	-2368.52761	-2070.75773	1
6935	C	92.24000	79.53580	79.14890	-347.10386	-211.95636	816.11544	1
6936	H	92.99800	78.74380	78.96890	-2027.24786	2403.32760	-111.84286	1
6937	H	92.10900	79.69280	80.24090	1908.09932	919.17948	-2326.47637	1

6938	C	91.62700	82.88080	77.58990	248.42227	689.14329	-542.97228	1
6939	O	92.02600	83.95080	78.05690	149.28934	-171.04220	756.36267	1
6940	N	91.29900	82.78080	76.30590	-331.25744	596.28516	-497.37794	1
6941	H	91.10600	81.91780	75.84690	1445.82965	2792.18114	-107.36550	1
6942	C	91.14300	83.99380	75.47590	612.29400	-318.80955	-595.74116	1
6943	H	92.02900	84.60980	75.52090	341.74386	2835.43554	1319.75097	1
6944	C	90.89300	83.53080	73.98690	517.51697	-499.03601	-560.88346	1
6945	H	89.88900	83.05780	73.93690	2128.87328	1637.00740	1639.00321	1
6946	H	90.85600	84.47980	73.41090	-1256.47112	2228.18795	-1831.57992	1
6947	C	92.01000	82.69580	73.39690	-547.41416	493.30768	537.06264	1
6948	C	93.29400	83.19280	73.34590	786.37913	-200.80348	415.61620	1
6949	H	93.55400	84.19180	73.66590	2082.03614	1130.29365	-2070.21448	1
6950	C	94.39900	82.58680	72.68290	-618.47257	-290.02323	604.01093	1
6951	H	95.32400	83.13780	72.59590	655.95752	2022.12489	2319.25783	1
6952	C	94.10100	81.35380	72.07090	600.09640	408.89255	551.49089	1
6953	H	94.80900	80.81280	71.46190	2045.02833	-1258.14154	-2033.01875	1
6954	C	91.83500	81.41480	72.88390	-370.64793	-315.48317	-771.06516	1
6955	H	90.85900	80.95880	72.95990	2820.84396	1337.61107	-389.69505	1
6956	C	92.82900	80.73080	72.21990	278.11087	868.36814	-6.49039	1
6957	H	92.53500	79.82280	71.71490	666.69203	-2802.82065	1264.09824	1
6958	C	90.05300	84.85580	75.95490	652.77190	565.18946	-293.08825	1
6959	O	90.15667	86.03541	75.72062	380.31096	-233.26686	-126.19142	1
6960	N	88.89800	84.23980	76.38290	-68.55996	-686.47804	486.53851	1
6961	H	88.83200	83.24980	76.48090	1531.30311	541.27594	-2694.50503	1
6962	C	87.77100	84.95680	77.05290	-791.18086	69.28925	447.97639	1
6963	H	87.56591	85.73597	76.26534	-3168.52356	-2493.67218	-735.78353	1
6964	C	86.55800	84.09580	77.20590	170.10671	496.42605	745.70496	1
6965	H	85.74200	84.75480	77.57290	-13.09365	1988.53377	2437.98856	1
6966	H	86.63600	83.28580	77.96190	-1439.65630	-2248.20643	1664.68730	1
6967	C	85.94200	83.48480	75.94290	-435.11005	-533.77840	-597.67121	1
6968	C	86.43200	82.68380	74.93490	-338.30142	779.26114	331.29328	1
6969	H	87.49000	82.51880	74.79890	2684.63309	-1076.73425	1237.58425	1
6970	N	85.42800	82.11980	74.20990	-285.59101	719.79103	336.17099	1
6971	H	85.59200	81.26780	73.76190	-655.80785	1782.74557	-2507.97937	1
6972	C	84.25200	82.63580	74.59690	748.67870	-449.43296	-262.56661	1
6973	C	84.51500	83.48880	75.69290	567.91079	473.39531	533.69019	1
6974	C	83.41000	84.02980	76.41090	-681.13713	147.45827	588.01299	1
6975	H	83.66700	84.57280	77.30890	-3135.43706	-243.59415	-89.00881	1
6976	C	82.13800	83.76480	75.96090	-655.08090	-465.58235	430.75873	1
6977	H	81.32000	84.18880	76.52390	2399.43516	-859.68149	1844.51993	1
6978	C	82.96000	82.40980	74.11690	-616.67597	-657.02197	139.58467	1
6979	H	82.82800	81.82880	73.21690	3104.40561	-417.61983	294.08451	1
6980	C	81.86200	82.98280	74.83290	-43.05539	653.94095	634.00195	1
6981	H	80.85600	82.74780	74.51690	1531.88442	-1265.78041	2439.13024	1
6982	C	88.03123	85.60355	78.53719	954.07649	-352.42094	-405.71230	1
6983	O	87.39763	86.64195	78.85063	-198.28949	-466.08465	-354.28237	1
6984	N	88.88700	84.89880	79.22090	-38.26233	140.60432	-831.52794	1
6985	H	89.17100	83.95280	79.08290	-2208.21740	-2231.00887	-211.19081	1
6986	C	89.44174	85.43823	80.44629	704.16894	-1753.39508	119.06103	1
6987	H	88.46815	85.73064	80.85129	-3350.48547	-3335.77854	-1374.58969	1
6988	C	90.14400	84.27080	81.25390	380.34768	-503.85067	657.96744	1
6989	H	90.98300	83.74980	80.74590	2224.12780	1539.57874	-1606.60483	1
6990	H	89.46800	83.42280	81.49390	-1277.95220	882.25521	-2736.18167	1
6991	H	90.53800	84.71780	82.19190	-2540.64013	-1854.78556	-56.07572	1
6992	C	90.45716	86.66080	80.09901	-974.45098	-275.31493	705.64910	1
6993	O	90.46544	87.56046	80.90246	-288.35472	-128.83139	286.28041	1
6994	N	91.18512	86.54072	78.96793	726.17878	-193.30812	1118.02558	1
6995	H	91.26586	85.62818	78.53088	2369.72227	1755.95245	-50.39321	1
6996	C	91.93322	87.73976	78.70019	-355.00702	-579.38056	-67.05916	1
6997	H	92.54401	87.96405	79.61294	-770.19043	-845.21914	-1573.74015	1
6998	C	92.90305	87.55792	77.48869	631.91982	437.27099	280.86849	1
6999	H	92.42395	87.23112	76.55419	993.77069	558.23366	295.69066	1

7000	C	93.69180	88.91328	77.43520	7.86219	-345.94779	1089.03858	1
7001	H	94.58281	88.83085	76.70269	-1389.01566	1035.22495	-480.28540	1
7002	H	92.99944	89.69523	76.91508	1084.39961	912.14522	-4150.68521	1
7003	H	94.07746	89.23722	78.38465	4787.34973	-502.42298	-2007.45619	1
7004	C	93.95351	86.38215	77.94881	670.87528	-1364.53411	-872.69131	1
7005	H	94.65986	86.19312	77.16915	-2136.11969	513.10716	1677.02835	1
7006	H	93.34628	85.45166	78.00786	-1077.14090	-1282.19408	652.23034	1
7007	H	94.53339	86.54592	78.92070	3402.48907	-2625.53839	1719.87640	1
7008	C	90.82825	88.98381	78.46753	-282.32372	-1325.56533	-687.66863	1
7009	O	90.94231	90.09939	78.96908	261.34669	-456.25710	-16.66491	1
7010	N	89.97724	88.59401	77.56306	-578.20778	-268.37493	68.16522	1
7011	H	90.04060	87.64830	77.27201	2584.45271	1034.30767	488.82674	1
7012	C	89.01784	89.50622	76.92048	276.17262	-224.26755	448.61941	1
7013	H	89.76203	90.29228	76.57731	-1120.23282	-1912.47483	2365.56709	1
7014	C	88.19893	88.87851	75.76680	94.58798	-319.49767	277.33165	1
7015	H	88.83589	88.27610	75.14022	951.00822	5337.45112	943.96329	1
7016	H	87.43283	88.12724	76.11419	2929.79409	1022.46575	3648.31925	1
7017	C	87.18181	89.75204	74.86791	-139.54104	556.43428	-145.13964	1
7018	O	86.35886	89.13089	74.14209	-276.95099	697.85692	178.13098	1
7019	O	87.41452	90.95244	74.75651	-254.99440	-399.22756	-110.64066	1
7020	C	88.07478	90.24220	78.01335	450.26095	325.90925	-606.51056	1
7021	O	87.61177	91.37393	77.81883	-519.62830	361.79627	-10.84374	1
7022	N	87.72879	89.45092	78.97528	745.91099	1197.36273	-320.49765	1
7023	H	87.89749	88.44956	79.09332	-2508.94819	1697.59413	102.49146	1
7024	C	86.73397	90.04188	79.84305	-13.06120	-751.45210	-187.80049	1
7025	H	86.37848	90.95581	79.23604	-1593.18728	-1179.54139	11.80994	1
7026	C	85.67539	88.87149	79.86831	-41.00614	178.67701	5.57704	1
7027	H	85.79966	88.19377	80.79665	367.27803	1480.99045	-1290.75310	1
7028	H	84.66887	89.22840	79.80762	958.61612	1505.50967	585.91880	1
7029	H	85.72893	88.20758	79.00456	780.84123	1543.23852	-1653.23587	1
7030	C	87.15558	90.29599	81.40365	-782.66126	1353.19841	586.17902	1
7031	O	86.70750	89.84336	82.45710	-807.31535	482.54820	-235.83995	1
7032	N	88.19568	91.11951	81.20058	875.38267	-164.85704	852.27280	1
7033	H	88.46478	91.32374	80.28329	797.57884	-636.15600	-1173.63201	1
7034	C	88.98097	91.61315	82.31940	-488.65770	168.52201	-123.19385	1
7035	H	88.19615	92.12561	83.00876	1200.07286	741.80615	-2691.99824	1
7036	C	89.94785	90.59329	83.06333	-955.91073	-676.14739	156.97695	1
7037	H	89.41905	89.70839	83.48429	-1475.09310	-695.81014	53.33137	1
7038	C	91.21803	90.24960	82.20391	33.87078	274.84894	352.15886	1
7039	H	90.85422	89.46214	81.45525	-223.88277	-991.52962	-1080.66190	1
7040	H	91.75591	91.01073	81.63286	-4978.33390	-658.63158	-556.94486	1
7041	H	92.05528	89.73612	82.84324	-805.32674	226.84703	-2127.52677	1
7042	C	90.47175	91.44757	84.24232	627.48658	-736.60896	904.13333	1
7043	H	89.71474	91.98946	84.79263	-1828.82557	-151.64621	2235.70490	1
7044	H	91.30658	92.16388	83.93564	224.81218	-844.09088	-1037.21856	1
7045	H	90.93956	90.71806	84.95203	-1092.23533	1145.96683	-1012.96400	1
7046	C	89.79832	92.80772	81.55242	-400.88170	87.90720	-251.75240	1
7047	O	89.83218	93.83862	82.18598	-594.58375	764.21476	-778.78882	1
7048	N	90.37811	92.51826	80.36587	350.50317	725.61920	-61.98133	1
7049	H	90.31440	91.53386	79.98922	-5117.72520	547.53876	154.39344	1
7050	C	91.10843	93.55725	79.70993	-759.68117	482.55306	867.76291	1
7051	H	90.90920	94.48201	80.34148	-616.31012	1294.16679	304.30631	1
7052	C	92.62179	93.11454	79.73164	476.26914	-849.08727	29.07737	1
7053	H	92.93434	92.42145	78.90285	-822.33106	1858.38300	2785.53236	1
7054	H	93.23075	93.98387	79.41331	547.36328	1163.96018	-584.35613	1
7055	H	92.99587	92.78236	80.77520	-2790.24250	-1830.52245	-806.05950	1
7056	C	90.40511	93.75919	78.25594	900.06684	577.89223	739.90875	1
7057	O	89.87026	94.83786	77.96059	-235.20281	482.51857	568.61053	1
7058	N	90.69167	92.66454	77.56320	-17.99058	-386.67293	-54.10191	1
7059	H	91.22608	91.77272	77.93641	-2357.12780	-419.24652	-1687.49191	1
7060	C	90.83751	93.00024	76.19024	135.01845	700.84774	159.26595	1
7061	H	89.93460	93.55163	75.79835	-1739.46359	-768.94188	-546.88196	1

7062	C	92.05240	93.98938	76.20159	-50.83490	162.55353	481.76258	1
7063	H	92.19527	94.45748	77.14670	3464.30898	2773.62535	-309.72070	1
7064	H	92.91673	93.23799	76.16203	2876.40784	678.18411	241.89273	1
7065	C	92.13761	95.06878	75.06154	152.35350	475.05424	687.15870	1
7066	O	92.62416	96.17401	75.20182	320.47882	-213.19088	342.64754	1
7067	N	91.64063	94.64519	73.84608	687.54219	-470.92986	638.61838	1
7068	H	91.41947	93.55606	73.63202	-980.92066	-2716.06040	-1597.55991	1
7069	H	92.32170	94.82647	73.10474	210.40255	-2099.41751	-295.07217	1
7070	C	91.19512	91.59282	75.41885	-1249.71286	-85.65245	-844.90149	1
7071	O	92.02166	90.79055	75.79266	-176.22707	134.98767	-207.10670	1
7072	N	90.30609	91.38379	74.40649	32.67651	-108.44679	-164.21383	1
7073	H	89.59608	92.12591	74.32278	-1682.14477	-551.83073	-2226.70481	1
7074	C	90.72641	90.66536	73.27364	-344.33061	731.85074	621.80285	1
7075	H	91.12910	89.70608	73.55154	2441.97650	-1672.08049	-4520.32698	1
7076	C	89.44598	90.57833	72.26851	-260.18203	-238.89347	588.48653	1
7077	H	89.29023	91.63213	72.02506	813.43243	152.87458	-739.69101	1
7078	H	88.55396	90.32948	72.83012	1458.09536	838.36867	2024.84345	1
7079	C	89.50659	89.72312	71.01213	242.27659	-128.67682	-652.20833	1
7080	C	89.93054	90.01349	69.70930	-1015.88793	-492.32286	-45.17147	1
7081	H	90.12185	91.09873	69.35927	508.53396	-208.80160	2626.28292	1
7082	N	90.11058	88.87317	69.03186	596.36469	456.35351	190.07013	1
7083	H	90.60067	88.84017	68.07203	260.56930	220.97247	-806.97652	1
7084	C	89.69569	87.79798	69.68989	137.49391	-804.67939	-642.34934	1
7085	C	89.24112	88.26446	71.02774	497.09816	163.99405	-392.72886	1
7086	C	88.60425	87.41137	71.95712	325.87923	-349.55088	-1339.45653	1
7087	H	88.30737	87.74345	72.90221	2323.24699	-1120.26923	-1535.38582	1
7088	C	88.55754	86.03858	71.59049	640.52581	-257.25948	-925.95502	1
7089	H	88.13293	85.33987	72.23287	-1112.36067	-265.98478	-2492.51271	1
7090	C	89.58564	86.39333	69.32783	-315.47363	859.17666	138.46405	1
7091	H	89.85615	86.01190	68.34053	859.88007	1926.41069	-114.27788	1
7092	C	88.98740	85.61190	70.25405	390.11850	-141.04079	239.40516	1
7093	H	88.91171	84.52831	70.03959	-120.20056	138.61771	3415.06217	1
7094	C	91.81736	91.41358	72.31106	103.12506	438.74499	199.48961	1
7095	O	91.86207	92.64140	72.28489	302.84477	208.96815	27.85096	1
7096	N	92.51369	90.53726	71.64324	619.45866	124.77877	-629.34081	1
7097	H	92.11191	89.62282	71.81170	-1892.87437	419.73913	1575.59632	1
7098	C	93.85079	90.65543	71.22493	-522.49226	-1308.79749	449.81414	1
7099	H	94.06768	91.75682	71.04818	-1306.71997	3362.91619	275.10043	1
7100	C	94.84147	89.92481	72.24851	39.43928	-322.61044	-241.94158	1
7101	H	94.47372	88.94966	72.49483	541.10639	-1546.81659	-1073.90252	1
7102	H	95.85388	89.84846	71.76977	920.68148	1180.80586	-1996.56220	1
7103	C	94.99027	90.72233	73.55495	398.00475	-219.13214	581.26246	1
7104	C	95.44861	90.13231	74.75174	-180.16517	57.64429	127.34446	1
7105	H	95.84234	89.02780	74.81647	-1072.69454	1418.09460	-1343.59347	1
7106	C	95.36712	90.98568	75.89111	173.27812	53.41695	507.34328	1
7107	H	95.71569	90.42986	76.77225	218.24928	-480.88605	2537.27922	1
7108	C	94.98550	92.36689	76.00846	-743.12172	323.26750	167.96630	1
7109	O	95.06039	93.21337	77.10456	798.89706	-614.58254	206.09155	1
7110	H	94.78904	94.10359	76.69290	405.62185	-186.03431	402.65796	1
7111	C	94.54572	92.08417	73.52714	92.55886	-37.51456	-510.45716	1
7112	H	94.18652	92.56427	72.56264	-739.41364	2189.51800	-1619.38819	1
7113	C	94.52360	92.80366	74.73023	1130.89412	78.04030	669.50463	1
7114	H	94.16178	93.87491	74.62944	-1610.70002	-2666.35567	2115.04722	1
7115	C	94.21385	89.74268	69.91787	-182.28808	294.70952	27.57054	1
7116	O	95.32707	89.81373	69.41888	86.89385	295.56373	-322.63191	1
7117	N	93.24297	88.86804	69.48664	256.15042	384.14534	773.21961	1
7118	H	92.51849	89.08494	70.20787	-386.58563	2766.12628	-1702.45917	1
7119	C	93.64238	87.67447	68.90952	-258.75842	490.65468	-453.32392	1
7120	H	94.77743	87.64692	68.99854	-4992.86221	1202.75627	-1356.42151	1
7121	C	93.04868	86.48477	69.83551	322.14261	290.35284	-133.75347	1
7122	H	93.71475	85.63211	69.62643	-2296.41760	-1345.60217	2235.21860	1
7123	H	91.93449	86.31690	69.67076	-1185.05176	1247.93462	-5057.84125	1

7124	C	93.26506	86.75997	71.33885	-326.28923	-164.16469	-304.99796	1
7125	C	94.52898	86.61862	71.97120	-49.87148	-326.34183	158.82286	1
7126	H	95.39864	86.40414	71.32918	2674.02262	1103.67932	-2687.10472	1
7127	C	94.61780	86.82838	73.34250	116.59770	-177.56392	233.86175	1
7128	H	95.55560	86.90042	73.90939	272.34734	2986.29612	711.95105	1
7129	C	93.43222	87.05171	74.13610	404.41422	-498.20982	187.88205	1
7130	H	93.47405	87.20968	75.23887	-991.19322	1308.71575	1003.84738	1
7131	C	92.13783	86.94242	72.13963	-49.77198	68.01547	892.34058	1
7132	H	91.09468	87.03603	71.74048	-2613.14027	1789.07621	1576.94875	1
7133	C	92.17465	87.15074	73.54900	-137.14740	-368.04094	135.37472	1
7134	H	91.25558	87.38938	74.09268	-1930.77592	43.67455	-965.19005	1
7135	C	93.22030	87.53686	67.36226	-119.56760	-369.15644	739.36940	1
7136	O	93.43880	86.53820	66.74236	-302.81490	-154.47395	-344.05981	1
7137	N	92.47744	88.60706	66.92819	-542.67294	-504.60211	-483.94770	1
7138	H	92.65556	89.48748	67.44259	3270.29582	-751.65484	-1519.85715	1
7139	C	92.42033	88.61795	65.42893	-72.69676	-166.46070	510.43035	1
7140	H	93.19900	87.85634	65.10829	1505.25344	-1104.09539	2934.19296	1
7141	H	92.74793	89.63047	65.10771	300.92000	546.37033	2374.45310	1
7142	C	90.91773	88.32649	65.09784	475.12307	637.25428	-94.64185	1
7143	O	89.97444	88.10123	65.84637	471.54403	-69.39737	604.60811	1
7144	N	90.82018	88.49374	63.69221	-275.84776	-81.47426	-365.92513	1
7145	H	91.72683	88.38873	63.31808	1663.08160	356.81262	470.33156	1
7146	C	89.69542	87.89942	63.04437	135.29324	-486.00947	452.74065	1
7147	H	89.08394	88.13273	63.96319	-1090.49678	2301.43610	-1865.75898	1
7148	C	89.27297	88.82224	61.76317	100.09343	527.40829	795.25211	1
7149	H	89.81006	88.45511	60.81036	-2630.86710	746.37737	-1080.81310	1
7150	H	89.62316	89.89904	61.73585	-1625.31863	-1678.83497	724.31273	1
7151	C	87.76444	88.64984	61.41367	-142.88915	312.74836	-1160.50495	1
7152	O	87.25744	89.41400	60.64303	651.61575	230.05688	-69.11906	1
7153	N	87.10318	87.59078	61.97881	68.71661	-159.84505	-51.50833	1
7154	H	87.48476	86.79290	62.43014	-4387.45360	-4299.80407	1281.57143	1
7155	H	86.03289	87.43157	61.98152	-5.85796	-1497.59454	1290.43140	1
7156	C	89.89314	86.32332	62.76301	-291.12393	-632.24397	973.85450	1
7157	O	88.92498	85.61951	62.61893	60.71869	-446.34225	-37.26749	1
7158	N	91.19626	86.05500	62.73912	-402.67347	-799.97036	-441.55472	1
7159	H	91.88549	86.76149	62.73717	-2465.42760	-263.72247	945.80237	1
7160	C	91.51800	84.51480	62.52590	-303.85369	327.99406	-794.69732	1
7161	H	90.87200	84.13680	61.74790	653.10532	1475.78820	-2700.69044	1
7162	C	92.98800	84.28580	62.01190	-238.70131	369.43906	798.74118	1
7163	H	93.08100	84.82880	61.04690	1085.24458	-2922.78161	-421.68479	1
7164	H	93.75600	84.78580	62.63890	1128.55225	-2204.32737	1940.49914	1
7165	C	93.37900	82.83780	61.76390	608.72225	-553.81916	-392.67362	1
7166	C	93.09300	82.24380	60.53090	-468.98586	-656.18359	-425.35439	1
7167	H	92.55800	82.73080	59.72890	-1607.52473	-1776.61513	-2039.05104	1
7168	C	93.42400	80.89180	60.32490	-625.83448	-653.59781	112.21452	1
7169	H	93.07600	80.44380	59.40590	-1045.66976	1143.19553	2738.23026	1
7170	C	94.15700	80.14080	61.27890	579.68301	666.09819	-227.44627	1
7171	H	94.35300	79.09980	61.07090	1124.86553	-373.46759	2914.34825	1
7172	C	94.09900	82.07280	62.66490	462.54836	-777.13699	-116.43932	1
7173	H	94.24300	82.65980	63.55990	-85.87457	-3127.46285	331.40295	1
7174	C	94.50800	80.76380	62.47290	675.66046	106.19139	-603.04007	1
7175	H	94.97700	80.15980	63.23490	1560.44302	-1618.92325	-2200.52978	1
7176	C	91.15900	83.68080	63.73290	-511.73531	21.65640	754.39312	1
7177	O	90.49700	82.62580	63.60990	165.21243	358.61325	-683.90688	1
7178	N	91.54500	84.08880	64.97890	410.80864	-705.33174	215.44300	1
7179	H	92.25500	84.78180	65.07190	2449.11558	-1691.15549	1019.82949	1
7180	C	91.05900	83.46380	66.12890	-632.30974	219.01402	-619.40960	1
7181	H	90.97300	82.39880	65.96990	-1278.42454	-1123.25045	-2646.16049	1
7182	C	91.97900	83.68480	67.32190	679.12662	291.88879	533.89041	1
7183	H	92.00800	84.76880	67.56390	105.77246	2278.40069	2167.00916	1
7184	H	91.54900	83.17080	68.20790	2791.06047	1226.09723	-777.74883	1
7185	C	93.41300	83.09980	67.07090	463.97143	782.73025	59.28629	1

7186	H	93.86800	83.56380	66.16990	36.40771	2133.23610	2312.18607	1
7187	C	94.41000	83.62580	68.14990	-600.67703	-670.61488	-144.61603	1
7188	H	94.13600	83.23380	69.15290	1342.01646	-1105.45353	-2622.05846	1
7189	H	94.50000	84.72780	68.25790	-2084.70444	2346.69202	-212.76793	1
7190	H	95.41400	83.22980	67.88390	-2814.07102	-49.33852	-1405.98586	1
7191	C	93.41700	81.60480	66.91190	-587.30337	-417.38709	558.85040	1
7192	H	92.78300	81.17580	66.10690	69.58549	-2208.91414	2239.21469	1
7193	H	93.12900	81.18280	67.89790	-687.56433	1506.23164	-2675.20985	1
7194	H	94.45700	81.21880	66.84390	-1156.29635	-2827.12469	754.03643	1
7195	C	89.61400	83.83780	66.42890	-551.54040	-574.51235	-444.06052	1
7196	O	88.85000	83.03980	67.01290	275.76398	-630.50100	387.36281	1
7197	N	89.26699	85.06767	65.89515	182.15401	-353.84353	71.71544	1
7198	H	90.03133	85.51605	65.28241	1041.09300	1339.37489	-2235.48960	1
7199	C	87.85405	85.47624	66.17081	-146.33241	246.08806	587.50903	1
7200	H	87.90735	85.59658	67.27633	2523.72919	824.30489	2837.07741	1
7201	C	87.51160	86.95031	65.77138	670.79714	-483.76843	-87.63080	1
7202	H	87.88312	87.16743	64.75435	-3429.05353	-3589.33914	40.37964	1
7203	H	88.12587	87.62734	66.45499	-2446.30051	1868.43414	-622.66488	1
7204	S	85.71903	87.04428	66.05966	173.04040	0.87845	215.15603	1
7205	C	86.67300	84.54580	65.53490	468.55176	-778.06349	-80.79270	1
7206	O	85.70400	84.06480	66.09490	-54.92999	-671.22255	412.39570	1
7207	N	86.85900	84.23180	64.25690	66.16328	-769.66710	340.45157	1
7208	H	87.68800	84.53680	63.79390	-135.63952	1068.33728	-2956.09263	1
7209	C	86.09400	83.32380	63.49490	130.49446	-830.37783	-353.40467	1
7210	H	85.03600	83.53880	63.49790	2368.38846	-1149.97036	-1722.36190	1
7211	C	86.54900	83.31080	62.03090	112.81255	636.57212	-643.03987	1
7212	H	86.13700	82.48080	61.41790	-304.47146	-3122.02448	-241.83976	1
7213	H	87.65600	83.22380	61.99490	2937.06650	-918.11379	654.93028	1
7214	C	86.19500	84.62180	61.36690	-497.36283	-287.74757	-708.01311	1
7215	H	86.41142	85.52573	62.00224	1964.32044	-591.97918	1567.50183	1
7216	H	85.09100	84.55380	61.26190	-2298.96645	-1784.27605	1195.54945	1
7217	C	86.79500	84.65480	59.96290	660.26666	303.50348	-550.80358	1
7218	H	86.34400	83.82380	59.38090	2426.74497	-1992.59634	-196.71027	1
7219	H	87.86800	84.41480	60.12190	-1387.40064	-1541.07747	-2366.09931	1
7220	C	86.49573	86.03755	59.26389	-865.28944	-168.25863	719.34471	1
7221	H	86.74049	86.04727	58.19427	3744.31990	1691.21782	-1462.22169	1
7222	H	87.00491	86.89124	59.76247	980.66461	-2472.76020	-566.20482	1
7223	N	84.97503	86.16868	59.37344	-399.54779	-319.40839	221.82335	1
7224	H	84.55862	86.89386	58.60105	1666.17049	293.58599	349.90022	1
7225	H	84.59159	86.65016	60.27522	-809.83821	-123.80305	-196.37482	1
7226	H	84.40530	85.21527	59.23449	-2785.86651	-503.77552	2214.22902	1
7227	C	86.02200	81.92880	64.05690	-25.20875	-730.95805	544.53269	1
7228	O	84.99900	81.30480	64.09590	-669.60571	-145.24746	392.63036	1
7229	N	87.20100	81.39480	64.42590	664.46358	323.69454	-407.89985	1
7230	H	88.05400	81.83980	64.16690	1874.68390	1570.92865	-1978.88092	1
7231	C	87.36500	80.09380	65.00890	-806.66962	406.06459	-125.88355	1
7232	H	86.88200	79.29380	64.46790	-840.29316	742.92660	-2939.42064	1
7233	C	88.86800	79.76980	65.00690	384.14217	412.45196	716.77694	1
7234	H	89.28500	79.59280	63.99190	242.40516	2840.98077	-1329.77225	1
7235	H	88.98400	78.87080	65.64790	-2622.91723	1509.52797	860.14927	1
7236	H	89.43500	80.62280	65.43790	-671.05250	313.67905	-3057.69852	1
7237	C	86.72700	79.92780	66.35090	447.81818	-666.23100	432.48831	1
7238	O	85.95200	79.01880	66.54290	18.07445	-533.90771	581.58671	1
7239	N	86.90000	80.80780	67.33590	52.24553	-1.42966	-842.57976	1
7240	H	87.40500	81.66380	67.25290	-635.55545	3074.58441	-203.04230	1
7241	C	86.19000	80.52680	68.62890	-45.17959	-746.01266	522.37431	1
7242	H	86.32400	79.48480	68.87990	2489.32848	-1413.08181	-1305.63002	1
7243	C	86.84000	81.26180	69.83390	897.64650	-110.01010	-116.53127	1
7244	H	86.44200	80.90480	70.80790	1408.17935	2475.00587	1337.76048	1
7245	C	88.33400	81.07680	69.72290	-582.43885	632.82097	-302.90858	1
7246	H	88.48300	79.98080	69.82890	-1210.19525	2649.47509	1189.09016	1
7247	H	88.82500	81.27280	68.74590	-2159.66932	-2208.90610	595.64124	1

7248	H	88.77100	81.69980	70.53290	-2075.46351	-2104.57188	1077.70805	1
7249	C	86.58200	82.78080	69.82590	-583.50057	-481.36666	509.17996	1
7250	H	86.96400	83.25980	70.75290	2213.50099	-179.52086	-2228.54478	1
7251	H	85.55100	83.08380	69.54390	624.68477	2755.71629	1383.48217	1
7252	H	87.13100	83.11580	68.91990	-244.60913	3125.03068	-269.39903	1
7253	C	84.70900	80.73080	68.63990	-624.07646	-121.06114	653.70006	1
7254	O	84.02200	80.17280	69.49290	-238.44104	571.68688	489.84406	1
7255	N	84.24600	81.55880	67.65790	-151.63758	-810.04598	183.04056	1
7256	H	84.91200	81.97480	67.04290	1977.50723	1873.26611	1574.34604	1
7257	C	82.80800	81.69580	67.40890	499.75622	-247.95496	721.25797	1
7258	H	82.37200	81.78180	68.39290	-348.33637	-218.96637	-3119.12515	1
7259	C	82.41500	82.92780	66.52990	742.69846	-31.02271	528.09810	1
7260	H	81.41600	82.87480	66.04590	896.14559	-2284.10859	-1969.26312	1
7261	H	83.13300	83.04280	65.69090	-1146.78510	1807.43618	2305.70697	1
7262	N	82.95338	85.43630	67.27554	548.05513	-96.33975	1417.83324	1
7263	H	83.54174	85.72333	66.47539	-217.88683	1816.66167	79.55679	1
7264	C	82.39900	84.15480	67.43290	902.00239	-124.80661	-47.60248	1
7265	C	82.60496	86.32339	68.20354	-727.83993	-105.20763	685.23799	1
7266	H	82.97967	87.30753	68.44535	-1816.83778	3702.77545	-1462.13906	1
7267	N	81.72527	85.69308	69.00202	-110.12599	-414.41266	109.15644	1
7268	C	81.65600	84.41580	68.51590	145.69151	-483.20267	-759.43411	1
7269	H	80.87200	83.84280	68.99590	-3021.51565	347.01583	-805.13936	1
7270	C	82.16700	80.46780	66.77990	725.62175	110.67695	-540.99418	1
7271	O	81.09700	80.01880	67.19390	479.04239	-454.87964	432.70097	1
7272	N	82.89000	79.89280	65.78590	188.12333	734.94736	-370.31646	1
7273	H	83.69400	80.36680	65.43590	1914.81718	-549.16846	2435.18283	1
7274	C	82.59700	78.59880	65.20790	54.12027	769.66613	-485.93832	1
7275	H	81.57800	78.58580	64.84890	-1049.03304	2426.50211	1705.82632	1
7276	C	83.57500	78.33080	64.01290	596.97102	-687.01777	55.52647	1
7277	H	84.59400	78.72480	64.21390	-496.89337	2038.51344	-2344.30931	1
7278	C	83.59900	76.78780	63.77490	232.22169	-880.38005	-49.54850	1
7279	H	84.31500	76.28780	64.46290	246.70180	201.97220	-3129.94755	1
7280	H	83.98300	76.51480	62.76890	-2337.88053	281.78683	2086.41728	1
7281	H	82.64600	76.27180	64.01990	-2667.66253	262.47740	-1647.09090	1
7282	C	83.00400	79.04680	62.75690	-678.67608	258.77949	551.25580	1
7283	H	81.91100	78.88580	62.63890	3119.82534	-308.84410	-263.68804	1
7284	H	83.47200	78.73680	61.79890	-191.64151	3022.17448	-853.20641	1
7285	H	83.14800	80.14080	62.88390	1772.08540	-2410.22431	-974.04228	1
7286	C	82.54300	77.54080	66.30590	-631.12913	145.22344	641.90122	1
7287	O	81.51500	76.91780	66.54690	-130.07486	580.52320	519.32704	1
7288	N	83.59100	77.46180	67.16990	126.88737	-117.38196	826.31311	1
7289	H	84.39600	78.01380	66.96890	1956.94730	-1116.92560	-2195.69140	1
7290	C	83.61000	76.47880	68.21290	172.84335	-885.22278	-134.00303	1
7291	H	83.48300	75.48980	67.79590	2001.37120	-2191.18902	-1044.71538	1
7292	C	85.03500	76.38780	68.80890	-548.43571	-706.59961	-177.16170	1
7293	H	85.44800	77.41780	68.87090	-1703.84352	1680.71119	2042.14431	1
7294	C	85.07400	75.72080	70.18590	-539.66435	-539.81379	498.81306	1
7295	H	86.10000	75.62280	70.60190	-2611.82489	1740.15603	-220.12259	1
7296	H	84.55100	76.30080	70.97590	-496.85295	-1171.17159	2877.45034	1
7297	H	84.66100	74.69080	70.12890	2368.40023	-2056.67944	242.85024	1
7298	C	85.97700	75.72480	67.76590	-89.73891	-245.42260	873.59354	1
7299	H	85.69100	74.65480	67.67490	-1508.14052	2268.84120	-1573.56220	1
7300	H	85.74100	76.16480	66.77290	1471.34731	1867.64784	2060.40163	1
7301	C	87.47200	75.97180	67.95890	398.49030	399.48319	716.28881	1
7302	H	88.05300	75.45780	67.16290	1584.70168	-2599.63602	-792.99393	1
7303	H	87.73000	75.66880	68.99590	1408.83570	-3.37167	2813.07605	1
7304	H	87.69600	77.04780	67.79490	1761.32265	-1730.37664	-1949.81164	1
7305	C	82.51700	76.61280	69.28290	-612.13101	80.81315	-670.98127	1
7306	O	81.96700	75.61980	69.76790	-700.48536	235.55583	278.31806	1
7307	N	82.13600	77.82380	69.67790	-397.17551	-497.81979	554.16546	1
7308	H	82.59400	78.62980	69.31090	651.88955	2517.34254	1770.94686	1
7309	C	81.05000	78.07380	70.56590	654.19916	-590.42628	-234.24616	1

7310	H	81.27600	77.50580	71.45590	-377.49390	-3116.51217	-207.54877	1
7311	C	81.05200	79.58980	71.00790	-114.37893	862.88896	271.64518	1
7312	H	80.98000	80.15680	70.05590	943.25906	-572.63602	-2946.28182	1
7313	H	82.02300	79.80180	71.50490	-1748.26127	656.72251	-2531.90132	1
7314	C	79.92200	80.03280	71.97990	452.51212	528.19214	589.65825	1
7315	C	79.38500	79.12780	72.88490	754.59482	199.91169	-471.24620	1
7316	H	79.82100	78.13980	72.84190	2344.68839	-2090.15074	178.69654	1
7317	C	78.46300	79.55580	73.85390	-193.29632	798.69741	-395.18348	1
7318	H	78.13700	78.88380	74.63390	509.82928	2843.38580	1246.37776	1
7319	C	77.98700	80.85580	73.88990	709.78619	190.32186	-539.84457	1
7320	O	76.96700	81.12580	74.81990	334.16104	-638.41461	-323.09504	1
7321	H	77.08100	82.02380	75.14090	1606.67949	-1710.99670	2095.06505	1
7322	C	79.47200	81.38480	72.01490	-504.04825	738.87999	177.32097	1
7323	H	79.94600	82.09480	71.35290	2005.67626	-799.99938	2288.11931	1
7324	C	78.48900	81.79280	72.93090	691.47901	405.71107	-434.40339	1
7325	H	78.06400	82.77980	73.03490	51.16103	757.40718	-3053.18574	1
7326	C	79.67300	77.54080	70.07190	-591.54483	-271.63962	-638.54337	1
7327	O	78.96500	76.79380	70.76590	480.63820	-472.80926	-411.17582	1
7328	N	79.39400	77.68380	68.75890	-742.13666	-402.33044	5.97397	1
7329	H	79.95300	78.19680	68.11190	-1152.78188	-985.56835	2756.44249	1
7330	C	78.20500	77.02080	68.19390	61.86485	795.84696	440.73955	1
7331	H	77.43900	76.92980	68.94890	2957.23336	311.72141	1027.53435	1
7332	C	77.48800	77.80880	67.07390	365.22154	-641.60525	-535.17000	1
7333	H	76.97700	77.12180	66.36490	1489.23193	-2376.00632	1426.53721	1
7334	O	78.48200	78.54080	66.33890	-429.72842	-403.07271	-525.82612	1
7335	H	77.96600	79.06380	65.71990	-574.08783	2164.89805	2209.49448	1
7336	C	76.51200	78.84980	67.67590	697.50266	558.61072	181.37007	1
7337	H	76.14500	79.53180	66.87990	2249.53106	-1717.20658	-1374.42272	1
7338	H	77.06600	79.47580	68.40790	2634.55936	-1601.01892	627.74326	1
7339	H	75.64300	78.39980	68.20290	-713.51949	1849.88532	2442.75264	1
7340	C	78.36700	75.56380	67.75190	-7.02825	-797.23219	442.51829	1
7341	O	77.49200	74.70580	67.73790	240.06474	726.04181	-197.12798	1
7342	N	79.64800	75.13880	67.41590	-408.58583	723.26836	150.37549	1
7343	H	80.37000	75.81880	67.31490	490.41974	-2731.32403	-1482.42496	1
7344	C	79.99100	73.68980	67.21490	96.94854	903.87318	-71.17058	1
7345	H	79.38000	73.32380	66.40290	1636.03180	79.93332	2686.11929	1
7346	C	81.38900	73.44280	66.61790	753.31258	-143.30555	493.39100	1
7347	H	82.10200	74.18380	67.03690	1.26167	-3129.15480	326.51929	1
7348	C	81.96200	72.04380	66.97190	590.03942	163.45730	675.71162	1
7349	H	82.88300	71.83080	66.38890	1734.49980	-1908.04658	-1802.52460	1
7350	H	81.18600	71.31880	66.64490	2503.40734	-883.74296	-1688.24652	1
7351	H	82.34400	71.99180	68.01390	424.99352	-1858.61728	-2502.62833	1
7352	C	81.32400	73.80080	65.10990	471.76441	434.85651	647.91139	1
7353	H	80.97800	74.84980	64.98990	2747.00389	-1517.00860	-225.56764	1
7354	H	82.37400	73.66580	64.77390	-1751.98534	1436.13269	-2183.18495	1
7355	H	80.63300	73.08980	64.60990	682.85022	-2983.27233	729.40251	1
7356	C	79.75400	72.79980	68.47990	-611.60228	619.69360	-270.87543	1
7357	O	79.20000	71.70380	68.33390	539.82664	389.62199	424.74596	1
7358	N	80.08100	73.22380	69.70090	180.51449	-501.80127	654.43280	1
7359	H	80.50800	74.12280	69.76890	-623.22305	-2689.20612	-1509.30106	1
7360	C	79.61600	72.58280	70.91190	-758.21121	77.84343	-500.50691	1
7361	H	79.83700	71.53080	70.80090	-2388.70021	-667.93170	1935.51150	1
7362	C	80.32000	73.15880	72.15090	173.62257	886.27264	125.80548	1
7363	H	80.52000	74.24680	72.04990	-487.35254	2917.52556	-1071.80145	1
7364	H	81.33400	72.70680	72.18690	-1942.63109	-1104.31059	-2214.70287	1
7365	C	79.57500	73.06880	73.50490	0.53602	-710.39638	571.65348	1
7366	O	78.59100	73.73680	73.79790	503.15830	-70.38296	-604.57025	1
7367	N	80.05400	72.13480	74.36090	397.13462	-702.76268	247.14571	1
7368	H	80.91400	71.64380	74.22290	2443.43042	1919.69813	-492.57803	1
7369	H	79.62900	72.06180	75.26290	-1603.97196	-1825.56446	1998.20284	1
7370	C	78.06400	72.62880	71.06090	-123.19949	902.26504	-46.80486	1
7371	O	77.44500	71.63380	71.38190	-387.17212	282.86592	627.46462	1

7372	N	77.42000	73.74480	70.75490	-507.13097	-667.59190	-99.05314	1
7373	H	77.98600	74.52280	70.49790	-2034.56775	-2307.93209	657.42663	1
7374	C	76.00300	73.97580	70.88590	-846.11252	99.95548	-324.88999	1
7375	H	75.75900	73.92180	71.93690	1782.92205	-2460.45939	815.81541	1
7376	C	75.56400	75.38480	70.54190	-253.18701	-871.19825	91.43828	1
7377	H	75.41200	75.53680	69.45190	2147.36810	1424.51941	1804.93239	1
7378	H	76.35700	76.10880	70.82590	2127.62731	-2289.29574	-361.32158	1
7379	C	74.25900	75.91580	71.28290	-525.10873	544.33656	509.32263	1
7380	H	73.50300	75.10180	71.26190	-1666.29387	-2300.37864	1352.75610	1
7381	C	74.54200	76.24980	72.74990	-617.90918	-485.30478	462.72943	1
7382	H	74.82100	75.38380	73.38690	-351.36839	2865.56617	-1250.31876	1
7383	H	73.69400	76.78080	73.23390	-1920.77585	2242.40229	1086.49821	1
7384	H	75.40100	76.95280	72.71390	-589.63127	-2948.43239	925.90908	1
7385	C	73.71700	77.15380	70.58690	-87.72335	480.98790	769.67932	1
7386	H	72.74800	77.35680	71.09090	-1276.29460	2225.82568	1820.71370	1
7387	H	73.66100	76.90080	69.50690	-2203.76964	934.25333	2041.76304	1
7388	H	74.31300	78.05480	70.84590	-1234.75030	-2563.91468	1341.62567	1
7389	C	75.09600	73.04480	70.08690	-823.19531	386.69312	-65.33692	1
7390	O	74.19500	72.43780	70.57690	526.45364	454.78628	-373.68869	1
7391	N	75.58000	72.79280	68.84390	443.93448	-712.83705	-86.35858	1
7392	H	76.37800	73.29880	68.52390	601.87010	1445.94777	-2728.59188	1
7393	C	75.03800	71.79380	67.92590	40.82754	-550.16236	-726.02031	1
7394	H	73.97500	71.68380	68.08490	-943.64116	2265.16292	1968.96027	1
7395	C	75.21300	72.27780	66.44590	0.42648	-911.21787	-33.65742	1
7396	H	74.68000	71.57580	65.76990	-390.88671	2219.09751	2195.68669	1
7397	H	76.30400	72.25780	66.23490	1252.60414	1664.08903	-2357.96879	1
7398	C	74.58800	73.64280	66.30190	26.48589	860.96915	299.13478	1
7399	C	73.40500	74.05580	66.90090	-621.48891	167.06086	-645.98236	1
7400	H	72.87400	73.31580	67.48090	2145.74123	2086.75121	-969.27303	1
7401	C	72.89700	75.36980	66.79290	-857.74780	244.13350	-190.04880	1
7402	H	72.03100	75.61380	67.39190	1603.14685	2173.95579	1613.09101	1
7403	C	73.59500	76.30480	66.07290	-539.21799	452.23959	-579.80541	1
7404	O	73.11000	77.58880	66.04690	460.31102	-255.30135	588.69535	1
7405	H	73.77800	78.08480	65.56790	2107.07791	-2267.33556	563.59415	1
7406	C	75.25300	74.59480	65.48390	-684.91077	80.98427	-596.48118	1
7407	H	76.17700	74.26580	65.03190	52.89202	-2929.72220	1145.49398	1
7408	C	74.76400	75.91180	65.39090	335.61882	465.96907	708.29643	1
7409	H	75.26000	76.67480	64.80990	2047.39318	-735.56354	-2272.74144	1
7410	C	75.55000	70.36280	68.08790	-730.70072	225.96520	-496.45462	1
7411	O	74.98700	69.48580	67.47890	492.52319	-467.35595	-403.26983	1
7412	N	76.64500	70.10980	68.85690	332.02813	-574.83824	-521.52719	1
7413	H	77.20900	70.81580	69.27890	-332.30311	-1613.18258	2680.56763	1
7414	C	77.21400	68.74780	68.93090	-683.50515	-67.23577	-599.79252	1
7415	H	76.76200	68.11280	68.18290	-2599.98571	1610.27686	738.45040	1
7416	C	78.76800	68.59680	68.72990	603.28981	448.25783	516.29190	1
7417	H	78.91700	68.76980	67.64290	2145.86021	-2299.79467	66.74314	1
7418	H	79.12100	67.55780	68.90390	-2639.78228	-698.79261	1562.51867	1
7419	O	79.43400	69.45380	69.61290	760.86385	211.04121	13.23026	1
7420	H	79.36600	70.29480	69.15390	-3047.61140	-664.88082	410.15176	1
7421	C	76.83600	68.12980	70.21990	505.51926	593.75309	-472.60824	1
7422	O	76.31600	67.01880	70.22490	-305.41886	529.60808	-499.86181	1
7423	N	76.90800	68.88580	71.39690	82.91860	470.09816	-696.27905	1
7424	H	77.09200	69.86380	71.34290	-1866.32202	2134.50234	1363.43982	1
7425	C	76.65900	68.29280	72.72790	499.97309	463.04944	-605.85735	1
7426	H	77.37300	67.49480	72.86990	-351.75708	-47.79780	-3126.05319	1
7427	C	76.99100	69.27280	73.89690	725.69444	72.90043	-547.26969	1
7428	H	78.08900	69.43780	73.90890	367.04990	3123.02768	-100.98865	1
7429	H	76.72300	68.86880	74.89590	2930.09636	78.26983	1143.08153	1
7430	O	76.37400	70.60180	73.75590	279.79270	520.02189	-524.32862	1
7431	H	76.99100	71.20580	73.33690	534.48385	2596.34613	-1694.56189	1
7432	C	75.22200	67.71180	72.98090	202.29665	-549.82311	698.72857	1
7433	O	75.04700	66.54180	73.22690	544.77936	-309.00250	-480.99910	1

7434	N	74.23400	68.54880	72.77190	-752.15878	-381.67568	-35.39965	1
7435	H	74.49300	69.49780	72.60890	1268.04132	2607.15182	1221.90704	1
7436	C	72.81700	68.20780	72.84690	710.04538	-428.18661	-379.39792	1
7437	H	72.69700	67.79180	73.83690	-686.59231	-1500.55204	-2678.64907	1
7438	C	71.92400	69.42580	72.75590	209.06955	-36.19039	886.80955	1
7439	H	72.28100	70.22380	73.44090	-2085.32984	2284.08993	576.67919	1
7440	C	71.88500	70.06880	71.32090	499.76581	-492.78721	-582.10471	1
7441	H	72.95400	70.30580	71.12690	2779.33005	739.84867	1275.21553	1
7442	H	71.46800	69.35080	70.58190	1524.64378	-1888.52651	-2001.78800	1
7443	H	71.31100	71.01980	71.33190	2637.64247	-1630.49978	-531.54386	1
7444	C	70.59100	69.04780	73.37790	-372.81460	-735.77503	388.70989	1
7445	H	69.91400	69.92780	73.42990	1625.06971	2261.93045	1463.23112	1
7446	H	70.01500	68.20180	72.94690	-864.21140	-2007.22371	2263.27592	1
7447	H	70.85600	68.68180	74.39290	-469.47901	2020.33590	2365.59898	1
7448	C	72.36900	67.11980	71.85690	629.43342	358.41755	-553.89659	1
7449	O	71.52900	66.26080	72.13090	-589.69875	363.08965	-379.53724	1
7450	N	72.91100	67.09180	70.61690	-449.40910	168.04409	-694.59696	1
7451	H	73.50900	67.85780	70.39290	1964.75811	-654.85447	-2368.35754	1
7452	C	72.45400	66.06380	69.71790	468.66728	-462.33048	630.91402	1
7453	H	71.39000	65.90280	69.80790	2191.61940	1245.69789	-1882.35688	1
7454	C	72.66000	66.54280	68.23090	-170.29364	-613.54213	652.69988	1
7455	H	72.52100	65.61380	67.63890	-2061.86786	-957.50340	2174.88261	1
7456	H	73.68700	66.96680	68.24990	2005.53283	408.55536	-2389.38210	1
7457	C	71.72500	67.59780	67.72090	128.59630	-727.81848	534.03582	1
7458	C	71.74100	68.95780	67.92090	894.52228	-29.63960	174.36279	1
7459	H	72.58600	69.44280	68.38690	2030.21511	2058.12856	1241.19285	1
7460	N	70.70500	69.55680	67.31790	727.30233	420.89478	-80.93944	1
7461	H	70.35400	70.42880	67.57890	-1973.75192	-1651.95424	1809.30284	1
7462	C	69.94900	68.58180	66.73890	243.32934	-63.35365	-876.48625	1
7463	C	70.55000	67.30580	66.99790	-190.94289	172.77976	874.72223	1
7464	C	69.90800	66.17080	66.61990	-93.85484	-660.48461	621.61271	1
7465	H	70.39900	65.26380	66.93990	2048.96375	-2016.74493	1277.77684	1
7466	C	68.76100	66.27480	65.85090	-377.12460	-617.76491	554.61208	1
7467	H	68.26800	65.37480	65.51390	1730.73166	-2328.72526	1216.48379	1
7468	C	68.83000	68.69180	65.97190	730.54797	-304.43379	-452.84736	1
7469	H	68.33200	69.62280	65.74690	-2320.43694	1339.02085	1649.49137	1
7470	C	68.20200	67.49880	65.54590	-244.50619	-641.80439	599.79567	1
7471	H	67.29300	67.52580	64.96390	-1265.65520	2117.35612	-1952.72789	1
7472	C	73.19300	64.74780	69.88990	-482.85355	-411.10843	-655.20478	1
7473	O	72.67800	63.69780	69.58190	-227.20677	516.73750	-552.25598	1
7474	N	74.40600	64.73880	70.51790	306.62036	443.17883	-649.80671	1
7475	H	74.96100	65.55880	70.63090	541.35490	-2263.20012	-2117.33000	1
7476	C	74.94700	63.53980	71.09390	211.47599	668.35783	583.11810	1
7477	H	75.05800	62.74180	70.37490	1193.44186	-1526.63374	2478.57059	1
7478	C	76.44200	63.74480	71.56290	-164.41428	-877.45988	-185.69629	1
7479	H	76.37000	64.76080	72.00790	-1630.38460	2144.49160	1625.18554	1
7480	C	76.85300	62.73380	72.62490	-608.62513	-648.12263	202.39444	1
7481	H	77.96400	62.74180	72.63890	2696.28003	-1620.77259	-37.36905	1
7482	H	76.59800	61.68380	72.36590	1179.64944	2730.85172	1024.25695	1
7483	H	76.41300	62.97180	73.61690	-1478.26273	1604.74732	-2266.66089	1
7484	C	77.39100	63.63880	70.36590	8.20750	265.60563	872.25987	1
7485	H	76.79400	64.06380	69.53090	462.68468	-2934.50414	-1035.77727	1
7486	H	77.58600	62.57880	70.09590	-1516.21961	1468.85257	2332.76155	1
7487	C	78.55700	64.57680	70.48490	839.58786	-355.09175	-21.28559	1
7488	H	79.21500	64.35480	71.35190	-436.62506	-2985.91408	-889.88870	1
7489	H	78.21700	65.63480	70.49190	2176.02064	-1949.66633	1167.03110	1
7490	H	79.23400	64.48180	69.60890	-331.58476	2196.46751	2227.96055	1
7491	C	74.09700	62.96180	72.24090	649.57505	638.24844	46.28366	1
7492	O	73.82900	61.77480	72.30290	-138.42758	177.31496	-756.98378	1
7493	N	73.51000	63.84680	73.06590	356.39596	-536.86647	545.37015	1
7494	H	73.79600	64.80180	73.04790	604.44629	2816.39918	1265.21403	1
7495	C	72.53000	63.56280	74.09690	-367.57465	819.53089	157.19097	1

7496	H	72.92800	62.80480	74.75590	-2230.80755	-2203.91626	-253.92325	1
7497	C	72.31300	64.68880	75.09590	-713.56169	533.97940	-192.73483	1
7498	H	71.43000	64.41080	75.70990	737.94673	-1447.00282	2694.40971	1
7499	H	71.98400	65.56780	74.50090	988.30864	-2623.77034	1427.34070	1
7500	C	73.46500	64.97780	76.06990	315.59796	810.29507	-274.35532	1
7501	H	74.37300	65.14780	75.45290	-1407.76648	-148.86095	2809.67261	1
7502	C	73.19900	66.08480	77.11390	-686.19111	-497.15689	-336.79043	1
7503	H	74.07700	66.31080	77.75590	175.12160	-2544.02273	-1842.69015	1
7504	H	72.87400	67.00380	76.57990	-2609.81228	-1501.90045	911.81200	1
7505	H	72.38300	65.70780	77.76590	1615.89084	-2455.22836	-1122.04132	1
7506	C	73.79100	63.67480	76.88490	651.44052	173.93095	-613.86015	1
7507	H	74.66400	63.90280	77.53190	1930.19295	-2010.98147	1458.94995	1
7508	H	72.87900	63.35080	77.43090	-537.77902	2884.37451	1135.51911	1
7509	H	74.16100	62.87780	76.20390	843.70987	-2804.94804	-1148.32328	1
7510	C	71.22700	62.91880	73.51690	187.75238	-389.88903	-802.61235	1
7511	O	70.71800	61.98380	74.14690	577.28224	-43.37584	537.11357	1
7512	N	70.70300	63.40180	72.34790	128.20291	632.22047	544.54896	1
7513	H	71.10300	64.26580	72.05290	186.89101	98.28880	-3139.05038	1
7514	C	69.73400	62.58180	71.58590	654.06218	-578.57456	-262.49789	1
7515	H	68.87900	62.38480	72.21590	1298.20440	-2813.05665	-547.36078	1
7516	C	69.26800	63.38280	70.33890	-409.82423	454.41187	676.02141	1
7517	H	68.28800	62.96680	70.02090	2106.20782	-2278.35270	520.79157	1
7518	H	69.96100	63.29480	69.47590	-2163.36909	25.16517	-2284.16881	1
7519	H	69.03900	64.45180	70.53990	1007.43167	948.51124	-2825.53253	1
7520	C	70.21000	61.21680	71.12590	491.19168	598.24155	-481.96346	1
7521	O	69.50700	60.27980	71.39790	-532.73410	-403.46037	-420.76280	1
7522	N	71.39700	61.10080	70.48690	-225.28400	-777.07639	240.98069	1
7523	H	71.96500	61.91780	70.43290	2166.94562	691.93797	-2173.42926	1
7524	C	71.91600	59.80780	70.10590	-126.00536	575.75589	695.75772	1
7525	H	71.21400	59.26580	69.48990	-690.27769	-1789.79050	-2493.67057	1
7526	C	73.26300	60.01580	69.27590	224.21008	184.41705	-864.39065	1
7527	H	73.86400	59.08180	69.30890	-1619.40231	-2123.66932	-1663.06675	1
7528	H	73.85400	60.81780	69.76790	1913.52656	-1741.36255	-1790.05552	1
7529	C	73.07700	60.37180	67.86290	-622.17021	-263.70164	612.22274	1
7530	C	71.99300	61.12680	67.38390	-153.95335	-692.81968	-572.49477	1
7531	H	71.19200	61.52980	67.98490	-1051.61428	-1867.79130	2302.97401	1
7532	C	71.80300	61.37380	66.02090	-108.51949	-460.74910	-779.34895	1
7533	H	70.93800	61.91180	65.66190	-2696.83752	568.12273	-1517.40904	1
7534	C	72.70500	60.88880	65.10690	558.68542	-586.75041	418.38447	1
7535	H	72.48900	61.01780	64.05590	-1393.58512	1798.98202	-2172.51247	1
7536	C	73.97600	59.87980	66.90290	-668.38031	-292.36310	-547.03070	1
7537	H	74.74700	59.17780	67.18090	-519.74511	-1949.36202	-2414.14145	1
7538	C	73.75000	60.08480	65.52790	345.24016	-765.15780	356.08113	1
7539	H	74.35200	59.44180	64.90390	1616.51876	-2429.04107	1176.79770	1
7540	C	72.12500	58.72180	71.18490	-303.75585	855.95742	-80.74823	1
7541	O	71.74000	57.56280	70.96290	-445.51117	517.35292	-396.85386	1
7542	N	72.61100	59.07480	72.37390	624.43315	-41.74067	566.58030	1
7543	H	72.89000	60.02280	72.50490	-2034.23856	-302.64010	-2380.86301	1
7544	C	72.68100	58.14080	73.49390	713.61045	-433.99477	365.86837	1
7545	H	73.09600	57.19180	73.18990	-1633.72734	654.31360	-2607.87939	1
7546	C	73.64600	58.74880	74.51190	260.21211	-18.29780	873.73100	1
7547	H	74.62300	58.87080	73.99490	-2067.64718	-1943.85280	-1358.12284	1
7548	C	73.16700	60.07580	75.15390	440.04924	-542.59235	-586.00444	1
7549	H	72.36900	59.90880	75.90790	-1735.24072	-1838.97854	-1872.25100	1
7550	H	72.74200	60.71680	74.35090	2076.29169	1145.42748	-2067.66413	1
7551	H	73.98700	60.55380	75.73090	61.29541	-2003.23385	-2425.18520	1
7552	C	74.00800	57.66680	75.58290	-407.78799	564.90514	-588.25347	1
7553	H	74.22300	56.72280	75.03790	-1794.03469	1567.45159	-2054.93583	1
7554	H	73.10600	57.48480	76.20490	-1525.73716	1839.86572	-2045.78750	1
7555	C	75.17000	58.18180	76.40990	765.16157	229.69992	-439.56423	1
7556	H	76.07100	58.47080	75.82890	2386.89484	-203.53102	2039.49366	1
7557	H	74.83000	59.07680	76.97390	-1837.93490	2218.18707	-1264.85874	1

7558	H	75.49500	57.43180	77.16290	2558.80596	729.98521	1678.64822	1
7559	C	71.27200	57.86480	74.12990	-473.64884	546.29694	-555.57847	1
7560	O	71.00500	56.75880	74.66690	-269.51525	338.64344	660.53719	1
7561	N	70.33700	58.79980	73.99790	646.29447	534.45494	96.61090	1
7562	H	70.55600	59.61580	73.46790	781.07339	-2098.00231	-2210.55127	1
7563	C	68.93700	58.59380	74.35490	593.35796	568.41995	-395.31771	1
7564	H	68.88800	58.26980	75.38390	207.37911	2077.34144	-2353.69341	1
7565	C	68.03700	59.88580	74.21290	-217.45794	-817.13132	341.26157	1
7566	H	66.94500	59.71580	74.32590	-659.08708	-2535.99944	1741.41819	1
7567	H	68.26200	60.32580	73.21790	-1033.35935	-2156.23168	-2044.76396	1
7568	O	68.38100	60.83480	75.21390	-253.99409	745.99177	51.09315	1
7569	H	69.14200	61.29780	74.85590	803.33209	3021.09575	-354.77355	1
7570	C	68.26600	57.55280	73.49690	-30.08678	-625.98435	-662.33630	1
7571	O	67.62400	56.66180	74.00890	-147.26451	764.27598	-133.50141	1
7572	N	68.41900	57.71580	72.14690	-287.87827	-29.02419	-793.06745	1
7573	H	68.91000	58.48880	71.75390	1145.58148	-2423.08517	1647.58234	1
7574	C	68.00800	56.73880	71.10290	159.68382	-403.84943	-801.78409	1
7575	H	66.93000	56.69380	71.05990	-2629.37076	1715.92865	-200.56050	1
7576	C	68.42200	57.32980	69.74790	-560.24413	-688.18695	-209.70514	1
7577	H	68.40100	56.60980	68.90190	705.45967	2170.66254	-2165.35841	1
7578	H	69.46400	57.71380	69.75790	-2176.69301	979.14654	2049.75751	1
7579	C	67.53700	58.48480	69.21390	-503.21823	77.51028	756.44866	1
7580	H	67.35400	59.16180	70.07590	1502.90016	-2763.10212	69.16678	1
7581	C	68.30300	59.44180	68.21290	-889.39703	87.46079	-181.03738	1
7582	H	67.50000	60.12880	67.86990	-467.28716	2715.87637	-1517.85523	1
7583	H	68.58400	58.83980	67.32290	3139.17701	-199.59344	-62.89984	1
7584	H	69.13000	60.00380	68.69590	-2149.99199	625.97437	-2209.95854	1
7585	C	66.27600	58.00980	68.50990	-855.61590	268.32927	-165.44437	1
7586	H	66.46300	57.26280	67.70990	-2981.96851	-570.26593	825.15865	1
7587	H	65.65900	58.82780	68.07890	802.82144	-1280.83377	-2759.19713	1
7588	H	65.59800	57.65380	69.31590	1210.31431	2486.21506	-1500.69990	1
7589	C	68.65300	55.42080	71.41890	391.22034	-381.16090	-730.14657	1
7590	O	67.96100	54.39280	71.36790	455.71177	545.16498	-344.59999	1
7591	N	69.99700	55.34680	71.65690	351.48327	563.15960	521.51995	1
7592	H	70.50300	56.19780	71.54090	-1979.51661	-2341.54775	704.90735	1
7593	C	70.66600	54.11680	71.95390	435.66842	173.61348	-781.98618	1
7594	H	70.37400	53.43580	71.16790	863.62376	2358.74427	-1894.38795	1
7595	C	72.21100	54.42880	71.99990	391.20592	677.24236	-468.77683	1
7596	H	72.41300	55.16980	72.80390	351.82945	-486.90668	-3088.26232	1
7597	H	72.52700	54.79380	70.99990	-2874.21529	-490.39723	-1181.78815	1
7598	C	72.99600	53.16680	72.28990	-158.05239	897.39430	33.96919	1
7599	O	73.09800	52.74080	73.45190	-319.86522	-36.92665	721.07551	1
7600	O	73.42800	52.48280	71.30890	21.67933	-572.38710	543.62693	1
7601	C	70.16900	53.41580	73.19190	746.88087	11.67975	522.95655	1
7602	O	70.09800	52.19680	73.28190	-322.11435	-301.26398	655.06457	1
7603	N	69.80300	54.19280	74.24790	-534.60853	-443.75660	479.52694	1
7604	H	69.85400	55.18780	74.23790	-98.47031	2179.77530	2266.51924	1
7605	C	69.17300	53.66180	75.45390	489.20023	634.45007	435.43913	1
7606	H	69.73600	52.83980	75.86990	-2529.30393	-1780.19729	-575.97347	1
7607	C	69.09800	54.71380	76.61790	-508.57795	603.74851	-456.38494	1
7608	H	69.19700	55.75280	76.23590	-2706.36543	520.13211	-1517.65444	1
7609	H	68.12200	54.60580	77.13890	1669.27123	1344.82401	-2302.86955	1
7610	C	70.26100	54.47080	77.66490	628.80261	-236.01511	616.72940	1
7611	H	70.11000	55.20080	78.48890	-1946.14455	1913.91686	1564.50308	1
7612	H	70.18700	53.40880	77.98390	-1769.25170	-2205.48983	1379.77870	1
7613	C	71.68300	54.73580	77.10590	323.18171	728.31266	443.35680	1
7614	H	72.30700	54.92680	78.00490	1725.79829	1879.44631	1840.52385	1
7615	H	71.52300	55.67780	76.53890	1230.80889	-706.21838	2807.95144	1
7616	N	72.29500	53.58780	76.26790	-646.18371	-481.90583	250.77015	1
7617	H	72.33300	53.71780	75.27790	-2297.33232	1210.76458	-1776.10235	1
7618	C	72.51900	52.36480	76.67390	661.82706	237.93006	580.36647	1
7619	N	72.45100	51.90980	77.92390	523.04594	587.03562	307.38317	1

7620	H	72.43900	52.51280	78.72190	-1787.39077	2469.37472	778.23451	1
7621	H	72.53400	50.92280	78.06190	619.34052	36.08832	3084.37047	1
7622	N	72.86300	51.48580	75.77490	-499.76751	365.50436	573.85650	1
7623	H	72.93300	51.87680	74.85690	428.56464	-2759.31526	-1449.39224	1
7624	H	73.24600	50.61580	76.08390	2888.30830	25.41442	-1247.09883	1
7625	C	67.78400	53.02580	75.23090	419.40290	-701.88434	403.62183	1
7626	O	67.57600	51.90080	75.66890	739.58384	-7.74335	-276.73636	1
7627	N	66.94800	53.66880	74.42790	272.18759	-526.80115	-600.88830	1
7628	H	67.26800	54.51680	74.01190	-114.68577	570.29813	3091.89803	1
7629	C	65.70600	53.17180	73.94890	802.44318	-342.17193	-265.43233	1
7630	H	65.24000	52.91680	74.88890	-773.61628	2935.24407	827.09510	1
7631	C	65.01600	54.39180	73.21590	-514.19369	-573.38898	-488.14028	1
7632	H	65.75700	55.08780	72.76690	586.04189	-1171.70827	-2860.39872	1
7633	H	64.48300	54.96280	74.00590	-1918.41273	-1950.05892	-1554.08784	1
7634	C	63.96000	54.00580	72.20890	589.46538	-651.03714	-245.21870	1
7635	C	62.81500	53.27380	72.56890	82.15858	-902.01760	105.19132	1
7636	H	62.64500	52.99980	73.59990	-1367.78945	-1996.15587	2010.65660	1
7637	C	61.86200	53.00680	71.55590	-399.62295	295.36783	764.53276	1
7638	H	60.98800	52.51080	71.95090	-292.73603	-3089.36869	-518.00862	1
7639	C	62.07000	53.38380	70.23690	-273.52043	79.29525	866.22736	1
7640	O	61.17200	53.02380	69.23190	495.62397	-74.81991	-610.23446	1
7641	H	61.57000	53.06280	68.35890	851.61547	-2247.43352	2030.27581	1
7642	C	64.22300	54.25280	70.86090	650.27815	-305.94784	-561.23547	1
7643	H	65.19200	54.70680	70.71490	1349.63683	2773.39621	-620.46766	1
7644	C	63.28000	53.95980	69.85490	-277.81554	535.08939	684.06789	1
7645	H	63.50300	54.29180	68.85190	1275.25847	-1228.78225	-2600.39156	1
7646	C	65.83400	51.91380	73.11590	574.02176	142.30897	-694.04480	1
7647	O	65.14200	50.94680	73.39390	552.31917	520.35186	-218.64288	1
7648	N	66.72600	51.85580	72.13990	422.02364	574.53356	-452.19411	1
7649	H	67.18100	52.70080	71.86790	1203.14880	-1030.59614	2718.18520	1
7650	C	67.06100	50.73780	71.34590	790.22595	424.03887	-164.87872	1
7651	H	66.18800	50.37980	70.82090	-2262.06129	-451.42444	-2139.51418	1
7652	C	68.18900	50.95680	70.27890	613.00707	645.78500	196.55807	1
7653	H	68.49600	49.97580	69.85790	1447.96023	1574.31117	2307.20215	1
7654	H	69.07300	51.42780	70.75990	-522.29934	3100.87838	99.91442	1
7655	C	67.74500	51.90280	69.18490	-391.16536	-815.71745	114.21783	1
7656	H	67.22000	52.78380	69.61290	-1776.43918	1361.34034	2211.16316	1
7657	C	68.90400	52.46280	68.26490	510.25515	640.32723	-401.33741	1
7658	H	69.21300	51.65180	67.57190	-814.81842	2419.76861	1838.21028	1
7659	H	69.81900	52.69180	68.85290	2307.23219	-1576.31507	-1445.73049	1
7660	H	68.67000	53.44480	67.79890	-512.84722	2259.63912	2128.20229	1
7661	C	66.79800	51.18780	68.16290	113.62520	245.58611	-870.76276	1
7662	H	67.28100	50.33580	67.63890	-1961.02823	-2100.52277	-1280.78047	1
7663	H	66.50300	51.92080	67.38290	-1866.41494	477.41028	-2487.32807	1
7664	H	65.90400	50.68680	68.59190	-1249.88407	1244.38661	-2605.28655	1
7665	C	67.57100	49.59980	72.22890	-510.18512	-755.64773	12.59556	1
7666	O	67.16500	48.45580	72.05690	170.02894	-395.46220	-662.06271	1
7667	N	68.39700	49.92080	73.24090	644.36919	409.26202	-360.50692	1
7668	H	68.72700	50.85680	73.34190	1479.30347	-47.64056	2776.25969	1
7669	C	69.08400	48.91580	74.02090	-270.91730	-767.29334	411.47996	1
7670	H	69.46000	48.13080	73.38090	1797.65204	435.01954	2545.07983	1
7671	C	70.26000	49.50580	74.88190	468.22097	-770.57178	135.79122	1
7672	H	69.96200	50.21280	75.68490	2054.26700	1367.04935	1951.76572	1
7673	H	70.89000	50.10780	74.19090	-2146.73375	1282.63419	-1909.08616	1
7674	H	70.83600	48.64580	75.28590	1459.47504	2739.95025	-510.71662	1
7675	C	68.12500	48.26380	75.04290	756.15586	506.05180	-59.92406	1
7676	O	68.45400	47.23480	75.64590	296.21782	-703.34129	202.96123	1
7677	N	66.89700	48.82080	75.37790	97.57007	399.55034	737.23259	1
7678	H	66.81100	49.74780	75.01990	-1511.28522	28.39929	-2759.24568	1
7679	C	65.93700	48.35880	76.39690	-624.55313	501.03365	-436.29082	1
7680	H	66.38800	47.45080	76.76890	-1511.13383	-1840.62939	2055.91445	1
7681	C	65.75500	49.42180	77.42890	-341.69308	-696.41013	479.28047	1

7682	H	65.76800	50.45180	77.01090	-1462.77981	1153.28881	2535.43416	1
7683	C	64.37800	49.29580	78.19190	-248.81438	762.72529	-433.35037	1
7684	H	64.35700	50.15180	78.89890	1472.39796	2763.45699	305.90179	1
7685	H	63.54600	49.42280	77.46690	1387.58266	-2563.18625	-1184.44790	1
7686	H	64.34900	48.32980	78.73890	2105.62272	-2040.34506	1140.86423	1
7687	C	66.94300	49.36980	78.37390	601.89979	-537.61864	424.42177	1
7688	H	67.87300	49.13980	77.81290	1558.10070	2341.21922	-1410.40454	1
7689	H	66.93800	48.50780	79.07490	1414.57683	694.44056	-2723.04075	1
7690	C	67.20200	50.71380	79.14890	-595.51929	367.18638	584.79222	1
7691	H	68.24400	50.65780	79.52990	-1747.67030	852.83322	-2473.16604	1
7692	H	66.39500	50.70680	79.91290	1661.18725	-1989.41852	1783.50697	1
7693	H	67.23000	51.56080	78.43090	2692.93388	-1447.99748	741.37483	1
7694	C	64.68400	47.94480	75.66090	12.54828	-908.34415	78.76834	1
7695	O	64.12400	46.89680	75.93190	-369.21429	-539.63082	-442.83926	1
7696	N	64.12500	48.67480	74.69190	88.43404	127.31748	829.84454	1
7697	H	64.58500	49.51780	74.42290	1222.07498	2313.77896	-1746.76440	1
7698	C	62.87300	48.23880	73.93890	700.69683	574.78948	-100.45899	1
7699	H	62.32800	47.76380	74.74190	1626.40524	-736.02938	2590.61633	1
7700	C	62.19700	49.49980	73.38790	-825.74470	64.46257	381.36763	1
7701	H	62.95800	50.04680	72.79190	30.59940	2226.53833	2222.56990	1
7702	C	61.03600	49.08980	72.50190	-498.83728	-243.21960	-723.50301	1
7703	H	61.35600	48.76480	71.48890	-2526.11441	1854.13627	-281.33770	1
7704	H	60.40500	48.31080	72.98290	-2242.58347	-1795.54235	1282.60410	1
7705	H	60.31000	49.90180	72.28490	2313.48785	-1447.36120	-1565.61354	1
7706	C	61.82500	50.37880	74.60090	-591.38656	-661.95142	208.64624	1
7707	H	61.06500	51.09380	74.21890	1955.52936	-432.03524	2426.41231	1
7708	H	62.72800	50.86480	75.02890	1190.10654	-2493.82458	1504.23124	1
7709	H	61.21500	49.71080	75.24590	-2259.28048	2110.24103	-583.74717	1
7710	C	63.20100	47.23580	72.87290	417.80222	307.40444	749.92988	1
7711	O	62.38700	46.38080	72.49590	-492.71843	595.46477	-162.10330	1
7712	N	64.47400	47.13380	72.43890	-193.69306	672.65699	-471.89815	1
7713	H	65.23300	47.65180	72.82590	470.99995	-1159.54275	-2886.49370	1
7714	C	64.77200	46.31680	71.22390	-609.91446	214.90419	-642.86199	1
7715	H	64.08400	45.51580	70.99690	-2480.15667	1231.58407	-1493.40210	1
7716	C	64.96500	47.11680	69.95990	-646.88090	640.06767	57.52811	1
7717	H	65.19000	46.42980	69.11690	790.08686	-2387.03599	-1891.04420	1
7718	H	65.80000	47.84180	70.06290	-1996.62865	-1793.95742	-1641.16332	1
7719	N	62.80000	47.30780	68.67190	248.17708	-160.52799	-790.76620	1
7720	H	62.85700	46.39880	68.25890	-1772.11809	2275.94912	1256.13665	1
7721	C	63.74700	47.92880	69.43990	-677.71136	604.87165	79.30073	1
7722	C	61.90700	48.23880	68.29190	398.74466	-522.32628	632.16213	1
7723	H	61.02100	47.93880	67.73390	-685.14795	487.19339	-3031.73896	1
7724	N	62.23400	49.43580	68.75890	414.44244	-668.32608	-307.00163	1
7725	C	63.35500	49.21480	69.53490	-529.59590	698.22968	-251.90175	1
7726	H	63.91700	50.02480	69.98390	-1320.23936	1001.53031	2674.34689	1
7727	C	66.09300	45.60480	71.41390	748.32666	-202.42896	-480.08408	1
7728	O	67.00800	45.60980	70.60490	549.98168	-566.01703	27.78668	1
7729	N	66.26200	44.96680	72.58690	-401.93304	-341.53202	659.14945	1
7730	H	65.54000	44.88280	73.26990	-1650.61831	1008.01634	2481.44887	1
7731	C	67.55100	44.53680	72.97490	-444.39073	536.63254	-588.21204	1
7732	H	68.36100	45.24380	72.87890	2748.24951	-1450.17862	492.27311	1
7733	C	67.54100	44.11380	74.52790	684.43262	130.49388	-588.19583	1
7734	H	67.20500	45.01580	75.08290	1852.05488	-1067.55999	-2308.34023	1
7735	H	66.79700	43.31280	74.72290	2410.20495	595.60692	-1932.45718	1
7736	H	68.52800	43.74880	74.88590	-1383.08883	-911.40774	-2674.81353	1
7737	C	68.08100	43.25480	72.25790	-398.17893	100.57878	814.11821	1
7738	O	69.24900	42.90780	72.37290	636.46954	-463.33057	-62.11712	1
7739	N	67.23100	42.50780	71.53190	4.30664	598.47252	595.38591	1
7740	H	66.32800	42.91980	71.44090	2912.59593	-475.07240	1090.55829	1
7741	C	67.54800	41.26580	70.93090	-335.31234	258.58779	807.55742	1
7742	H	68.32300	40.86780	71.56890	-2010.33196	1752.49858	-1668.99382	1
7743	C	66.43900	40.21380	70.95290	658.31779	513.60753	-366.43690	1

7744	H	66.01200	40.24680	71.97790	-1852.94001	1355.80876	-2150.95843	1
7745	O	66.96200	38.92080	70.87490	550.85539	82.34729	559.82541	1
7746	H	67.72100	38.72880	71.43090	-1576.56453	-1211.14979	2438.39839	1
7747	C	65.34400	40.37980	69.88590	749.87638	-35.58720	-517.56156	1
7748	H	64.40400	39.92280	70.26290	1715.98814	2070.02727	-1633.58441	1
7749	H	65.72800	39.97280	68.92590	-218.60340	-3067.59484	663.55156	1
7750	H	65.10900	41.45680	69.74290	1934.06509	1985.81936	-1487.99863	1
7751	C	68.04700	41.39180	69.50990	-678.69371	-598.30908	113.36708	1
7752	O	68.49600	40.41480	68.88190	293.00025	-344.02636	-647.62948	1
7753	N	67.97800	42.58880	68.90590	-98.72521	-227.23125	807.02638	1
7754	H	67.40400	43.31080	69.28390	1231.01158	1517.88517	2465.53469	1
7755	C	68.25700	42.84080	67.50690	-681.96376	472.33319	378.52053	1
7756	H	69.24300	42.47480	67.26390	1563.84161	-1931.99102	-1928.73957	1
7757	C	67.21300	42.10680	66.52190	757.31941	496.00431	109.07811	1
7758	H	67.50300	42.52180	65.53290	-2122.92264	366.82424	2292.78557	1
7759	H	67.39400	41.01280	66.44490	1704.69488	-133.87949	-2640.89339	1
7760	C	65.73100	42.38580	66.82990	-606.63431	-671.11848	-114.21820	1
7761	O	65.28300	43.17080	67.69590	700.57820	200.82518	304.11620	1
7762	N	64.85100	41.84280	65.95390	-470.70949	144.07806	685.81803	1
7763	H	65.23300	41.18080	65.30890	1897.93127	-1554.74088	-1969.48317	1
7764	H	63.87600	42.02380	66.07990	-976.37974	-1779.46187	-2403.83533	1
7765	C	68.28700	44.37280	67.28890	603.54252	251.75734	635.45705	1
7766	O	67.32600	45.05080	66.84790	-283.11668	71.34098	-733.74562	1
7767	N	69.42800	45.01480	67.51390	-509.83989	439.26624	509.68691	1
7768	H	70.29900	44.54280	67.62790	3073.41697	96.42858	665.60942	1
7769	C	69.59800	46.39680	67.30590	-250.56010	-750.92999	-452.52049	1
7770	H	69.34300	46.64780	66.28690	2380.22491	527.76585	1988.52176	1
7771	C	68.81800	47.28080	68.35890	-751.25610	368.83109	-361.97915	1
7772	H	67.74200	47.08880	68.15690	-1135.32986	1162.85284	2693.88671	1
7773	H	68.95200	48.36380	68.15390	2621.79742	1598.95014	683.93200	1
7774	O	69.09100	46.87480	69.72790	82.97477	577.35857	-532.35279	1
7775	H	68.34100	46.30280	69.90690	-994.29190	-1709.16046	2447.11674	1
7776	C	71.05900	46.81080	67.33990	-598.58095	-246.29948	-642.25262	1
7777	O	71.31200	47.99080	67.04890	-119.88413	-416.63787	660.05144	1
7778	N	72.08300	46.00080	67.59690	-235.47629	186.73699	-788.89321	1
7779	H	71.88000	45.04780	67.80590	-1941.52766	367.00668	2448.26523	1
7780	C	73.48600	46.44780	67.59790	-117.31300	808.07841	405.82995	1
7781	H	73.52400	47.26880	68.29890	-94.15309	555.56409	-3095.27219	1
7782	C	74.37500	45.29980	68.15590	349.24143	-694.52830	476.56255	1
7783	H	74.02300	44.33880	67.72490	2187.56157	1734.49200	-1450.63369	1
7784	H	74.17000	45.24680	69.24690	-462.21592	-675.52413	3037.80345	1
7785	C	75.92100	45.26480	67.94090	-688.34064	-188.53166	-567.53325	1
7786	H	76.30900	44.56380	68.70990	900.64859	2483.23659	1708.97465	1
7787	H	76.31100	46.28280	68.15790	2722.79775	917.21387	1281.91941	1
7788	C	76.47700	44.90180	66.52690	-694.39980	62.00798	587.72011	1
7789	O	77.48800	45.40880	66.06490	-583.38469	-402.96791	-347.71597	1
7790	N	75.84000	43.91380	65.89590	677.82138	-414.44226	-285.42615	1
7791	H	75.05300	43.46880	66.32490	1601.33989	2239.89573	1522.10510	1
7792	H	76.20200	43.57880	65.02690	1908.02434	-180.88731	-2494.98479	1
7793	C	74.06300	47.03080	66.32090	522.08630	-575.61216	-477.01944	1
7794	O	74.69700	48.06380	66.27790	244.51640	-347.06706	665.87042	1
7795	N	73.75600	46.55480	65.10790	-757.58830	144.48831	-343.30071	1
7796	H	73.25200	45.70380	64.98290	-484.25524	488.11033	3070.09306	1
7797	C	74.08400	47.23980	63.86290	-161.53046	-750.43013	492.15193	1
7798	H	75.12800	47.51180	63.92690	-1065.13115	-2932.33163	406.39032	1
7799	C	74.06800	46.20880	62.72890	-731.28525	-469.71222	275.75953	1
7800	H	73.13500	45.60880	62.79690	-2009.06986	-1599.06496	1817.92623	1
7801	H	74.85700	45.42680	62.72790	-416.58161	-528.78603	3073.28347	1
7802	C	74.06200	46.76480	61.27790	-776.95958	-436.42055	193.18882	1
7803	H	73.11700	47.30680	61.06290	1417.32230	2737.90974	-627.11560	1
7804	H	74.90400	47.46680	61.10090	-1647.08289	868.00982	-2536.11970	1
7805	C	74.25100	45.71380	60.15490	787.69201	-432.25438	-155.39769	1

7806	H	75.13100	45.04580	60.27290	-2340.97760	1034.54472	1829.69051	1
7807	H	73.41700	44.99080	60.02890	-276.37492	2903.44781	1179.76013	1
7808	N	74.37500	46.45680	58.85890	-541.96141	-484.39141	429.31933	1
7809	H	73.83000	47.27780	58.68890	439.68406	2676.96414	1593.35092	1
7810	C	74.66200	45.80580	57.73890	412.49453	602.72693	-545.91163	1
7811	N	75.21300	44.60980	57.67290	343.28745	-484.01684	600.46125	1
7812	H	75.14000	43.94180	58.41390	1066.64886	1702.06179	-2421.46073	1
7813	H	75.29600	44.15880	56.78390	-2741.62249	591.53017	-1425.42078	1
7814	N	74.43800	46.41980	56.59390	-652.77470	441.51959	-302.68453	1
7815	H	74.35200	47.41580	56.55990	-366.14760	-834.01819	-3011.40761	1
7816	H	74.81700	46.00380	55.76690	-2089.51111	-2352.02812	-11.54432	1
7817	C	73.45900	48.66280	63.65890	367.37472	-648.97084	524.71294	1
7818	O	74.22500	49.62080	63.25590	591.72685	-305.57477	-424.39443	1
7819	N	72.19600	48.93680	63.88290	-569.87937	557.90511	-276.86041	1
7820	C	71.15200	47.91380	63.64390	554.89815	314.54020	651.61607	1
7821	H	71.01200	47.26380	64.53490	-408.21656	-2507.78575	1855.42343	1
7822	H	71.30300	47.24080	62.77290	2314.20547	-2085.90791	437.79846	1
7823	C	71.58800	50.28980	63.86990	223.43296	-572.17464	673.90274	1
7824	H	71.84300	50.86080	62.98890	2443.94981	-1878.97436	628.32388	1
7825	C	70.07700	50.06480	63.96190	-439.81422	-571.98101	557.54119	1
7826	H	69.46100	50.84980	63.47390	-2705.05160	792.16700	1397.63854	1
7827	H	69.73700	49.93580	65.01190	-1616.19085	-411.24491	-2667.77641	1
7828	C	69.87000	48.68880	63.34890	-607.08387	-680.02370	21.63219	1
7829	H	69.82900	48.81780	62.24590	2001.62042	2191.28034	-1044.04615	1
7830	H	68.94600	48.19980	63.72390	-1180.94778	-2507.16573	1489.19729	1
7831	C	72.06400	51.10980	65.08690	418.51034	-615.39546	-526.86671	1
7832	O	72.36800	52.25980	64.91690	-310.85032	-687.91968	231.87457	1
7833	N	72.14200	50.58980	66.34490	-289.32400	-596.50411	522.63444	1
7834	H	71.85400	49.64680	66.48990	1363.66697	2593.04601	-1146.62592	1
7835	C	72.81900	51.31980	67.35990	357.30677	628.45541	555.72176	1
7836	H	72.31400	52.25080	67.56990	2502.65950	1397.91440	1296.44011	1
7837	C	72.89600	50.49980	68.67390	-257.51074	-482.49481	-729.61495	1
7838	H	73.60400	51.00680	69.36290	-2483.46327	1672.50487	966.10759	1
7839	H	73.30500	49.50780	68.38590	-1677.63239	2346.91290	1255.29902	1
7840	C	71.62900	50.31280	69.43890	-163.66395	-590.59331	-675.17750	1
7841	H	70.76200	49.92680	68.86190	-554.84535	2989.57813	-807.95758	1
7842	H	71.29200	51.26680	69.89990	481.09859	-1476.23941	-2736.32739	1
7843	C	71.72500	49.24180	70.58390	446.76018	-774.28284	-179.84001	1
7844	H	70.75000	48.93880	71.02290	1486.63614	-1571.06313	2284.71002	1
7845	H	72.23500	48.32680	70.21490	-1807.91618	1953.25876	1677.63092	1
7846	N	72.53600	49.96180	71.58390	-293.05361	786.60279	-89.71019	1
7847	H	72.73100	50.93480	71.46790	-1194.06061	2648.21785	-1208.05119	1
7848	C	73.24800	49.36280	72.44790	810.67973	-416.96001	19.84276	1
7849	N	73.02000	48.12780	72.87290	-787.41695	-159.99390	258.93781	1
7850	H	72.19900	47.67380	72.52690	-2513.64235	-426.69839	1843.30052	1
7851	H	73.73800	47.68480	73.40890	1844.99598	1762.05733	1841.02417	1
7852	N	74.05500	50.13280	73.16390	-11.35797	841.95718	60.42671	1
7853	H	74.03900	51.12880	73.07790	-990.59967	-2636.73108	1401.63752	1
7854	H	74.58500	49.72780	73.90890	-1576.76848	1001.33361	2531.67106	1
7855	C	74.26400	51.75680	67.03390	490.81175	-88.58160	-763.35321	1
7856	O	74.70400	52.87880	67.34290	-97.63868	-781.84572	53.02065	1
7857	N	74.99000	50.84080	66.43790	391.45388	-416.25300	-621.42545	1
7858	H	74.53700	50.00780	66.12990	-2434.88356	1263.10961	-1540.81873	1
7859	C	76.32900	51.05180	65.91890	755.75258	424.99039	282.26265	1
7860	H	76.92000	51.30980	66.78590	2383.14925	975.35757	1807.62371	1
7861	C	76.94900	49.70280	65.47390	-127.10057	449.84396	-782.90284	1
7862	H	76.30500	49.24080	64.69590	-1462.01769	-776.97564	2675.26435	1
7863	H	76.96900	49.10280	66.40990	2351.35848	2038.64845	-461.79218	1
7864	C	78.38400	49.85180	64.90690	507.13821	429.47325	624.35131	1
7865	H	78.99800	50.42380	65.63490	1539.25316	2178.00992	-1668.89147	1
7866	H	78.48000	50.46080	63.98190	497.81871	1585.92457	-2671.18813	1
7867	C	79.08600	48.50880	64.76090	-465.49210	-579.50324	-528.15158	1

7868	H	80.13800	48.65880	64.43590	-1798.56283	2098.41842	-1503.34231	1
7869	H	79.13800	48.00180	65.74790	-1712.44281	2016.17196	1703.17835	1
7870	C	78.42400	47.54480	63.73590	-276.83746	-461.54264	736.06414	1
7871	H	77.43900	47.19580	64.11290	2062.78229	-900.72626	2198.14641	1
7872	H	78.43800	48.07180	62.75690	-581.77017	-1296.54614	2806.90894	1
7873	N	79.19100	46.31480	63.58490	668.80042	-48.88060	512.82451	1
7874	H	79.15700	45.54480	64.28290	-1455.35871	2733.96206	-552.81890	1
7875	H	78.84600	45.88880	62.70090	2802.27857	696.03767	-1249.39690	1
7876	H	80.20700	46.41180	63.38790	-1395.14776	167.54165	-2814.91008	1
7877	C	76.45600	52.09780	64.76190	-340.64362	379.01610	-756.14795	1
7878	O	77.33400	53.00380	64.73790	480.83886	274.14261	-563.26464	1
7879	N	75.49900	52.07180	63.80890	474.66355	163.46394	-678.70932	1
7880	H	74.82500	51.33980	63.87890	-1343.72188	-1828.90196	-2178.93446	1
7881	C	75.37200	53.05880	62.72290	505.86493	-644.58825	-400.07208	1
7882	H	76.24900	53.07880	62.09390	1996.30797	-1795.19527	1640.19958	1
7883	C	74.08200	52.69580	61.93290	467.02505	-635.74028	-457.35423	1
7884	H	73.19500	52.54980	62.58490	2992.05203	-698.08008	677.15216	1
7885	H	74.18000	51.73280	61.38690	-2643.66720	-1378.09349	1005.04144	1
7886	C	73.59900	53.60380	60.75090	746.41321	-148.09729	502.37985	1
7887	H	73.51200	54.61580	61.20090	-2259.59392	2000.75123	888.51342	1
7888	C	74.75200	53.70080	59.70190	392.86651	818.16838	-87.79179	1
7889	H	75.73100	53.99880	60.13390	973.97142	-2231.00409	-1993.04456	1
7890	H	74.40100	54.35980	58.87990	-2807.57231	-610.77700	-1281.68460	1
7891	H	74.77600	52.72380	59.17190	461.01885	-2966.66190	940.53442	1
7892	C	72.26900	52.99980	60.24790	145.82257	-611.60754	-660.39609	1
7893	H	72.31900	51.91280	60.01990	-2677.86183	717.21180	-1487.57839	1
7894	H	71.53100	53.17380	61.05890	2811.05797	716.38731	-1217.77196	1
7895	H	71.90400	53.53280	59.34390	-582.05890	1814.68262	-2503.26999	1
7896	C	75.26700	54.48680	63.29190	864.36087	-210.32899	-200.23236	1
7897	O	75.99400	55.39780	62.81990	-722.97101	-65.10869	-310.96785	1
7898	N	74.42500	54.77980	64.32690	56.26413	662.10682	-520.69299	1
7899	H	73.71000	54.13580	64.58490	1481.70092	2723.79880	-532.64312	1
7900	C	74.40000	55.99780	65.09690	135.32019	888.85078	151.93334	1
7901	H	74.15100	56.75380	64.36690	1816.38195	-1659.32307	1961.02774	1
7902	C	73.31000	55.86980	66.17990	147.39433	803.00974	-406.08038	1
7903	H	73.30000	56.73880	66.87090	-1879.52770	558.27214	2460.47436	1
7904	H	73.61800	54.94780	66.71790	-124.36038	1122.47502	2936.46225	1
7905	C	71.87600	55.65080	65.62390	-292.57289	-459.05976	-731.51640	1
7906	H	71.83700	54.60480	65.25090	853.61981	-51.96252	-3027.68217	1
7907	C	70.97400	55.48080	66.86590	-262.24589	276.38742	-828.42506	1
7908	H	71.23100	54.55980	67.43290	-35.86831	1339.43061	-2846.55324	1
7909	H	71.08600	56.36480	67.52890	690.15356	-2302.03786	2030.40291	1
7910	H	69.94100	55.32880	66.48690	789.05455	-2499.06386	1740.77540	1
7911	C	71.25800	56.61480	64.56090	507.07240	560.70252	-509.84435	1
7912	H	70.17700	56.37880	64.46190	-1746.50458	-1860.64461	1840.09500	1
7913	H	71.83700	56.72880	63.61990	1435.80627	2799.35657	17.01108	1
7914	H	71.32500	57.64680	64.96790	-602.34540	-2187.68669	-2179.31943	1
7915	C	75.73500	56.27280	65.77590	449.23342	690.57438	-390.82908	1
7916	O	76.34600	57.33580	65.63190	98.01944	-737.45968	-264.90119	1
7917	N	76.31200	55.24680	66.49890	474.00165	695.72037	62.99122	1
7918	H	75.88100	54.35180	66.58390	-2128.34693	2169.62168	813.08508	1
7919	C	77.48200	55.40080	67.33590	-188.92237	684.46151	-572.07673	1
7920	H	77.32600	56.29280	67.92390	-2248.40509	1524.77759	-1586.80624	1
7921	C	77.62100	54.17580	68.29490	656.69761	-251.44449	580.49541	1
7922	H	78.49700	54.34580	68.95590	-1355.25345	2557.13823	1233.91994	1
7923	H	76.75900	54.12480	68.99390	-186.38175	-699.89618	-3061.63901	1
7924	H	77.70900	53.20180	67.76690	763.93062	-1527.50127	2642.22938	1
7925	C	78.78300	55.65680	66.64290	-504.56942	517.63806	555.79811	1
7926	O	79.62000	56.37780	67.15490	-520.37260	-556.13294	208.70012	1
7927	N	78.96700	55.15180	65.41590	-170.22067	783.12437	-265.35529	1
7928	H	78.26300	54.58880	64.98890	-2830.38522	295.52187	-1341.57092	1
7929	C	80.24300	55.01480	64.81890	-742.71501	-319.79120	-421.37752	1

7930	H	80.93500	55.54480	65.45490	-1284.08264	1406.65318	2504.13355	1
7931	C	80.74100	53.60680	64.68090	369.62887	-790.28411	-265.09721	1
7932	H	81.54200	53.50280	63.91790	1367.07050	2829.87709	-145.39652	1
7933	H	79.93900	52.99380	64.21490	-1230.72456	-447.92394	-2860.57817	1
7934	C	81.19200	53.07180	66.00590	-439.81834	431.09233	672.43604	1
7935	H	80.21400	52.97080	66.52290	822.31980	-2077.29909	2215.13992	1
7936	H	81.98500	53.67880	66.49090	2425.71536	1965.56947	-388.15957	1
7937	C	81.80000	51.67080	65.81990	-194.87544	641.85926	-617.64978	1
7938	O	82.54700	51.38680	64.86090	490.51294	511.21769	348.82770	1
7939	O	81.46400	50.77080	66.62690	586.86452	97.56209	519.32543	1
7940	C	80.24800	55.64180	63.46990	-393.60719	-299.78151	765.93435	1
7941	O	81.28400	56.18180	63.05390	185.46925	-763.79646	-76.44188	1
7942	N	79.10300	55.73680	62.73990	1.18328	620.27752	-572.64884	1
7943	H	78.21300	55.39680	63.03490	-2991.28572	-323.39887	919.70058	1
7944	C	79.08500	56.37380	61.44790	456.82388	-551.93061	564.03506	1
7945	H	80.07800	56.57180	61.07090	2080.94848	-158.14349	2354.33011	1
7946	C	78.41800	55.43180	60.43790	595.38611	-262.83251	-638.65911	1
7947	H	77.80000	55.86380	59.62190	-1201.22448	1916.78934	-2186.59658	1
7948	H	77.61800	54.90880	61.00490	-2339.72894	2080.30056	-310.23263	1
7949	C	79.39200	54.30580	59.96390	523.91545	550.26969	-504.14965	1
7950	H	80.20100	54.78780	59.37390	1632.38826	612.06032	2618.95341	1
7951	H	79.81400	53.79280	60.85490	3082.36072	-630.18896	-11.85261	1
7952	C	78.69400	53.25980	59.05890	535.32051	-553.97053	-487.85204	1
7953	H	78.18300	53.69880	58.17490	-2896.45892	-1228.09288	-23.23467	1
7954	H	77.89200	52.86580	59.71890	574.79550	-3068.48749	-390.15494	1
7955	C	79.52300	52.08780	58.64990	119.91645	-217.39813	-877.38766	1
7956	H	78.88900	51.18480	58.52290	1550.97321	-136.94496	2733.85340	1
7957	H	80.17100	51.87080	59.52690	-1835.80481	76.09568	-2553.87086	1
7958	N	80.41500	52.29680	57.45590	-340.75312	-238.62309	734.58738	1
7959	H	81.01600	53.14280	57.39090	2077.51361	1710.64734	1629.67761	1
7960	H	80.99800	51.45480	57.27390	2036.95678	-1679.36001	-1711.36882	1
7961	H	79.79000	52.30380	56.62490	-136.84474	-2232.74320	2212.31949	1
7962	C	78.36900	57.66680	61.44790	-436.04995	495.04796	-629.47515	1
7963	O	78.89200	58.71780	61.08490	-87.52700	-612.14327	491.16888	1
7964	N	77.09500	57.58980	61.86190	607.50853	527.28763	-256.07310	1
7965	H	76.77100	56.72180	62.22990	1458.51518	-1997.19696	-1944.77865	1
7966	C	76.09900	58.66480	61.66090	133.28248	-784.46330	445.31350	1
7967	H	76.35500	59.15680	60.73390	-2975.33665	-993.06191	243.77466	1
7968	C	74.63500	58.10880	61.42090	-235.67123	686.81576	-551.53802	1
7969	H	74.40700	57.32080	62.17090	-2592.77985	286.31803	-1758.90331	1
7970	C	73.63900	59.25180	61.53490	412.54753	67.66444	810.35613	1
7971	H	73.66300	59.64980	62.57190	1124.66712	1030.89139	-2751.47470	1
7972	H	72.61900	58.85480	61.34290	-2442.61912	-1685.69764	1044.15588	1
7973	H	73.85800	60.07080	60.81690	1055.85425	-1531.17459	2537.49924	1
7974	C	74.54200	57.54180	59.97590	-322.67470	385.89947	760.53510	1
7975	H	75.40900	56.88280	59.75790	1220.58053	-2103.52528	1995.89348	1
7976	H	73.71200	56.81880	59.81990	2015.11253	1366.60431	1992.47093	1
7977	H	74.61300	58.32480	59.19190	301.43086	-2515.68369	1865.12768	1
7978	C	76.21100	59.84480	62.65990	-12.43828	6.78298	-911.72928	1
7979	O	75.93300	60.98580	62.30390	576.43795	213.03201	-495.94745	1
7980	N	76.85000	59.71980	63.88290	-395.10264	459.78809	-587.50414	1
7981	H	76.85700	58.81880	64.30890	-1745.59768	-2615.25319	-107.54412	1
7982	C	77.20900	60.88380	64.76190	682.57926	-366.07454	481.17147	1
7983	H	76.28000	61.42980	64.83790	-1968.94770	1636.93714	1828.08861	1
7984	C	77.73400	60.39280	66.08790	-528.03511	-107.94521	-735.51190	1
7985	H	77.00500	59.71580	66.58190	2074.08785	1543.57762	1792.69461	1
7986	C	79.03700	59.53180	65.95890	-159.07311	-559.93267	-701.87047	1
7987	H	79.91700	60.21080	65.96790	3081.88190	-14.18254	632.47849	1
7988	H	79.30200	58.94780	65.05190	-1119.62649	-2552.41944	-1459.38951	1
7989	H	79.18400	58.75480	66.73890	-2398.91850	585.98352	-1949.36902	1
7990	C	77.96200	61.63780	66.98490	237.71013	-728.35172	494.41751	1
7991	H	78.82900	62.29580	66.75890	2530.62891	1755.47006	-642.23704	1

7992	H	78.00300	61.31880	68.04790	-1566.25258	1835.16075	2019.22364	1
7993	H	77.05900	62.28480	66.98290	-1195.10023	2422.04621	-1613.58416	1
7994	C	78.17500	61.78680	63.99590	591.43949	297.00416	-627.24705	1
7995	O	78.09900	62.98780	64.12390	-680.00288	401.52001	-2.23548	1
7996	N	79.04000	61.27880	63.15690	461.53381	222.71467	-670.86288	1
7997	H	79.21600	60.30180	63.07090	-351.47570	1952.59601	2441.73297	1
7998	C	79.83300	62.16880	62.23990	-743.29342	-451.56983	273.95362	1
7999	H	80.38500	62.91080	62.79690	-567.46054	2257.40796	2116.67760	1
8000	C	80.87800	61.35180	61.53590	247.62975	876.88086	-34.79164	1
8001	H	81.46900	62.00780	60.86190	1668.15668	-2662.34459	165.53182	1
8002	H	80.48200	60.49880	60.94490	3032.26998	320.36756	775.19650	1
8003	C	81.78800	60.76180	62.55890	-542.31176	452.41814	-576.77273	1
8004	C	81.47900	59.48980	63.13990	610.43304	80.23188	-672.59598	1
8005	H	80.54500	58.99280	62.92390	2094.09441	-2307.64190	-433.34013	1
8006	C	82.33100	58.99680	64.14690	-627.84855	-285.72860	596.33579	1
8007	H	82.11600	58.00880	64.52490	1288.86116	-2499.37535	-1410.73952	1
8008	C	83.50600	59.67180	64.52090	597.32487	558.50971	-403.38680	1
8009	O	84.34300	59.10380	65.48790	784.82525	-16.16578	-86.11168	1
8010	H	85.16400	59.59980	65.50190	1989.31837	2340.00078	-682.08136	1
8011	C	82.96400	61.42180	62.94590	-743.72146	-227.65914	-475.92091	1
8012	H	83.22800	62.37680	62.51590	-1601.44261	-1953.72382	-1875.25225	1
8013	C	83.79600	60.81880	63.85490	-646.60004	642.81176	-12.34635	1
8014	H	84.68400	61.36680	64.13590	-1077.47896	1761.32941	2373.81213	1
8015	C	79.07200	63.01480	61.18490	755.97992	-504.10201	76.33172	1
8016	O	79.35300	64.19780	61.05590	305.27495	532.93805	496.39850	1
8017	N	78.11400	62.42880	60.51990	-330.48286	752.95759	-191.07130	1
8018	H	77.89300	61.46280	60.63090	-1800.74236	-2418.28065	-898.59439	1
8019	C	77.45200	63.00280	59.37490	-171.02718	887.28241	122.19095	1
8020	H	77.88600	63.93180	59.03590	1745.28610	-293.13041	-2601.20688	1
8021	C	77.51400	62.02580	58.15990	496.29923	423.73091	-636.85963	1
8022	H	78.58700	61.74980	58.07590	-1987.58359	1594.16214	1845.63940	1
8023	C	76.64800	60.74380	58.20490	-838.08345	59.05954	354.37142	1
8024	H	76.89000	60.04880	57.37290	1950.03968	-933.72632	-2285.54733	1
8025	H	75.57900	61.03780	58.26890	-1395.33314	2687.81368	852.60148	1
8026	H	76.88300	60.24480	59.16990	-855.71685	683.96007	2949.26661	1
8027	C	77.07000	62.83080	56.90790	-570.77126	-609.60883	366.12599	1
8028	H	77.53500	63.83980	56.88090	476.65632	-683.53386	3033.77759	1
8029	H	77.24600	62.12980	56.06390	-2189.15145	-1811.11047	1351.19245	1
8030	H	75.98500	63.07180	56.90790	-1330.65511	-1417.88160	2473.29638	1
8031	C	75.96700	63.43180	59.71690	-272.22670	-592.10152	-637.77693	1
8032	O	75.23100	63.95280	58.88690	-83.50511	410.59184	-669.37917	1
8033	N	75.55600	63.14580	60.96990	-150.57332	825.49864	92.47680	1
8034	H	76.07500	62.48980	61.51290	504.16011	2415.79102	1951.41040	1
8035	C	74.24300	63.52480	61.53090	-523.91201	361.70244	-652.79288	1
8036	H	73.64800	62.66780	61.80990	-1282.59050	2670.70883	1058.53775	1
8037	H	73.74100	64.17580	60.82990	-2164.17609	-669.96139	-2183.05287	1
8038	C	74.39400	64.47380	62.76890	667.40836	-593.81190	-182.76899	1
8039	O	73.38900	65.08080	63.16490	213.44088	492.89450	578.90002	1
8040	N	75.62000	64.65580	63.34290	407.76159	-528.08353	517.23356	1
8041	H	76.40600	64.05980	63.19790	-1565.45391	-724.90537	2630.98698	1
8042	C	75.80700	65.65780	64.37690	248.54503	560.24445	675.13149	1
8043	H	74.96800	66.32780	64.49790	-134.98160	2855.56669	-1313.67617	1
8044	C	76.01200	64.93380	65.67590	278.61279	-370.56758	785.17870	1
8045	H	76.89500	64.26080	65.65490	2093.60022	-2303.69237	-456.14232	1
8046	C	76.30800	65.94080	66.83790	659.81054	-153.30146	-610.40947	1
8047	H	77.32300	66.35880	66.66890	2604.30123	1417.98064	-1051.27172	1
8048	H	76.23100	65.35680	67.77990	1842.88595	1275.58512	2207.91308	1
8049	H	75.48500	66.68680	66.80890	2557.02413	-1828.61020	-126.64340	1
8050	C	74.73100	64.15080	66.04990	-260.84914	590.19267	-644.26807	1
8051	H	73.85200	64.82480	66.13390	-1559.89301	-2590.09786	-869.68563	1
8052	H	74.86500	63.63880	67.02690	-1583.21081	890.33354	-2568.84720	1
8053	H	74.49800	63.28680	65.39090	-1477.86579	-1563.69327	-2295.43074	1

8054	C	76.98200	66.54980	64.00090	-311.36156	-663.92101	541.95376	1
8055	O	76.81300	67.75280	63.82890	493.09283	-568.06205	240.40009	1
8056	N	78.17500	65.95380	63.88490	669.45657	322.63646	-400.50705	1
8057	H	78.34800	64.98480	64.04090	-1952.26483	-1901.95370	1571.45169	1
8058	C	79.38000	66.79380	63.80390	275.33721	269.64065	-826.39842	1
8059	H	79.33300	67.52180	64.60090	435.59070	-1565.41234	-2694.06221	1
8060	C	80.72500	65.95580	63.88190	783.96094	-408.45164	-223.65934	1
8061	H	81.57500	66.47980	63.39390	952.56650	2545.70453	1584.37108	1
8062	H	80.62700	65.05980	63.23190	-935.60924	-1361.43225	-2677.56677	1
8063	C	81.07600	65.46380	65.23690	756.59391	-502.07413	-83.29604	1
8064	C	81.17800	64.13780	65.68490	-792.75719	-351.50764	-281.83227	1
8065	H	81.15400	63.23580	65.09090	409.44274	1620.97532	-2665.14950	1
8066	N	81.54500	64.11680	67.03990	-628.07833	249.30732	-505.99977	1
8067	H	81.89000	63.41080	67.61890	-799.53679	1852.52640	-2413.94140	1
8068	C	81.67300	65.44380	67.41590	799.83290	-399.14944	-179.99461	1
8069	C	81.36600	66.28480	66.35090	-261.53011	-603.09923	631.92114	1
8070	C	81.43800	67.69780	66.49390	449.92375	-625.12954	-488.09085	1
8071	H	81.35400	68.36680	65.64990	2137.35506	1826.49301	1412.04209	1
8072	C	81.95200	68.19480	67.67890	795.64160	-402.47773	190.83272	1
8073	H	82.20600	69.23880	67.78590	-1100.00132	2894.86718	554.94806	1
8074	C	81.95100	65.96580	68.65390	-476.80441	764.53960	139.95628	1
8075	H	82.12500	65.34080	69.51690	2152.14988	774.02491	2160.40796	1
8076	C	82.16800	67.36880	68.71590	112.25910	-691.74216	-583.38811	1
8077	H	82.68500	67.67280	69.61390	-1251.40173	-1419.70961	2513.29357	1
8078	C	79.54100	67.60780	62.56990	-662.04951	-398.77358	-483.86060	1
8079	O	79.68900	68.83180	62.62190	-72.69763	683.15442	389.41279	1
8080	N	79.43900	66.98780	61.39490	234.11088	-475.89358	-656.80263	1
8081	H	79.52900	65.99580	61.36090	-1658.50736	-143.70214	2669.63092	1
8082	C	79.40100	67.72880	60.09790	664.72391	-587.29714	211.36507	1
8083	H	80.27400	68.36380	60.06790	816.95783	600.97156	-2978.19397	1
8084	C	79.57800	66.71580	58.97690	-89.51908	129.76712	898.10792	1
8085	H	79.06400	65.76680	59.23990	1520.52353	1979.92785	1914.71150	1
8086	C	79.02300	67.18080	57.59490	-566.26586	586.52737	408.38661	1
8087	H	79.08700	66.33780	56.87390	-745.45430	-1568.61513	2623.35104	1
8088	H	77.97200	67.53780	57.64990	2928.32411	1084.36958	-383.77957	1
8089	H	79.57700	68.09680	57.29790	2043.77050	-2084.93708	-1172.29081	1
8090	C	81.08100	66.50980	58.92390	388.43729	695.20120	444.14273	1
8091	H	81.56100	66.51280	59.92590	2721.90919	-1233.68186	983.59831	1
8092	H	81.53800	67.31980	58.31590	1799.36522	2401.52655	945.08269	1
8093	C	81.48100	65.22680	58.17990	554.61258	-314.94345	-651.66442	1
8094	H	82.58100	65.23080	58.01990	-548.99997	-2333.92582	-2037.06051	1
8095	H	81.14600	64.38880	58.82690	-1062.72655	1845.77819	2315.58662	1
8096	H	81.07500	65.34680	57.15190	-2526.76737	-1845.25930	-329.68320	1
8097	C	78.20300	68.68480	59.97390	-169.06395	509.15556	737.31201	1
8098	O	78.39300	69.81780	59.50690	-730.96421	-163.19824	250.36949	1
8099	N	76.94300	68.38580	60.25590	382.34420	-450.46081	602.96788	1
8100	C	76.40600	67.04980	60.23790	101.55111	39.63848	-905.29949	1
8101	H	76.84500	66.50280	61.09990	-35.26389	-2364.76667	-2074.81596	1
8102	H	76.61900	66.55080	59.26890	-2215.49163	1831.81047	-1278.39488	1
8103	C	75.89100	69.36780	60.47890	-503.71622	-382.96712	-656.54944	1
8104	H	75.63800	69.83980	59.54090	2410.32531	1718.91546	-1064.84167	1
8105	C	74.79500	68.58480	61.07990	322.65296	-422.80851	740.66121	1
8106	H	74.84900	68.53780	62.18890	-1040.70574	-1901.65108	-2280.10547	1
8107	H	73.81200	69.09380	60.98690	2242.03676	-2148.05451	-507.30583	1
8108	C	74.91000	67.23780	60.38990	-325.40783	-656.23778	-543.05867	1
8109	H	74.48000	66.36180	60.92190	2405.11862	197.92356	2018.52840	1
8110	H	74.36300	67.34880	59.42990	-56.49788	846.00936	3029.73636	1
8111	C	76.27700	70.60180	61.32290	703.01954	-46.61631	-578.82766	1
8112	O	75.93900	71.65980	60.85690	-723.71387	-201.97021	-243.05039	1
8113	N	76.98300	70.49280	62.53090	441.73769	351.29978	627.79660	1
8114	H	77.22900	69.59880	62.89790	-998.57522	-2127.28062	2091.82956	1
8115	C	77.34300	71.60280	63.34590	51.77988	707.65465	-572.70825	1

8116	H	76.43300	72.10680	63.63490	2898.13603	-1172.21801	-353.46674	1
8117	C	78.07100	71.11780	64.56590	-253.11347	659.10138	-577.03548	1
8118	H	77.40400	70.42680	65.12390	-1411.15697	-2314.43961	-1596.94444	1
8119	H	78.32800	71.98480	65.21090	-2709.75096	367.84358	1555.68861	1
8120	H	79.06500	70.67980	64.33290	-3067.13397	137.45548	-687.03816	1
8121	C	78.26200	72.58380	62.57290	682.49780	447.18425	407.03071	1
8122	O	77.99600	73.79480	62.52490	-478.25785	550.39124	303.25920	1
8123	N	79.28600	72.04380	61.88190	-190.06427	-631.23312	-527.34487	1
8124	H	79.45000	71.06180	61.82190	1714.14310	1948.78440	-1778.25167	1
8125	C	80.16600	72.83480	60.97290	-481.45767	-367.76633	681.46712	1
8126	H	80.56600	73.62780	61.58790	1.92333	3141.55384	-169.88815	1
8127	C	81.26100	71.99780	60.26490	-642.24492	-600.79952	240.85763	1
8128	H	80.87300	71.21680	59.57690	1253.90065	-2877.67719	-211.97497	1
8129	H	81.86300	72.79880	59.78490	1351.93614	-2410.42112	-1503.45100	1
8130	C	82.21600	71.17680	61.14290	37.20441	698.82925	584.55497	1
8131	H	81.67600	70.33280	61.62390	-1335.69003	-1079.49409	-2636.06731	1
8132	C	83.30900	70.67280	60.22790	-647.67314	-293.02833	571.05596	1
8133	H	82.82200	70.02180	59.46990	-334.40520	1911.46601	2476.42829	1
8134	H	83.81700	71.51980	59.71990	-1094.50796	2151.03179	2018.25192	1
8135	H	84.03400	70.09680	60.84190	2169.42575	-2232.25064	-457.02871	1
8136	C	82.83200	72.00880	62.34890	-734.31262	-29.66428	-539.77404	1
8137	H	81.97800	72.18080	63.03890	1618.46271	2641.76034	547.63768	1
8138	H	83.61500	71.40980	62.85990	1034.92887	1218.91969	-2709.49871	1
8139	H	83.28400	72.93580	61.93590	904.06768	2719.56616	1298.01685	1
8140	C	79.39800	73.56380	59.85490	-412.89558	811.61597	-47.41066	1
8141	O	79.60700	74.74080	59.58190	-265.26780	686.81507	285.56135	1
8142	N	78.44400	72.86480	59.19490	630.45625	456.03448	-327.45955	1
8143	H	78.25100	71.91980	59.44990	-2228.30596	1238.06642	1843.92796	1
8144	C	77.51900	73.42580	58.26290	466.52900	-601.72352	501.72752	1
8145	H	78.15500	73.93980	57.55690	1337.24937	-2722.63665	-835.00899	1
8146	C	76.60000	72.37380	57.56490	309.95694	430.93829	-741.39725	1
8147	H	75.90000	72.97980	56.94990	342.40933	-2245.93785	2176.40650	1
8148	H	76.05600	71.96080	58.44090	1084.66154	928.89903	-2803.36979	1
8149	C	77.41200	71.39580	56.68990	866.46906	252.80207	129.51252	1
8150	H	78.23700	70.92380	57.26490	-1870.34412	-1592.98019	1965.31250	1
8151	C	76.51500	70.32580	56.03890	-579.50716	-525.10325	468.92328	1
8152	H	75.79800	70.79480	55.33190	1948.98959	-2450.34638	308.97967	1
8153	H	77.06300	69.52180	55.50390	935.83366	-2836.40874	988.54796	1
8154	H	76.02800	69.82180	56.90090	-2204.04567	997.94039	-2011.10017	1
8155	C	78.08700	72.20080	55.55590	-548.67517	-215.89980	695.55290	1
8156	H	78.93000	72.84180	55.89090	2446.53965	-890.45067	-1766.28638	1
8157	H	77.35600	72.90380	55.10290	-19.42709	-3080.31590	-639.92405	1
8158	H	78.47800	71.55980	54.73690	-1972.30071	-1450.31055	1976.07071	1
8159	C	76.65800	74.51080	58.81890	231.98561	562.33357	-679.27508	1
8160	O	76.44500	75.53780	58.13990	714.06837	-40.17815	-334.84222	1
8161	N	76.13800	74.39180	60.04090	617.36970	286.62132	-499.37476	1
8162	H	76.10800	73.55980	60.58990	2165.59712	-1853.48418	-1331.54487	1
8163	C	75.18900	75.41980	60.53390	701.13198	-525.05250	253.34724	1
8164	H	74.52600	75.63580	59.70990	942.78482	-2944.10920	584.46903	1
8165	C	74.32700	74.98880	61.72290	-449.78881	-343.47278	-714.95978	1
8166	H	73.68700	75.85480	61.99690	2635.01368	188.31622	1708.64454	1
8167	H	75.08200	74.73680	62.49790	-2836.22068	1121.91519	771.61179	1
8168	C	73.43400	73.79580	61.37990	-400.29774	366.91327	732.52125	1
8169	H	73.87200	73.05280	60.67990	-2481.98041	-1112.62012	1581.16285	1
8170	C	73.20600	72.96180	62.64590	524.56692	373.61649	-645.51628	1
8171	H	72.47500	72.15780	62.41390	-135.19921	1449.58460	-2789.02347	1
8172	H	72.89900	73.58880	63.51090	-219.67440	-1200.96979	2899.59324	1
8173	H	74.09900	72.35780	62.91390	1564.87649	1580.78756	-2224.97157	1
8174	C	72.04600	74.18280	60.80190	-273.69235	416.04256	763.84036	1
8175	H	71.38500	73.30880	60.62390	749.99034	-2806.24561	1208.60509	1
8176	H	71.56400	75.00680	61.36990	1626.87072	-1973.16836	-1832.51863	1
8177	H	72.15400	74.59180	59.77490	-2157.38483	-596.93883	-2210.78741	1

8178	C	75.85100	76.71480	60.91390	422.05272	-388.77636	-708.64338	1
8179	O	75.24100	77.76980	61.06290	-536.29828	147.64734	560.54585	1
8180	N	77.17700	76.61080	61.06990	435.26067	426.40441	-584.29420	1
8181	H	77.61500	75.74080	60.85690	3076.65370	-173.31295	634.34286	1
8182	C	78.06900	77.62580	61.56690	-385.31104	623.44216	-542.50003	1
8183	H	77.44900	78.34180	62.08490	1219.20639	2253.68843	1825.55484	1
8184	C	79.05700	77.17280	62.62790	-209.66098	-676.59296	574.20837	1
8185	H	79.78300	77.96780	62.90290	-2046.86423	791.12563	2254.48293	1
8186	O	79.81600	75.99880	62.30490	-537.29814	487.37630	-312.09339	1
8187	H	79.18000	75.28680	62.20490	1726.20155	-1706.24308	2001.79644	1
8188	C	78.13500	76.76780	63.83490	244.30263	-860.47520	177.05836	1
8189	H	77.36500	77.55080	64.00490	-1786.84574	-1433.28235	-2156.64328	1
8190	H	78.74600	76.71880	64.76190	-1218.63170	2026.93918	2074.77241	1
8191	H	77.51500	75.84680	63.79690	-466.71224	-692.76123	3033.23059	1
8192	C	78.80100	78.28280	60.43990	-665.85034	456.81807	-423.57004	1
8193	O	79.82000	78.91780	60.65690	-552.27533	557.56958	87.95085	1
8194	N	78.35900	78.17880	59.20190	-162.28026	-574.47720	596.91989	1
8195	H	77.57900	77.59780	58.98190	-367.52315	-1901.80390	-2479.17222	1
8196	C	78.86300	79.05080	58.16390	-14.04506	-447.73381	-794.22174	1
8197	H	79.93700	78.96980	58.24790	-1992.67779	-1609.82420	1826.45216	1
8198	C	78.55500	78.55580	56.73090	655.95336	-529.40855	-347.71078	1
8199	H	77.45400	78.54380	56.58590	-2215.42451	2227.87174	-163.42572	1
8200	C	79.23400	79.47680	55.69190	-159.48417	502.42681	744.03166	1
8201	H	79.23300	79.06580	54.66090	2879.15674	-1266.80384	62.37558	1
8202	H	78.67300	80.41380	55.48890	3132.71444	-55.29409	-285.07721	1
8203	H	80.26600	79.78080	55.97290	-366.21256	-1156.54205	-2902.84775	1
8204	C	79.06900	77.10780	56.54390	-394.22383	621.10379	-538.76587	1
8205	H	79.00500	76.45980	57.44390	-2499.35262	-1550.88304	1116.34425	1
8206	H	80.15200	77.14780	56.29690	700.62728	2262.72359	-2070.61093	1
8207	C	78.26600	76.33080	55.51690	-565.96897	-633.65471	-331.07678	1
8208	H	78.23500	76.94280	54.59090	-1800.90823	-2245.03912	-1270.73015	1
8209	H	77.16900	76.27180	55.68190	2418.72941	-1963.84501	437.36376	1
8210	H	78.74700	75.33680	55.39290	667.24415	-2148.85118	2198.96568	1
8211	C	78.55300	80.52180	58.35990	641.49862	-13.07469	-647.88856	1
8212	O	79.45400	81.34280	58.28290	429.95962	-391.11820	-534.59191	1
8213	N	77.30800	80.94280	58.79090	-701.89462	110.25088	455.91773	1
8214	C	76.06600	80.31780	58.47990	-458.25423	444.20150	-651.25962	1
8215	H	75.80500	79.49080	59.17390	1834.49021	2545.03429	235.94993	1
8216	H	76.09400	79.92480	57.44090	-2289.01874	1680.45934	1354.50206	1
8217	C	77.11200	82.34380	59.28390	685.39954	588.08551	125.83284	1
8218	H	77.25900	83.06080	58.48990	-2803.66106	-1131.60613	-870.16002	1
8219	C	75.62100	82.35380	59.68890	265.07419	809.50247	-325.41118	1
8220	H	75.54600	82.00980	60.74290	-1970.85200	2004.33411	-1413.01571	1
8221	H	75.08500	83.32580	59.65190	-1975.54576	246.85397	2436.08462	1
8222	C	75.00600	81.34580	58.64290	-729.52436	511.26967	-194.54699	1
8223	H	74.62200	81.75380	57.68290	27.38355	2677.86276	1651.21997	1
8224	H	74.09500	80.94680	59.13790	-1442.41782	-2487.04692	-1277.59722	1
8225	C	78.03700	82.78180	60.40490	-288.39612	-864.61200	-26.92155	1
8226	O	78.48700	83.90380	60.44290	71.24541	-687.37751	-382.18253	1
8227	N	78.30300	81.91980	61.40090	198.69635	742.53901	349.03850	1
8228	H	77.87300	81.02280	61.32790	-2899.48114	1090.08704	550.40495	1
8229	C	79.25100	82.16380	62.47790	-722.98745	417.40509	-366.76032	1
8230	H	78.89200	83.09180	62.89790	1628.09794	-2323.51493	-1359.70648	1
8231	C	79.28600	81.04580	63.50590	819.55453	342.94851	205.34772	1
8232	H	80.16800	81.03780	64.18090	-2671.41909	1114.04009	-1233.15082	1
8233	H	79.41000	80.13580	62.87990	-1620.82808	-1182.19392	2423.54288	1
8234	C	78.00000	80.97680	64.30490	482.25145	637.00377	-439.44368	1
8235	O	77.75200	81.96580	65.02190	-547.32903	563.75195	79.00572	1
8236	O	77.25500	79.98480	64.24790	471.88587	-373.17630	511.55685	1
8237	C	80.65900	82.48880	61.91190	-606.37378	-460.62791	501.58127	1
8238	O	81.35100	83.42380	62.34390	426.03667	-539.98626	387.98817	1
8239	N	81.09300	81.65880	60.95190	222.40387	228.73368	781.59434	1

8240	H	80.60900	80.81980	60.71590	878.16134	-204.40596	-3014.17934	1
8241	C	82.35100	81.84880	60.18090	-65.79329	-908.34534	45.06656	1
8242	H	83.14500	81.81080	60.91190	960.33334	-2233.31578	-1997.06954	1
8243	C	82.61200	80.57680	59.36790	656.24266	-411.00044	-481.53422	1
8244	H	81.68500	80.38480	58.78690	2137.83445	256.08662	-2293.97248	1
8245	H	82.65500	79.66680	60.00390	1811.37974	2258.80147	1230.83126	1
8246	C	83.86900	80.51280	58.43890	592.11703	-547.29352	-425.81478	1
8247	C	85.11900	81.10280	58.74990	458.80924	-635.21661	-466.30992	1
8248	H	85.29600	81.67880	59.64590	-1969.18704	-1703.49115	1765.96900	1
8249	C	86.16200	81.10780	57.83790	-577.35659	-705.72029	-8.32061	1
8250	H	87.06200	81.63480	58.11890	917.19045	2209.95698	-2042.81131	1
8251	C	85.98200	80.43580	56.65890	-883.29316	208.07235	89.16331	1
8252	H	86.69700	80.46980	55.84990	-1065.22346	-984.63313	-2791.77772	1
8253	C	83.79600	79.72480	57.31990	462.88303	622.13985	-479.72107	1
8254	H	82.86100	79.25980	57.04390	-888.21074	1701.64388	-2492.73264	1
8255	C	84.80600	79.76980	56.36290	531.78267	-487.63267	-557.55948	1
8256	H	84.81800	79.17080	55.46490	-2241.90357	-1139.90078	-1890.16423	1
8257	C	82.49700	83.11280	59.39990	-4.58079	-673.93494	-614.20006	1
8258	O	83.51000	83.80280	59.50090	289.26115	-607.22467	413.80360	1
8259	N	81.49500	83.40680	58.56490	-483.96202	-633.02836	-278.79768	1
8260	H	80.75700	82.74780	58.43890	-2093.70205	-2006.71631	1219.72440	1
8261	C	81.46900	84.64280	57.71890	451.47373	-784.39792	111.09623	1
8262	H	82.41100	84.77380	57.20590	-1818.09101	-1530.39103	-2061.71642	1
8263	C	80.38000	84.70980	56.67890	591.42356	-262.21945	-642.58084	1
8264	H	79.41800	84.79380	57.22890	-1933.84250	-1014.42248	-2264.82372	1
8265	C	80.45686	85.88293	55.79994	413.04579	141.05967	-645.30895	1
8266	H	80.68751	86.80430	56.45108	-931.50006	1914.90435	325.54677	1
8267	H	79.55866	86.14063	55.22972	2176.19515	2042.98896	-4003.35956	1
8268	H	81.28014	85.80988	55.08561	-173.47066	-802.50749	1787.08957	1
8269	C	80.27800	83.41680	55.77490	71.22585	-730.26392	541.38017	1
8270	H	80.08400	82.53880	56.42690	1881.30631	2002.94117	-1532.03769	1
8271	H	81.26700	83.29280	55.28390	586.69067	2093.17112	2274.34715	1
8272	C	79.15000	83.46480	54.79990	521.37426	-376.54092	-646.40298	1
8273	H	79.31000	82.70080	54.00990	-857.53232	1957.92398	2308.54895	1
8274	H	79.14200	84.43280	54.25390	1805.22892	-574.56076	-2511.82299	1
8275	H	78.13300	83.27280	55.20590	1499.02114	-2753.28145	-265.71247	1
8276	C	81.38667	85.93525	58.68576	-475.58116	-254.48192	-487.36571	1
8277	O	81.97184	86.98951	58.42863	-351.06907	716.89081	1217.01555	1
8278	N	80.63890	85.80162	59.82376	9.51262	467.27370	-128.09444	1
8279	H	80.02851	85.02462	60.05358	-14.41479	-1372.21897	-532.25364	1
8280	C	80.33376	87.11158	60.27496	-422.47009	-495.31332	232.28871	1
8281	H	80.76132	87.91241	59.53880	-70.04854	2162.44828	1003.53519	1
8282	C	78.74030	87.29488	60.37232	-241.24973	166.09362	230.35635	1
8283	H	78.28586	86.58599	61.06598	1095.78749	789.36063	-1226.43986	1
8284	H	78.47875	88.29338	60.75210	-243.40348	-886.45688	75.49631	1
8285	C	78.07715	87.18127	58.98954	193.24388	464.59047	821.11010	1
8286	C	77.99095	88.32427	58.07941	-483.53674	723.55425	-312.72950	1
8287	H	78.44477	89.27134	58.35781	-298.71723	427.96880	1880.68178	1
8288	C	77.61558	88.18080	56.74189	316.16586	148.20284	-173.20898	1
8289	H	77.85181	88.98145	56.02474	-2617.48983	1836.44737	3331.77924	1
8290	C	77.14616	86.88906	56.31924	-444.80536	190.24870	-87.46002	1
8291	H	76.74979	86.88161	55.20684	125.19324	1541.01590	819.77797	1
8292	C	77.49418	85.96407	58.59942	-390.31865	-250.14350	270.59737	1
8293	H	77.34229	85.11443	59.31524	-231.21311	-215.66281	-1582.92903	1
8294	C	77.12350	85.80126	57.19613	749.52960	-1028.16510	462.24438	1
8295	H	76.57401	84.90397	56.87830	263.06003	-2326.48142	-908.55069	1
8296	C	80.82092	87.27440	61.83894	-141.65363	-501.28005	-304.43783	1
8297	O	80.30564	88.14267	62.49908	707.78839	77.40343	758.48117	1
8298	N	81.85324	86.51339	62.15908	-35.87483	832.22019	21.49138	1
8299	H	82.24734	85.92183	61.41448	938.37710	-819.27174	2590.91883	1
8300	C	82.60536	86.81547	63.34131	294.70287	-234.19260	-703.22315	1
8301	H	81.95926	87.29646	64.14949	-3407.26324	-654.61196	-2487.01207	1

8302	C	83.25771	85.43093	63.73554	614.65099	796.93054	228.21695	1
8303	H	84.05400	85.51755	64.54360	-51.44944	2750.95283	-147.92748	1
8304	H	83.68000	84.87680	62.92990	-2797.18605	-1173.47946	834.81879	1
8305	H	82.44800	84.78880	64.16490	741.18275	1458.74523	-2687.18007	1
8306	C	83.74932	87.80119	62.72744	975.72568	527.25563	114.50578	1
8307	O	84.43103	87.54542	61.68632	-551.33096	742.22006	61.15466	1
8308	N	83.86412	88.82423	63.49933	82.63079	5.84391	-32.23886	1
8309	H	83.34657	88.92537	64.37052	521.01442	3826.39061	-470.05453	1
8310	C	84.66968	89.93853	63.10244	-989.12613	-579.69111	18.27059	1
8311	H	85.23576	89.56734	62.22574	2514.30643	-457.84553	2482.50536	1
8312	C	83.62089	91.12787	62.81422	116.00373	58.61662	453.80894	1
8313	H	82.98174	90.84031	61.92566	1010.45014	3606.86006	-1439.55050	1
8314	H	84.26569	91.98904	62.62340	-937.49838	699.75035	551.04376	1
8315	C	82.51980	91.59240	63.83254	272.42179	613.82162	-504.93275	1
8316	O	82.62591	92.57319	64.52464	-438.28667	-475.76738	3.20152	1
8317	N	81.39390	90.78449	63.76465	-378.61342	-337.11005	272.29801	1
8318	H	81.48813	89.91236	63.17041	-155.35808	198.24426	-2180.59128	1
8319	H	81.08326	90.46871	64.68746	-1743.33838	904.24840	5276.01707	1
8320	C	85.67646	90.36592	64.30829	475.33637	-159.60417	183.10774	1
8321	O	85.25979	90.28544	65.44358	647.12791	76.60527	113.23229	1
8322	N	86.86691	90.75119	63.87660	-443.98815	935.47706	308.10848	1
8323	H	87.01282	90.75094	62.87830	-2182.22477	-1999.66522	-620.26786	1
8324	C	87.62619	91.74852	64.61301	447.26403	-518.21727	-206.06407	1
8325	H	87.56915	91.28356	65.66179	391.87631	601.02803	172.10359	1
8326	C	89.10173	91.65341	64.18704	857.41899	40.23868	-260.40795	1
8327	H	89.26266	90.59120	63.90645	1737.18446	-1246.06655	-1043.44175	1
8328	C	89.35880	92.52449	62.99770	-237.21556	354.76581	-599.25918	1
8329	H	89.84387	93.50932	63.44540	1460.50915	-780.45079	-194.61286	1
8330	H	88.46013	92.71952	62.42951	-2708.13910	815.73151	-62.70498	1
8331	H	90.06178	92.07318	62.22331	2795.54626	466.12536	1843.40910	1
8332	C	90.00252	91.95926	65.33841	108.75261	-803.27256	-382.11586	1
8333	H	89.69255	92.86882	65.87063	1643.64777	-43.23614	-718.73441	1
8334	H	89.92489	91.14459	66.12001	3084.87723	-1769.95916	-1351.19340	1
8335	H	91.07827	92.13416	65.07974	127.39898	-2993.19454	-1340.39978	1
8336	C	86.99011	93.29315	64.50166	271.57999	-163.85338	664.03473	1
8337	O	86.70968	93.85606	63.46306	-407.92164	-536.13715	238.32188	1
8338	N	87.20999	93.93451	65.67052	25.69568	333.69893	563.45035	1
8339	H	87.47886	93.17402	66.33185	-2010.11008	-1676.22003	837.29704	1
8340	C	86.14516	94.93079	65.83724	426.11849	-551.12093	-768.73063	1
8341	H	86.21907	95.53550	64.88032	-1101.53068	635.51119	1693.57634	1
8342	C	84.79652	94.15612	65.85904	281.43076	-121.24254	1314.10285	1
8343	H	84.99626	93.20944	66.37933	-1007.27599	-946.78283	1470.78178	1
8344	H	84.37228	93.92033	64.85651	4162.58653	3819.75298	-1138.45243	1
8345	O	83.46979	94.97094	66.22639	38.05995	-522.70423	702.40690	1
8346	H	82.90378	94.18564	66.15491	770.92107	-1198.18178	823.14265	1
8347	C	86.50039	95.69179	67.22580	29.92230	-621.63284	546.71296	1
8348	O	87.64609	95.95988	67.52200	384.37102	-57.99822	-469.93178	1
8349	N	85.39360	95.81692	67.94694	-484.70859	59.76843	-155.37227	1
8350	H	84.41343	95.63681	67.59731	-1292.33810	-501.23832	-609.03395	1
8351	C	85.61236	96.28502	69.29573	-595.50292	896.45011	1088.53855	1
8352	H	86.59937	95.80408	69.62881	-518.17295	2491.58506	56.83088	1
8353	C	85.63485	97.85631	69.13991	-160.76880	-89.36055	215.16332	1
8354	H	84.90252	98.24357	69.89678	-928.62455	1072.92023	-216.49209	1
8355	H	85.34127	98.09892	68.09854	-1929.67108	446.02703	3929.48446	1
8356	C	87.04016	98.45753	69.17387	36.99528	-0.41535	-65.72457	1
8357	H	87.48509	98.30408	70.15874	1371.38950	-129.69585	-0.95491	1
8358	H	87.68772	97.96097	68.37528	1342.92802	406.66728	2318.26168	1
8359	C	86.99091	100.05146	68.94509	426.64957	778.26126	-255.43428	1
8360	O	88.10852	100.54829	68.74980	-410.56447	231.29216	-669.94526	1
8361	O	85.93472	100.67784	69.00671	-265.04733	683.72904	-819.25098	1
8362	C	84.32975	95.99414	70.26331	465.84884	-239.58224	53.14136	1
8363	O	83.16903	95.70512	69.97979	-619.69794	-236.20082	228.70104	1

8364	N	84.87334	95.93255	71.50998	44.95605	-1087.72783	910.20387	1
8365	H	85.79426	96.33745	71.45691	-383.12752	1596.17933	355.83587	1
8366	C	83.95832	96.18800	72.58071	21.16823	586.78791	-287.80267	1
8367	H	82.98109	96.54699	72.28155	191.18863	-2668.85495	1682.41540	1
8368	C	83.78786	94.89043	73.47929	702.31363	-544.45829	-806.43504	1
8369	H	82.97714	95.07777	74.24571	720.10593	-1443.15323	3277.05570	1
8370	H	84.80083	94.71510	73.94383	3040.24938	-1046.20419	2745.60251	1
8371	H	83.53851	94.00234	72.87606	514.25029	181.93329	-545.96032	1
8372	C	84.78295	97.28986	73.44111	-448.71127	-101.19640	-57.87145	1
8373	O	86.01181	97.35468	73.31323	865.61573	43.19804	-110.12352	1
8374	N	84.09935	98.04601	74.28230	-1123.92728	-310.20480	-361.64510	1
8375	H	83.14214	97.58813	74.49825	33.66125	-245.49355	-327.72936	1
8376	C	84.84389	98.59528	75.40689	452.87195	-329.96150	-246.43860	1
8377	H	84.01651	99.14127	76.01016	-2411.57216	1656.62518	854.34896	1
8378	C	85.72169	97.59514	76.29611	-869.61517	571.02633	131.32169	1
8379	H	86.41827	96.97769	75.61140	482.36421	-1850.17661	1367.81530	1
8380	H	86.45491	98.13553	76.96107	3125.42981	2324.94928	180.32540	1
8381	C	84.90688	96.54865	77.10342	99.63753	557.72629	-129.94243	1
8382	O	83.70543	96.49892	77.17789	-289.29289	-381.61815	509.17930	1
8383	O	85.59701	95.56523	77.80676	882.40183	185.60464	1.21402	1
8384	C	85.86036	99.62183	74.69244	173.88814	281.26081	37.50868	1
8385	O	86.84256	100.01648	75.31337	278.46326	74.92960	475.61248	1
8386	N	85.44080	100.21620	73.54816	521.35975	-223.89592	-692.51473	1
8387	H	84.52535	99.79622	73.29341	1124.74761	782.43681	1105.80377	1
8388	C	86.29580	100.87519	72.60988	469.95105	-216.42265	556.39649	1
8389	H	85.72842	100.76638	71.64521	1615.57653	1850.41641	642.90871	1
8390	C	86.33311	102.36203	73.09961	-284.72611	636.50845	148.19692	1
8391	H	86.93820	102.81460	72.22359	4946.79778	-1425.47675	-905.09515	1
8392	H	86.93067	102.57855	74.11646	-519.08385	1090.80958	-959.35539	1
8393	C	84.91240	103.03265	73.20799	189.38283	-178.81596	-135.09836	1
8394	O	84.90637	104.13337	73.83363	-531.29117	-477.53355	-567.83585	1
8395	O	83.83215	102.51801	72.71427	91.49310	-348.99294	-6.61733	1
8396	C	87.88112	100.41803	72.56776	78.03473	-14.15609	-528.50321	1
8397	O	88.76009	101.22903	72.54309	-425.03561	57.32298	-630.18618	1
8398	N	87.92252	99.10091	72.27554	-206.34314	236.89178	-138.57500	1
8399	H	87.18766	98.38085	72.45236	1590.46478	987.20913	2685.99503	1
8400	C	89.30859	98.63303	72.14959	1331.85475	193.89408	145.34070	1
8401	H	89.87029	99.61766	72.06763	-1352.94568	-1698.54797	-3386.26569	1
8402	C	89.75520	97.70348	73.35192	768.72735	413.74473	-756.37924	1
8403	H	89.63037	96.66563	72.96672	-852.74182	-123.84866	23.70901	1
8404	H	90.83610	97.84431	73.59529	-1929.11605	-748.92233	4135.94110	1
8405	C	88.94989	97.74278	74.67609	197.44886	469.45063	1201.65313	1
8406	H	87.96279	98.18975	74.38574	1093.43699	6710.82575	-2643.20797	1
8407	H	89.26660	98.58368	75.27135	-3309.36834	375.55837	-1151.84802	1
8408	C	88.87726	96.39703	75.53600	190.80271	588.11670	716.80120	1
8409	H	88.28268	96.53624	76.50773	-3164.76811	-865.70071	-2567.46435	1
8410	H	89.88896	95.92934	75.84819	-354.33983	847.37022	1835.08818	1
8411	N	88.16046	95.51430	74.64918	249.01627	-668.97081	-40.15919	1
8412	H	87.83008	95.83828	73.74050	663.02271	3289.91120	210.90721	1
8413	C	87.75936	94.32475	74.90116	-328.02999	-727.28151	-456.97049	1
8414	N	86.99382	93.56190	74.00399	246.50669	115.84984	1048.90536	1
8415	H	86.81622	93.78188	72.96768	-1286.71124	-1002.07078	1334.73951	1
8416	H	86.88097	92.52394	74.26961	1432.13413	1816.21356	-2262.70483	1
8417	N	88.09499	93.72645	76.14292	-401.43757	-252.64164	1021.47138	1
8418	H	88.55775	94.29058	76.87854	1267.46391	-584.54587	544.52163	1
8419	H	87.70038	92.89699	76.61748	1351.94164	-976.95011	-2353.35122	1
8420	C	89.59333	97.69828	70.82188	-402.66099	375.27984	-650.85956	1
8421	O	90.41053	98.05150	70.01046	-242.83182	-430.37827	237.91031	1
8422	N	88.85565	96.55629	70.86489	203.81714	326.68702	41.12683	1
8423	H	88.31556	96.46754	71.70502	1401.02113	-1499.64576	-2196.11543	1
8424	C	89.10879	95.46779	70.03204	-611.91592	-72.02405	421.51517	1
8425	H	88.96693	95.99514	69.05341	310.29661	3117.20018	-147.87687	1

8426	C	90.61179	94.95915	70.33775	157.04107	-985.24914	60.08874	1
8427	H	90.64238	94.24109	71.25842	1740.41356	-882.21108	1582.18156	1
8428	H	91.23480	95.89280	70.66017	1082.28205	135.89736	-2177.42203	1
8429	C	91.24467	94.23278	69.14184	238.55351	243.50472	-836.75391	1
8430	C	91.30391	94.88903	67.87709	22.94787	-545.14234	-411.15703	1
8431	H	90.93018	95.90329	67.67878	991.28731	-3423.48930	-71.33105	1
8432	C	91.92991	94.26433	66.78971	-652.04214	-329.86708	655.01854	1
8433	H	91.97422	94.83127	65.81837	-1064.49394	1847.15292	1233.78730	1
8434	C	92.56561	92.98961	66.89573	110.51012	626.13696	168.06784	1
8435	O	93.24368	92.54663	65.75727	163.72355	704.99895	635.68365	1
8436	H	93.86912	91.88788	66.28952	-272.04675	-1296.77604	-577.90210	1
8437	C	91.77573	92.91637	69.22392	334.06746	-74.23468	449.99155	1
8438	H	91.86739	92.39441	70.24168	3084.01870	922.58004	1922.52707	1
8439	C	92.34590	92.29140	68.11159	-20.73098	17.03181	-965.28096	1
8440	H	92.66514	91.19085	68.20700	1033.18511	-1497.57256	7.86549	1
8441	C	87.99807	94.39828	70.47175	821.81982	-429.41061	185.03542	1
8442	O	87.52949	94.53929	71.60068	1137.25568	567.60905	-69.52345	1
8443	N	87.74036	93.48879	69.56661	317.53991	-39.25316	461.96714	1
8444	H	88.14724	93.44628	68.62384	3744.28559	1938.99611	2713.29174	1
8445	C	87.05411	92.28142	69.95388	205.10897	547.82132	144.64496	1
8446	H	87.67711	91.92004	70.75507	918.25984	640.54383	-1345.70670	1
8447	C	85.54080	92.65570	70.41136	-93.86961	-1062.94366	911.64402	1
8448	H	85.50382	93.45663	71.16972	176.74912	-1349.02710	4031.65579	1
8449	C	84.62262	93.08869	69.23366	-327.31710	210.07669	-402.29823	1
8450	H	85.02145	94.04347	68.87500	-73.76985	1814.61743	3133.41058	1
8451	H	84.53937	92.32085	68.39976	1673.76856	-3008.73850	-1341.60774	1
8452	H	83.57142	93.30722	69.55672	149.25374	-692.87439	1764.87814	1
8453	C	84.65498	91.53467	70.96466	229.60999	-1202.82854	73.69921	1
8454	H	84.62756	90.70580	70.20807	-269.54342	607.69568	-663.88000	1
8455	H	83.61588	91.89345	71.34739	1958.55351	2379.30098	-505.93744	1
8456	C	85.12001	90.96964	72.37209	-584.26990	140.72841	-691.78487	1
8457	H	85.15574	91.84274	73.05726	-1435.94424	-2426.97662	-1230.90230	1
8458	H	84.31746	90.24719	72.77304	-1783.37649	2181.44730	-924.67841	1
8459	H	86.09584	90.36286	72.25727	-546.70416	-1781.73665	-2960.41459	1
8460	C	87.06675	91.30836	68.68534	-173.30124	-401.51626	38.31902	1
8461	O	87.26229	91.58788	67.52331	-41.61573	261.43029	184.35275	1
8462	N	86.66564	90.05696	69.20281	-363.97297	-497.36444	-850.78330	1
8463	H	86.48258	90.18673	70.21861	291.94896	-2870.71598	-1943.85253	1
8464	C	85.93942	89.17816	68.31673	-161.62691	-31.62881	-917.41295	1
8465	H	86.12756	89.38051	67.20591	1270.67244	1831.18362	268.68240	1
8466	C	86.37075	87.79563	68.89158	-52.17779	-699.10388	0.18130	1
8467	H	87.50993	87.76152	68.81205	1750.80543	235.58722	-2680.11286	1
8468	H	86.19936	87.84577	70.03451	-4174.67728	-641.85866	-494.29405	1
8469	S	85.52198	86.47885	67.99002	-152.26887	-315.19606	570.85935	1
8470	C	84.33855	89.25035	68.63877	594.25454	-310.58746	-63.28855	1
8471	O	83.79438	88.82945	69.66138	390.78948	-403.76587	478.98870	1
8472	N	83.75475	89.91598	67.63585	411.57465	-888.00620	-315.13954	1
8473	H	84.26691	90.21625	66.73195	897.26896	897.32465	-3241.95973	1
8474	C	82.33880	90.00496	67.74562	883.01211	-509.18621	-898.03276	1
8475	H	82.16647	89.61768	68.86146	942.21023	934.38584	-336.85352	1
8476	C	82.06719	91.51655	67.45227	27.72311	625.89689	716.94826	1
8477	H	81.64441	91.73781	66.43074	-1518.30221	1868.59148	-740.90090	1
8478	H	83.02716	92.11828	67.70811	-2170.42145	2049.41541	-61.64802	1
8479	C	80.85722	91.93117	68.41600	255.05738	417.44246	18.49926	1
8480	O	80.33548	93.01724	68.16721	-288.01202	-825.38452	-104.70897	1
8481	O	80.59761	91.22076	69.41109	-548.13783	-256.34180	762.55758	1
8482	C	81.60201	89.14690	66.51551	-695.71261	-592.16265	286.98363	1
8483	O	82.29234	88.50517	65.72455	-210.60036	-164.12211	-237.86310	1
8484	N	80.32666	89.20755	66.62524	-960.26116	-121.94665	-561.70695	1
8485	H	80.06168	89.78987	67.34272	-1834.46459	-3400.64120	-2256.84906	1
8486	C	79.38100	88.42660	65.90610	514.16505	402.94169	265.19326	1
8487	H	80.02413	87.81546	65.12885	2482.85572	627.97064	-715.51614	1

8488	C	78.53719	87.55818	66.90744	-634.42496	-758.12191	-183.74631	1
8489	H	77.66401	88.25053	67.11056	2052.89449	-1260.65560	1071.84502	1
8490	H	79.04433	87.41031	67.95595	-1156.81808	1565.16366	-2527.88623	1
8491	C	77.97176	86.17876	66.38003	-97.06497	493.79047	-348.46209	1
8492	H	77.48333	86.33262	65.42276	-1024.80386	1937.54332	-734.22248	1
8493	H	77.22944	85.76523	67.05409	602.31916	2867.51790	-2929.39279	1
8494	C	79.26617	85.23981	66.51095	-254.28397	471.20277	663.58840	1
8495	H	79.85145	85.33841	65.56722	-872.45319	3374.17164	3315.06032	1
8496	H	79.75061	85.27246	67.55093	-310.13598	2286.52919	-2394.75943	1
8497	N	78.71300	83.93980	66.64390	139.49274	632.25749	541.72366	1
8498	H	78.51800	83.39480	65.82790	1546.00063	1711.60222	-2139.74908	1
8499	C	78.40500	83.36480	67.75690	-660.28185	376.69649	-503.56592	1
8500	N	78.10900	83.97080	68.86490	784.59473	306.33082	-56.96336	1
8501	H	78.26600	84.95480	68.95690	-1717.42843	1638.68264	-2064.79661	1
8502	H	77.74400	83.35480	69.56290	-1352.92526	1935.42880	-2078.92637	1
8503	N	78.05200	82.10080	67.70790	-565.40399	528.41277	-337.29892	1
8504	H	78.04200	81.66580	66.80690	-1268.65259	2583.95523	1269.61498	1
8505	H	77.44800	81.87880	68.47390	-1851.91353	1823.05462	-1773.44702	1
8506	C	78.34279	89.50023	65.24000	-191.25708	-1039.67988	-4.51786	1
8507	O	77.40088	89.92593	65.88281	205.62635	-843.73815	-300.52034	1
8508	N	78.59988	89.72579	63.92814	123.74416	-697.30614	-703.64508	1
8509	H	79.34752	89.28495	63.38726	816.07096	1822.74750	3512.33770	1
8510	C	77.90748	90.87888	63.53040	-266.69644	535.32696	-262.26583	1
8511	H	77.02182	91.05692	64.20936	1229.50607	-165.07414	-521.61279	1
8512	C	78.94977	92.06080	63.36749	-161.38504	740.20551	-645.11979	1
8513	H	79.91181	91.77736	63.84447	-567.52078	1237.76002	-865.34918	1
8514	H	79.14045	92.23226	62.26723	774.76254	1203.32556	1804.72387	1
8515	C	78.16366	93.17623	64.08690	-292.79067	-553.42921	958.38816	1
8516	C	78.62580	93.50177	65.42399	569.45677	184.11784	-807.08269	1
8517	H	79.59967	93.11406	65.79759	4.37172	-2950.76658	2306.07561	1
8518	C	77.86761	94.45844	66.13678	-165.90192	362.11525	295.76908	1
8519	H	78.14767	94.79861	67.14296	181.45528	2561.75492	1186.55822	1
8520	C	76.75534	95.08153	65.54370	-1102.73419	264.29587	-880.45640	1
8521	H	76.24733	95.81462	66.13869	1719.28294	-3381.42627	137.14102	1
8522	C	77.01203	93.78840	63.46830	95.94991	-13.53041	-37.86002	1
8523	H	76.70369	93.46401	62.44131	1086.27478	-640.09281	483.27030	1
8524	C	76.37158	94.81268	64.17437	-379.58367	512.37327	-248.19777	1
8525	H	75.57291	95.37816	63.69630	-538.88203	-1600.68762	2394.88455	1
8526	C	77.55927	90.68009	61.84060	-342.65700	-103.30159	-29.75598	1
8527	O	78.42946	90.40879	61.04597	121.51745	-872.84101	339.81987	1
8528	N	76.26200	90.83308	61.62183	-189.25414	536.19588	-95.33472	1
8529	H	75.88456	91.29651	62.44060	2346.07495	1739.53608	-1310.65771	1
8530	C	75.58244	90.08459	60.63529	847.59650	-1023.28119	408.22562	1
8531	H	76.36961	89.37183	60.27086	-88.40027	-1977.44808	-2065.50964	1
8532	C	74.25477	89.44268	61.28631	-396.51718	782.85084	-54.87195	1
8533	H	73.56909	89.04327	60.44308	3035.60702	2925.97863	-17.21000	1
8534	H	73.61440	90.27775	61.75645	1113.14905	149.91595	-805.45529	1
8535	C	74.66093	88.39196	62.29082	364.69064	-1123.95807	-1085.40206	1
8536	C	74.60115	87.00481	61.99636	-111.62325	-1428.14211	869.67407	1
8537	H	74.28990	86.75491	60.98287	2018.51260	334.61020	1530.78645	1
8538	C	74.74421	86.07201	63.02420	128.16864	689.69721	-189.91480	1
8539	H	74.54097	85.00905	62.87764	-2321.86884	2801.39844	2788.85245	1
8540	C	75.10321	86.50787	64.37151	480.39580	722.08477	-130.32975	1
8541	O	75.14942	85.61968	65.49835	629.02520	36.01810	482.09053	1
8542	H	75.54600	84.77580	64.99090	11.90255	-1173.96099	2918.88680	1
8543	C	75.10862	88.81402	63.58283	105.00368	-597.45474	-941.34327	1
8544	H	75.06815	89.89916	63.66145	-1102.98005	1424.53467	-161.05614	1
8545	C	75.34079	87.91139	64.57813	-505.14311	316.32548	-121.24479	1
8546	H	75.63179	88.27337	65.51127	-4536.32195	1541.88568	-725.03867	1
8547	C	75.12145	91.16183	59.53191	-509.98152	-264.36111	-499.80016	1
8548	O	75.07478	92.35135	59.70311	214.88198	689.79362	606.39100	1
8549	N	74.74806	90.47668	58.41013	261.23665	-12.39625	-53.04116	1

8550	C	74.82651	89.03707	58.16562	-346.92214	-733.51151	-1396.34786	1
8551	H	75.95626	88.88009	58.40549	1411.64871	-288.38954	-624.97035	1
8552	H	74.19013	88.35062	58.83906	-3331.88841	-1821.22496	474.01606	1
8553	C	74.33257	91.23085	57.27112	-10.70823	140.94064	1224.72303	1
8554	H	75.06617	92.05785	57.36728	1347.43548	2692.72690	-1552.40375	1
8555	C	74.55985	90.28829	56.01126	-337.03700	87.87420	-448.47510	1
8556	H	73.84786	90.58072	55.17741	1544.15993	100.21795	1090.17920	1
8557	H	75.57390	90.44031	55.56715	304.96446	-1024.40247	-3836.87817	1
8558	C	74.35674	88.86791	56.67221	-179.82550	-121.14797	229.88742	1
8559	H	73.26232	88.58556	56.70524	-1685.27734	206.38499	1259.68566	1
8560	H	74.91544	88.03421	56.14796	-1312.34708	-3111.58912	-1423.76312	1
8561	C	72.74583	91.62525	57.39506	-327.59201	924.10172	-50.61677	1
8562	O	72.30489	91.96786	56.29595	198.13508	140.14038	412.66154	1
8563	N	72.06013	91.34973	58.51355	247.02958	-31.26979	653.12705	1
8564	H	72.71849	91.03481	59.23472	1548.12177	1687.14880	1678.93535	1
8565	C	71.02944	92.26972	58.84489	-18.13075	307.45909	84.64113	1
8566	H	71.23684	93.36043	58.65575	1005.79743	2242.58546	-900.18756	1
8567	C	69.69350	91.86795	58.02159	-1627.55963	715.65000	162.61593	1
8568	H	70.07347	91.83412	56.97951	1325.67518	1977.16375	589.75238	1
8569	H	69.39628	90.80132	58.19583	861.21924	1534.89122	2584.56452	1
8570	C	68.56694	92.86501	58.14519	-83.25220	265.08301	-1131.10710	1
8571	O	68.29446	93.52825	59.18127	-203.18636	-904.62676	-59.17760	1
8572	N	67.69850	92.87748	57.08720	58.07429	-426.57066	-243.39960	1
8573	H	67.80770	92.39020	56.23546	127.86355	-26.86467	-2735.03710	1
8574	H	66.89117	93.46899	56.90958	3065.09629	4006.10451	-2711.80618	1
8575	C	70.93794	92.02598	60.44617	136.43046	-265.18471	194.71657	1
8576	O	71.78731	91.28792	60.87099	-146.67900	-231.36474	103.71072	1
8577	N	70.00733	92.74920	61.09012	128.88462	-1211.04541	-448.81245	1
8578	H	69.40334	93.42421	60.54600	-3376.42146	1757.71697	1642.98666	1
8579	C	69.40375	92.05552	62.24249	476.45665	82.68046	-385.50914	1
8580	H	70.20781	91.40998	62.57494	1533.58734	3898.89455	1006.13894	1
8581	C	69.09859	93.21509	63.22059	826.96726	50.16857	213.48069	1
8582	H	69.68257	94.07966	62.87519	-1501.14003	259.10799	702.79399	1
8583	H	68.05119	93.63565	63.03541	-2051.78226	-1392.61638	2215.99302	1
8584	C	69.42888	92.86430	64.77427	404.84303	-177.03687	-173.48959	1
8585	O	70.63244	92.87685	65.12411	941.36320	575.88919	-161.49260	1
8586	O	68.50008	92.70126	65.53971	-6.31688	3.83150	70.74667	1
8587	C	68.08195	91.24012	61.95098	-757.84099	-361.48897	-58.29884	1
8588	O	67.83260	90.33279	62.79404	-384.77348	640.95519	224.11388	1
8589	N	67.33010	91.60427	60.92187	658.56521	-124.87636	-323.10465	1
8590	H	67.78417	92.34544	60.29101	437.50617	1095.20958	3631.18879	1
8591	C	66.39450	90.59976	60.44194	277.32871	-1497.86424	142.73669	1
8592	H	65.65851	90.33412	61.20267	-2013.95744	-5313.78910	-761.90668	1
8593	C	65.73686	91.46568	59.33226	-708.83939	1049.40941	4.28744	1
8594	H	65.53062	92.47544	59.86914	607.14654	-394.82866	108.54781	1
8595	H	66.45571	91.76415	58.55384	2761.21269	-1102.24158	223.63392	1
8596	C	64.36890	91.07435	58.62186	-4.33159	-79.65384	152.46880	1
8597	H	64.52000	90.61587	57.62024	232.08933	-1231.78483	816.99141	1
8598	C	63.65948	90.04772	59.59402	465.14261	1435.00403	480.40771	1
8599	H	62.57107	89.99000	59.43559	-12.37848	-1979.21354	-1520.40345	1
8600	H	63.88195	90.28650	60.67806	42.89221	-1439.31324	13.80832	1
8601	H	64.06729	89.00302	59.50323	3597.47181	-2464.70211	42.83711	1
8602	C	63.45985	92.33902	58.41477	669.38693	-828.26492	-365.14642	1
8603	H	63.15022	92.80920	59.38854	4132.34464	1254.46036	1639.10680	1
8604	H	64.08264	93.18965	57.87451	-1183.17018	-142.97664	-1890.53710	1
8605	H	62.52703	92.14150	57.79681	-960.94612	-1880.41294	2918.58900	1
8606	C	67.04694	89.15639	59.89211	-255.49137	558.54667	-496.74140	1
8607	O	66.28911	88.25489	59.58738	-198.01649	173.84875	-211.00871	1
8608	N	68.32203	89.27286	59.53649	459.56268	785.84383	-202.18951	1
8609	H	68.68951	90.16414	59.93156	566.67136	1209.45612	-1959.15099	1
8610	C	69.10042	88.05948	59.54321	-11.27255	1049.40155	-5.10863	1
8611	H	68.42172	87.31174	58.99034	-1464.58541	-683.40745	-1861.80656	1

8612	C	70.50758	88.22242	58.78752	-586.57922	-13.52443	742.78871	1
8613	H	71.17267	87.36405	59.08454	-1366.75587	-2741.64145	598.33531	1
8614	H	71.13247	89.16327	59.07799	-2042.15676	-422.87675	-3650.57818	1
8615	C	70.19853	88.07343	57.31521	122.44735	4.80143	684.50254	1
8616	C	70.16255	88.94954	56.22180	-308.92772	-535.50068	878.62335	1
8617	H	70.41706	90.02973	56.03913	-2089.08558	1161.38969	70.89811	1
8618	N	69.81196	88.26556	55.13061	70.85981	-798.62983	-190.08134	1
8619	H	69.72795	88.80513	54.27325	2470.01953	3277.87806	-2190.83209	1
8620	C	69.67467	86.91792	55.36204	-141.80605	1096.82488	-178.68544	1
8621	C	69.81067	86.76110	56.82302	270.36541	-612.75657	-236.20599	1
8622	C	69.73458	85.46024	57.44397	391.72418	39.15720	-174.16530	1
8623	H	69.98933	85.24480	58.49650	-287.67505	1064.80955	-1022.78410	1
8624	C	69.68000	84.43180	56.55090	-249.17678	520.15760	706.25633	1
8625	H	69.73600	83.43380	56.95890	1509.78763	463.94103	2720.94217	1
8626	C	69.50253	85.79179	54.45120	355.40396	-183.56537	848.15577	1
8627	H	69.57747	85.93799	53.29714	-3883.37732	1197.37838	3543.29291	1
8628	C	69.46400	84.55980	55.13790	-726.02323	-516.91701	192.71243	1
8629	H	69.43900	83.61780	54.60990	-1237.27372	2881.62697	252.20224	1
8630	C	69.47100	87.55630	61.01389	1189.32426	-1.43135	146.37640	1
8631	O	69.72955	86.35006	61.14604	96.28068	143.89352	-13.94453	1
8632	N	69.76165	88.51866	61.91656	-405.89630	83.40689	804.74064	1
8633	H	69.29572	89.48289	61.87342	-304.00188	-2049.22001	3022.10860	1
8634	C	70.34804	87.87839	63.04713	-995.75521	-465.59528	-5.24245	1
8635	H	70.82373	86.93485	62.54570	-2070.47575	-832.82444	-504.57853	1
8636	C	71.17063	89.00348	63.83931	-441.76086	-443.82271	749.68964	1
8637	H	71.75312	89.68551	63.23884	-0.13437	3804.29348	-511.50439	1
8638	C	70.20934	89.71795	64.82896	134.09339	-33.44080	118.75907	1
8639	H	70.69892	90.63156	65.31818	-246.45870	-851.91970	2501.11950	1
8640	H	69.72914	89.03978	65.60124	-941.04791	150.48609	-1700.43279	1
8641	H	69.31912	90.10589	64.32232	3344.56695	-3223.60841	92.80256	1
8642	C	72.16645	88.21939	64.80788	335.80531	-611.07563	-572.18354	1
8643	H	72.82519	88.92494	65.31903	-3896.11705	-964.20812	-3387.43823	1
8644	H	71.64885	87.55812	65.57695	-1322.46287	-2838.90877	-2153.59406	1
8645	H	72.75039	87.45031	64.23638	2139.32188	1177.92032	548.25017	1
8646	C	69.25023	87.13708	64.02112	-681.94624	-959.79326	1106.38991	1
8647	O	69.74266	86.37588	64.80397	-195.58547	240.64682	-632.55509	1
8648	N	67.98314	87.50178	63.80797	372.73326	1009.15852	96.23802	1
8649	H	67.90002	88.27644	63.09022	4725.48392	-2226.46633	-996.64424	1
8650	C	66.78716	86.82731	64.36574	-210.36934	277.80558	19.38505	1
8651	H	67.09761	86.75058	65.46807	238.46928	-1062.61929	1314.39536	1
8652	C	65.57246	87.67641	64.06059	1043.45787	-908.68795	-317.26741	1
8653	H	65.34624	87.63394	62.95754	1390.48587	-2320.71210	-890.31477	1
8654	C	64.34091	87.16410	64.79271	-599.17299	411.41307	554.40357	1
8655	H	64.42514	87.20857	65.90634	1686.69841	3864.05234	-1552.03256	1
8656	H	63.43032	87.76474	64.44402	-3346.54231	-1469.93888	1533.45066	1
8657	H	64.07224	86.10348	64.52940	1624.95591	-239.93553	-4756.78740	1
8658	C	65.68840	89.15051	64.41279	-60.15871	-496.20239	317.57854	1
8659	H	66.24401	89.76317	63.54555	77.33987	-2576.30109	-392.44928	1
8660	H	64.69921	89.53793	64.68495	-2550.41425	-423.54708	2110.37332	1
8661	H	66.32712	89.17093	65.29590	-1574.74609	-307.98106	307.54121	1
8662	C	66.68231	85.40858	63.56945	-179.21973	-276.90879	-14.01820	1
8663	O	66.19800	84.42780	64.14390	-482.57715	592.64948	198.77909	1
8664	N	67.14638	85.35183	62.28202	-343.53351	68.89488	265.30728	1
8665	H	67.80594	86.09439	62.12500	-302.50677	-1679.67942	-2923.53546	1
8666	C	67.17300	83.92780	61.67790	685.68798	321.67274	507.74959	1
8667	H	66.24200	83.39480	61.79890	1649.61620	2256.69318	1443.72038	1
8668	C	67.57000	83.97580	60.15290	605.11168	-412.29603	543.41774	1
8669	H	68.48300	84.59580	60.02690	2104.62655	2018.10975	-1181.52712	1
8670	C	67.61400	82.57980	59.52390	-543.91757	453.41528	574.47303	1
8671	H	66.79600	81.88480	59.80990	1862.33532	-1444.02710	-2084.39898	1
8672	H	68.52000	82.02080	59.84090	2864.49075	1300.75818	-30.77500	1
8673	H	67.66500	82.68580	58.41990	-2611.94440	-1738.28447	-233.10893	1

8674	C	66.50700	84.79580	59.46790	834.42392	349.32340	-114.72088	1
8675	H	66.63300	84.77480	58.36390	-2506.74778	-471.96867	-1841.65343	1
8676	H	66.40800	85.88182	59.84108	2303.07971	-956.95724	-1769.23769	1
8677	H	65.54000	84.29880	59.69790	-1698.05578	-2195.07427	-1482.05322	1
8678	C	68.20200	83.10680	62.39890	550.50155	589.32564	-425.55181	1
8679	O	68.02100	81.91380	62.76490	265.05037	-645.49038	-369.75357	1
8680	N	69.35700	83.66280	62.70190	611.51693	-452.93843	-365.46698	1
8681	H	69.64500	84.55180	62.35490	-1783.86180	-1016.25432	-2383.96528	1
8682	C	70.38900	83.01780	63.55090	-417.00848	393.99101	708.74961	1
8683	H	70.48900	81.98180	63.26390	-1071.58594	2667.34841	-1278.74246	1
8684	C	71.76000	83.63580	63.31290	-484.47360	707.47680	310.18206	1
8685	H	72.58800	82.97480	63.64590	-2638.63833	1671.58017	376.34261	1
8686	H	71.82400	84.63980	63.78390	-798.91887	3040.56766	122.07846	1
8687	C	72.03300	83.72280	61.79390	-215.29745	-521.99840	715.97184	1
8688	C	71.81600	82.59080	60.95990	279.85305	-717.87178	-487.64063	1
8689	H	71.47000	81.69580	61.45590	-2316.48263	1909.86806	940.49903	1
8690	C	72.08100	82.67680	59.54890	606.64568	99.14528	673.49999	1
8691	H	71.79200	81.91980	58.83390	-2128.87791	1667.81113	-1607.64148	1
8692	C	72.48800	83.89180	59.02390	195.93976	854.07363	-252.22381	1
8693	H	72.66000	83.92580	57.95890	-2538.06704	1495.79316	1104.10359	1
8694	C	72.42300	84.92880	61.19290	-50.29512	126.63266	-901.60167	1
8695	H	72.50395	85.89272	61.76713	-1321.70914	-2082.90148	-1461.37561	1
8696	C	72.70238	84.99223	59.85766	-432.98429	-490.83777	-145.38737	1
8697	H	73.01897	85.89278	59.38421	-1895.56371	-1702.47407	-3038.91836	1
8698	C	70.05300	82.90880	64.99590	-703.64877	567.76549	118.20222	1
8699	O	70.29400	81.84380	65.59190	582.21902	-257.82227	-467.09306	1
8700	N	69.42700	83.89580	65.60790	-669.99197	-228.23948	-460.09759	1
8701	H	69.17200	84.72080	65.10890	-2598.22064	1215.83658	1291.98188	1
8702	C	68.97800	83.85380	67.00790	-783.83523	-179.54670	429.90268	1
8703	H	69.89000	83.70380	67.56490	346.22594	-2277.71589	-2142.51351	1
8704	C	68.19903	85.20585	67.46090	681.87297	51.56031	-152.30225	1
8705	H	67.22631	85.38521	66.95033	1389.28469	-574.96040	-1987.67425	1
8706	H	68.84072	86.08474	67.21789	338.23433	1053.83825	-238.65874	1
8707	C	67.99918	85.33896	69.00421	1257.63042	-271.50135	169.52143	1
8708	H	67.37700	84.47980	69.36990	-251.79211	455.35365	-3102.81808	1
8709	H	67.35645	86.18124	69.17199	645.54680	-152.24946	-693.25948	1
8710	C	69.36679	85.60018	69.80215	711.40873	319.18884	86.19525	1
8711	O	69.86384	86.67645	70.06156	325.14627	-345.90372	-415.02769	1
8712	N	70.01700	84.39780	70.10590	430.88271	-474.21138	-549.66895	1
8713	H	69.81800	83.47480	69.77790	1631.46249	1462.02418	-2258.10577	1
8714	H	70.95200	84.61280	70.38790	-1617.99244	-2635.09471	580.17461	1
8715	C	68.01400	82.64180	67.17590	-681.98160	-75.25730	-600.57343	1
8716	O	68.15500	81.79780	68.04290	503.60685	290.79634	534.27039	1
8717	N	67.09000	82.50080	66.23490	-542.00045	99.79091	-639.49165	1
8718	H	67.03700	83.21580	65.54290	-1827.24928	1527.47529	2055.77371	1
8719	C	66.19800	81.42780	66.04390	-649.22657	631.11082	107.95832	1
8720	H	65.61500	81.36480	66.95090	-749.82018	2991.41556	622.43786	1
8721	C	65.20800	81.57280	64.87290	376.31415	-425.96708	-713.01523	1
8722	H	64.70000	82.55680	64.95890	712.68056	-2278.81910	-2048.73038	1
8723	H	65.78400	81.60080	63.92390	-2781.34911	1454.07416	-219.07002	1
8724	C	64.14300	80.54880	64.85190	197.69820	-878.72599	142.15153	1
8725	C	64.10100	79.51580	63.85590	-289.94759	-542.79390	672.87159	1
8726	H	64.80100	79.56380	63.03490	2747.58171	331.57114	1496.35610	1
8727	C	63.15900	78.47080	63.93090	616.79588	321.75980	589.47814	1
8728	H	63.17600	77.65880	63.21990	2085.84444	1593.50673	-1734.42080	1
8729	C	62.29400	78.35380	65.04990	334.18835	-806.48764	263.33788	1
8730	H	61.65200	77.48780	65.10490	-1195.28903	-2707.66152	1066.80806	1
8731	C	63.23200	80.41480	65.92290	655.30633	-207.67647	599.07854	1
8732	H	63.26300	81.05080	66.79490	-1807.55544	938.41900	2397.98652	1
8733	C	62.34100	79.34080	66.02690	-637.91715	628.11748	-173.15066	1
8734	H	61.57100	79.40480	66.78190	-2428.13455	820.79013	1824.47044	1
8735	C	66.93500	80.04880	65.78090	195.05360	-792.53318	-406.56642	1

8736	O	66.63200	79.06580	66.49690	52.23850	680.28599	-397.62964	1
8737	N	67.94200	79.96780	64.95690	-147.37618	-825.15603	100.34977	1
8738	H	68.28900	80.79880	64.52890	641.78635	-2949.29133	887.70332	1
8739	C	68.76200	78.73780	64.76490	-283.59104	413.20314	761.76787	1
8740	H	68.18600	77.88280	64.44390	893.12959	-331.38519	-2998.45454	1
8741	C	69.92700	79.06480	63.73590	-20.02066	736.77696	-536.85183	1
8742	H	70.79800	79.64880	64.10390	720.16800	-286.26712	-3049.20242	1
8743	H	69.47600	79.59580	62.87090	-1766.34439	2477.45026	800.30865	1
8744	C	70.63800	77.74080	63.25190	-567.84164	-695.72988	-158.00889	1
8745	H	69.81100	77.09780	62.88090	1469.65111	2639.96115	-876.90192	1
8746	H	71.15600	77.18480	64.06190	1330.39681	2323.18840	1652.59379	1
8747	C	71.61500	77.98280	62.06390	-173.31241	676.02989	-586.85382	1
8748	O	71.30400	77.62580	60.88590	253.19284	748.00484	-3.06174	1
8749	N	72.76000	78.65180	62.30290	-756.73621	248.18430	280.04847	1
8750	H	73.02500	78.74080	63.26290	-76.03550	1762.26803	2605.15954	1
8751	H	73.53400	78.74680	61.67590	-1129.91214	2023.67923	-2127.49787	1
8752	C	69.42700	78.31480	66.03490	-551.28833	-311.69731	656.03123	1
8753	O	69.49300	77.10380	66.30090	607.35783	152.72270	481.06078	1
8754	N	69.91900	79.24580	66.90290	444.31337	-385.07350	-605.78570	1
8755	H	69.86900	80.20080	66.61990	2595.52861	35.76156	-1777.68910	1
8756	C	70.55000	78.86580	68.12590	-784.14317	-52.59372	462.38987	1
8757	H	71.32000	78.13480	67.92590	-462.13645	-2699.23387	1548.80362	1
8758	C	71.25000	80.09480	68.80590	197.12909	890.15955	14.39087	1
8759	H	71.58700	79.73080	69.79990	2746.32061	303.57606	-1504.58994	1
8760	H	70.61000	80.97980	69.01290	-3097.61543	-546.90067	-62.48631	1
8761	N	73.40700	81.20880	68.59690	-209.07347	622.14253	530.94185	1
8762	H	73.43300	81.28880	69.59390	-2040.68413	1011.31339	2170.50219	1
8763	C	72.35200	80.62980	68.01290	-248.12391	564.18458	-671.99799	1
8764	C	74.26900	81.55580	67.58590	-155.31937	-898.50238	-4.51232	1
8765	H	75.19500	82.08080	67.81790	973.62003	-220.44013	2983.57108	1
8766	N	73.76200	81.31280	66.40590	163.43278	-152.13122	814.13642	1
8767	C	72.56300	80.67780	66.66290	684.80954	300.46282	-521.73651	1
8768	H	72.02400	80.25780	65.82290	1199.36856	-2026.37391	-2086.51625	1
8769	C	69.64000	78.25780	69.17190	-747.16856	355.58843	383.07573	1
8770	O	70.02400	77.39280	69.98090	-534.25265	-579.67242	46.70353	1
8771	N	68.39300	78.68480	69.17490	45.48387	-842.94896	6.36779	1
8772	H	68.03400	79.38880	68.56790	-2083.58571	1357.88664	-1926.92519	1
8773	C	67.34400	78.10680	69.99190	-486.39842	359.06583	682.59747	1
8774	H	67.88300	77.80780	70.87890	1823.64178	-2248.54392	-1231.50603	1
8775	C	66.26800	79.14380	70.38190	354.39673	-755.01887	-368.51114	1
8776	H	65.65100	79.44880	69.50990	-1685.12818	2208.34413	1477.08682	1
8777	C	65.27500	78.49980	71.45990	818.16250	369.91638	158.81751	1
8778	H	65.85400	78.09680	72.31790	-704.60158	2358.52233	1959.37114	1
8779	H	64.71300	77.63880	71.03790	-1922.40656	1060.30325	-2253.51642	1
8780	H	64.49100	79.19980	71.82090	966.05373	2011.63690	2217.72032	1
8781	C	66.88300	80.46080	70.88990	578.45802	-638.70251	298.15505	1
8782	H	67.63100	80.93980	70.22190	1961.27994	-586.94183	-2388.95511	1
8783	H	67.49200	80.42380	71.81890	-2311.42056	1813.39268	1125.68567	1
8784	C	65.83800	81.51180	71.27090	-829.22184	-344.94732	-157.64989	1
8785	H	65.02200	81.53180	70.51890	1146.57994	789.58334	-2821.37180	1
8786	H	65.46700	81.24480	72.28390	429.82659	-2165.50649	-2241.44083	1
8787	H	66.38100	82.47880	71.20490	-2331.25248	-1872.54511	-978.29592	1
8788	C	66.76900	76.84280	69.45490	-340.18826	610.30084	-585.88040	1
8789	O	66.63400	75.81380	70.12590	101.89568	-622.84987	474.66044	1
8790	N	66.31500	76.98580	68.18590	158.99257	828.45462	32.50530	1
8791	H	66.41500	77.87280	67.74190	-2616.55087	-325.30913	-1716.40955	1
8792	C	65.74200	75.94280	67.37790	151.60799	-222.65958	-871.14220	1
8793	H	64.79300	75.72480	67.84490	332.72533	2444.91621	1951.89775	1
8794	C	65.55500	76.47180	65.99690	516.47904	744.65398	100.94974	1
8795	H	65.01800	77.43680	65.87590	-2309.33922	-1649.80974	1357.68420	1
8796	H	66.57200	76.68280	65.60290	-2378.86400	1325.20877	1575.77093	1
8797	C	64.89500	75.49180	64.95890	699.04891	-87.30804	578.92913	1

8798	H	65.50600	74.59380	64.72490	1876.96401	-2499.29325	358.83921	1
8799	H	64.58300	76.09980	64.08290	-1213.58057	2898.57565	153.97275	1
8800	S	63.30800	74.83580	65.62490	416.23263	-317.43383	192.86463	1
8801	C	62.41500	74.52080	64.05090	-723.11660	534.39399	151.57985	1
8802	H	61.57500	73.84080	64.30990	1894.43547	-1399.81738	-2085.62983	1
8803	H	63.09600	74.03980	63.31690	1019.44980	2208.15760	1995.74255	1
8804	H	62.01300	75.46580	63.62590	-1982.24411	1150.22911	2155.43673	1
8805	C	66.62700	74.71180	67.33690	574.44850	-552.29807	-443.20059	1
8806	O	66.22400	73.62780	67.63590	488.90100	-608.17075	121.37288	1
8807	N	67.94400	74.80680	67.04190	412.83426	217.61314	703.48041	1
8808	H	68.38100	75.69680	66.93390	-1566.75032	1034.45141	2524.56529	1
8809	C	68.78100	73.65580	66.86890	-596.84400	82.97288	684.35644	1
8810	H	68.16600	72.78480	66.69290	1497.15614	726.10748	2670.11566	1
8811	C	69.72500	73.87980	65.70990	-175.62620	-821.42401	-354.78026	1
8812	H	70.51200	74.64080	65.89490	2171.35181	2255.82464	-307.75434	1
8813	C	70.49500	72.60180	65.37190	378.51733	52.02063	-827.93085	1
8814	H	71.16400	72.77680	64.50290	-1830.41880	-1926.89381	1683.70826	1
8815	H	71.16100	72.19280	66.16290	-1694.63056	-1036.21179	-2439.81938	1
8816	H	69.76400	71.82480	65.06090	1340.02925	2669.43549	-988.26212	1
8817	C	69.01400	74.34080	64.41390	-814.01391	-209.93561	-353.21297	1
8818	H	68.75000	75.40280	64.60590	-2507.13629	1875.32597	309.26749	1
8819	H	69.68600	74.31480	63.52990	-1945.45291	-2290.22985	-931.81889	1
8820	H	68.06000	73.80680	64.21390	2327.78054	2116.14265	40.05353	1
8821	C	69.60800	73.28180	68.10590	732.54018	-357.93091	408.31525	1
8822	O	69.97600	72.13480	68.30190	1.35383	-550.82225	-565.88006	1
8823	N	69.88600	74.25980	68.99390	363.03646	-731.62391	213.54921	1
8824	H	69.62600	75.21180	68.84890	1755.34152	-2608.48845	-113.09448	1
8825	C	70.53000	73.95480	70.25190	897.70081	-103.05256	-122.32915	1
8826	H	70.92300	74.92080	70.53490	-36.69836	-2570.59466	-1813.53869	1
8827	H	71.34000	73.25280	70.12490	2707.14142	1502.01009	559.97968	1
8828	C	69.62700	73.38380	71.24690	-455.10011	563.46771	553.93053	1
8829	O	70.00600	72.62580	72.09890	-186.37563	-688.24524	339.42575	1
8830	N	68.35400	73.82580	71.22490	311.11183	604.43295	500.54223	1
8831	H	67.99000	74.44980	70.53890	1526.07374	630.11928	-2678.11031	1
8832	C	67.42000	73.44580	72.28490	488.89665	-662.84659	-391.23583	1
8833	H	67.91200	72.76780	72.96590	-202.70806	-176.52103	-3134.64129	1
8834	C	66.91300	74.68680	73.11490	284.28868	637.56471	586.63634	1
8835	H	66.12200	75.16780	72.50090	636.15078	1541.45354	-2667.85671	1
8836	H	67.73000	75.39380	73.37290	-1152.87383	-1009.69575	-2747.65767	1
8837	C	66.30000	74.35180	74.45690	529.35420	598.48763	-439.37193	1
8838	H	65.60900	73.48980	74.34190	-1404.50143	1893.60025	2083.23788	1
8839	C	67.30900	73.99080	75.58390	-356.46527	191.87426	-817.04821	1
8840	H	67.94500	74.88180	75.77790	-2886.42813	-572.73393	1112.98460	1
8841	H	67.87700	73.11080	75.21290	1554.72610	1907.30855	1960.41503	1
8842	H	66.84500	73.70680	76.55190	1700.32173	-1757.92658	1979.09737	1
8843	C	65.46100	75.57580	74.92890	-556.85359	-709.22100	135.53838	1
8844	H	66.10500	76.45080	75.16190	2764.59040	962.11966	1153.07932	1
8845	H	64.93300	75.42080	75.89390	-647.66229	-1903.03744	-2420.16700	1
8846	H	64.70300	75.83080	74.15790	-726.31647	962.86753	-2905.78333	1
8847	C	66.18200	72.68480	71.76890	-551.55292	145.25812	-711.43549	1
8848	O	65.92800	71.57280	72.17990	660.67273	-87.87243	423.57669	1
8849	N	65.43300	73.25880	70.81490	350.86310	-95.77548	-761.83622	1
8850	H	65.71600	74.14280	70.44990	-1155.90570	2419.27216	1645.97402	1
8851	C	64.18200	72.72380	70.30190	-367.08880	-590.07583	590.34509	1
8852	H	63.58800	72.69080	71.20390	-2345.06017	1344.25605	-1609.93625	1
8853	C	63.33000	73.64380	69.47090	-881.45777	-148.18660	-180.34394	1
8854	H	63.72500	73.82480	68.44790	-1263.21552	-2863.19262	-323.48226	1
8855	C	61.92300	73.14780	69.18390	-162.98024	889.47281	-117.16040	1
8856	H	61.36800	72.94880	70.12590	1868.77692	2273.08058	1113.10544	1
8857	H	61.30500	73.85280	68.58890	-2062.91018	1098.60995	-2106.10635	1
8858	H	61.96700	72.21880	68.57590	2163.49839	-1231.78059	-1923.59494	1
8859	C	63.22400	75.10980	70.05690	-710.87993	-201.85737	534.18567	1

8860	H	62.72800	74.93580	71.03590	-1722.85908	-2220.69218	-1413.68633	1
8861	H	64.20300	75.58080	70.29190	74.49284	-2991.69774	-970.78406	1
8862	C	62.38800	76.05980	69.16990	-901.93412	-89.79683	-99.51065	1
8863	H	62.69600	75.86280	68.12090	-2194.98692	-1319.68458	-1827.20860	1
8864	H	62.61200	77.12580	69.38790	-2958.87587	943.55482	502.97527	1
8865	H	61.29600	75.86780	69.23290	615.59011	228.60696	-3076.85130	1
8866	C	64.17900	71.32780	69.69790	615.77418	-500.64708	449.02746	1
8867	O	63.61300	70.39280	70.22690	672.86755	410.51495	-48.51765	1
8868	N	64.84000	71.21580	68.46890	30.93819	-690.30030	-484.97486	1
8869	H	65.25800	71.95580	67.94690	2834.41771	-1125.42655	773.12196	1
8870	C	64.86800	69.95580	67.69390	598.91025	-664.56113	176.39734	1
8871	H	63.81200	69.72680	67.68790	-2265.49285	-1205.97625	1819.72241	1
8872	C	65.36600	70.19380	66.22890	-475.69890	749.97196	206.64852	1
8873	H	66.39600	70.60980	66.18990	1947.96506	-2077.23152	1337.44816	1
8874	H	65.22500	69.21180	65.72890	-1103.00333	-1704.59296	2403.32535	1
8875	C	64.53200	71.18780	65.44590	645.79796	-525.54372	-371.75234	1
8876	H	64.74800	72.23680	65.73890	1034.52187	-432.58778	-2939.53373	1
8877	C	64.82900	71.16480	63.94490	-193.44510	495.40262	740.67958	1
8878	H	64.37600	72.06480	63.47790	1030.41163	-2830.14617	-909.25835	1
8879	H	64.51100	70.21780	63.45690	-1788.09069	1872.10513	-1787.78642	1
8880	H	65.92000	71.13280	63.73590	-2319.69691	430.01972	2081.42152	1
8881	C	63.01800	70.99680	65.50990	337.28319	463.18300	-709.33247	1
8882	H	62.67500	69.94880	65.36790	-2169.81831	-2099.82564	883.65550	1
8883	H	62.52000	71.27080	66.46390	1287.11327	-1973.07056	2085.31969	1
8884	H	62.58300	71.55980	64.65590	933.05301	2308.53467	-1923.09802	1
8885	C	65.59900	68.81180	68.33190	-487.30356	405.89265	-655.16212	1
8886	O	65.01500	67.77580	68.08990	51.76259	752.96699	-232.35441	1
8887	N	66.67700	68.82680	69.08290	716.34479	-416.55290	161.26411	1
8888	C	67.51000	69.99280	69.37990	-313.75432	-698.84754	494.59211	1
8889	H	67.00000	70.92280	69.70990	-1118.00607	2940.43275	46.30239	1
8890	H	68.07300	70.27080	68.46290	344.03567	2906.48788	-1154.20703	1
8891	C	67.20100	67.63480	69.73590	-534.45817	709.77158	205.01164	1
8892	H	67.07000	66.78880	69.07690	-857.55567	3023.80252	139.43755	1
8893	C	68.66500	68.04580	70.17490	481.33696	391.24665	668.35005	1
8894	H	69.12400	67.49880	71.02590	-2140.94963	-2003.45149	1140.50123	1
8895	H	69.38400	67.82280	69.35690	672.80993	2140.77173	2205.14159	1
8896	C	68.55100	69.51580	70.42490	-696.14943	-406.90384	-425.74198	1
8897	H	69.49600	70.06980	70.24090	-962.55716	2608.97393	1471.38199	1
8898	H	68.18300	69.79180	71.43690	-2261.40855	-1927.18248	-1034.51694	1
8899	C	66.39300	67.26680	71.00390	-453.74341	739.56402	280.38006	1
8900	O	66.32900	66.10480	71.31490	-137.54694	639.53244	442.38708	1
8901	N	65.84600	68.26680	71.68190	525.19233	644.56059	-146.24280	1
8902	H	65.99600	69.19580	71.35290	2330.43331	683.90243	-1999.89607	1
8903	C	64.95700	68.17180	72.79490	399.79504	-677.76227	460.70949	1
8904	H	64.63100	69.17880	73.00590	2056.58315	1120.06637	2100.98627	1
8905	H	65.55800	67.86280	73.63690	1733.48591	94.92812	-2623.78381	1
8906	C	63.76000	67.32980	72.57190	-10.08677	-839.03243	-356.89472	1
8907	O	63.42600	66.47880	73.44190	-437.01769	-217.15932	-620.87406	1
8908	N	63.06200	67.53680	71.42990	766.41190	160.47857	315.48648	1
8909	H	63.28600	68.31780	70.85290	-1861.68302	1369.43190	2134.71751	1
8910	C	61.89500	66.79280	71.11990	134.00087	-583.58071	687.69784	1
8911	H	61.24900	66.80980	71.98490	-1363.52244	-2722.36357	-792.31898	1
8912	C	61.08100	67.31480	69.93990	593.24576	-688.29568	-75.89158	1
8913	H	60.31700	66.55780	69.66190	1194.47358	2577.93466	-1351.18910	1
8914	C	60.20100	68.50380	70.43690	-62.19399	-708.20101	570.99408	1
8915	H	59.64400	68.05180	71.28490	1664.45034	1183.95113	2392.92520	1
8916	H	59.37700	68.71880	69.72290	-665.70437	3054.70418	-351.91805	1
8917	H	60.89200	69.32080	70.73390	1496.61065	-1903.13702	-2009.09239	1
8918	C	61.97000	67.64580	68.73790	-4.01097	820.47718	-397.80915	1
8919	H	62.59600	68.53580	68.96190	-5.14008	-236.63247	3137.22885	1
8920	H	62.67200	66.81080	68.52690	1511.82584	-448.24004	2722.44187	1
8921	C	61.18200	67.81180	67.43490	-828.62534	-319.95147	-206.06334	1

8922	H	61.83300	68.03080	66.56190	2986.70743	-737.51338	-658.69488	1
8923	H	60.42100	68.61980	67.48290	1471.44982	615.18607	2711.93800	1
8924	H	60.54100	66.91780	67.27590	1969.38797	-2313.68546	816.45382	1
8925	C	62.10100	65.27780	70.85890	542.50498	-411.58330	606.41449	1
8926	O	61.32600	64.41780	71.31790	-90.26999	-196.22098	-759.58929	1
8927	N	63.17400	64.90480	70.18990	-117.44128	375.04606	747.14141	1
8928	H	63.73500	65.66780	69.88090	734.43151	-2823.65248	-1177.20995	1
8929	C	63.66700	63.56780	70.06490	-589.92492	639.39638	-273.15172	1
8930	H	62.88200	62.91180	69.71890	1868.20173	2187.26408	-1274.33290	1
8931	C	64.85000	63.46980	69.11790	73.22357	-747.66018	516.81095	1
8932	H	65.76400	63.92480	69.55590	-60.91869	-1130.28062	-2935.46945	1
8933	C	65.11100	61.98380	68.79790	588.28790	-568.72396	-402.39460	1
8934	H	65.53400	61.39180	69.63790	2129.49122	1687.30096	1586.35080	1
8935	H	65.93800	61.98080	68.05590	869.28117	-2724.29525	1311.78956	1
8936	H	64.16200	61.56580	68.39990	-1383.60622	-1787.62488	-2188.20871	1
8937	C	64.66600	64.18280	67.82090	-511.99294	745.72906	114.90170	1
8938	H	64.71900	65.29080	67.87690	1588.00486	-188.69905	-2709.40205	1
8939	H	65.40800	63.84580	67.06590	1800.67259	-1935.62399	1705.62723	1
8940	H	63.66800	64.06080	67.34590	1347.81269	2032.19053	-1987.92073	1
8941	C	64.06000	63.02280	71.47490	-1.70514	752.11570	-515.52892	1
8942	O	63.68600	61.86980	71.71690	714.84410	-93.59885	-322.27999	1
8943	N	64.69800	63.81880	72.35490	551.30940	-398.39206	500.01400	1
8944	H	64.92200	64.75380	72.09190	1065.39191	2431.51348	-1688.46336	1
8945	C	64.99500	63.39580	73.70990	84.22080	855.54583	-303.97236	1
8946	H	65.58600	62.49180	73.72390	-1378.58275	-2174.01324	-1808.70182	1
8947	C	65.90700	64.41680	74.47290	-548.75752	-723.60389	81.93657	1
8948	H	65.40800	65.40280	74.35890	-798.90751	-3003.86307	486.60013	1
8949	C	65.96600	64.10380	75.97690	121.52595	468.18448	772.97202	1
8950	H	64.99500	64.04380	76.51390	1064.66948	1358.25911	-2630.55837	1
8951	H	66.52400	63.15380	76.11390	728.27879	-2508.23114	1754.02759	1
8952	H	66.62700	64.80880	76.52590	-2157.82906	216.12575	2279.31780	1
8953	C	67.28900	64.30380	73.77390	749.51981	-457.40855	-245.86273	1
8954	H	67.15200	64.24880	72.67190	-420.13663	-1908.78261	-2465.41282	1
8955	H	67.80800	63.36280	74.05590	1292.12572	-2513.34894	-1382.64763	1
8956	C	68.16400	65.49680	74.02690	-394.49375	463.21539	-679.15918	1
8957	H	67.70100	66.33980	73.47090	2086.51082	1736.69889	-1590.14961	1
8958	H	68.23500	65.67980	75.11990	2822.74157	-548.77616	1276.40157	1
8959	H	69.22100	65.29580	73.74790	1926.09764	-1485.74778	1995.22621	1
8960	C	63.73700	63.05580	74.48490	493.45836	-499.32038	-581.91839	1
8961	O	63.59500	61.94380	75.01890	-732.30512	90.81087	281.26470	1
8962	N	62.71100	63.97680	74.42690	-388.37517	-500.86328	-557.64953	1
8963	H	62.97700	64.85880	74.04390	1950.96197	-1152.01113	-2182.85226	1
8964	C	61.40000	63.89880	75.00690	-65.73122	687.61042	595.24979	1
8965	H	61.51400	63.67880	76.05790	-1951.21468	1538.10409	-1930.08375	1
8966	C	60.66100	65.21180	74.74190	522.64942	726.40915	-174.98094	1
8967	H	60.92700	65.60280	73.73690	-1874.72242	1772.08866	-1800.92861	1
8968	H	59.56300	65.07380	74.83190	-3107.24857	303.11924	-389.03888	1
8969	C	61.13800	66.33980	75.75290	-526.39631	-297.91956	682.35025	1
8970	H	62.24600	66.39680	75.69090	-1296.29539	1075.82747	-2657.14880	1
8971	C	60.60400	67.72780	75.32790	559.65290	571.52751	-437.71674	1
8972	H	60.92600	68.06380	74.31990	2176.88016	889.15141	2090.17434	1
8973	H	59.49500	67.79180	75.33190	-1717.87920	-2187.24171	-1470.74505	1
8974	H	60.93400	68.51280	76.04190	939.06574	2087.33093	-2158.57160	1
8975	C	60.79400	66.15080	77.20290	793.52293	-219.55549	-391.87721	1
8976	H	61.31900	65.24480	77.57390	-581.17914	1168.77396	-2862.59051	1
8977	H	60.95400	67.10180	77.75390	-2954.60589	506.49745	954.98199	1
8978	H	59.72800	65.90580	77.39990	1752.84334	232.71534	2602.23174	1
8979	C	60.68300	62.63780	74.55090	-422.82354	680.47202	435.46422	1
8980	O	60.15800	61.87580	75.38690	507.75188	597.42849	-94.31041	1
8981	N	60.66600	62.35580	73.27790	-572.47222	389.58514	482.87811	1
8982	H	61.20100	62.96480	72.69590	1749.94152	-2014.18665	-1667.02820	1
8983	C	60.10100	61.11180	72.65490	146.14881	299.24040	-848.85023	1

8984	H	59.04500	61.08180	72.87990	778.60536	-2130.16337	2180.45957	1
8985	C	60.12500	61.11180	71.07890	-81.54435	640.83186	643.53403	1
8986	H	59.92400	60.10280	70.65790	2240.83455	-2098.16604	688.90203	1
8987	H	61.15700	61.42380	70.81190	1734.81488	-2487.23910	-838.02460	1
8988	O	59.30200	62.05380	70.45490	-354.37435	-48.53850	704.05260	1
8989	H	58.40200	61.85880	70.72590	-972.02832	2985.12033	-206.01886	1
8990	C	60.70300	59.78680	73.11590	596.28258	-631.56435	277.53299	1
8991	O	59.91400	58.83680	73.29290	-337.54624	-10.70752	713.84530	1
8992	N	62.04400	59.67780	73.24190	215.16837	-355.06463	-735.05372	1
8993	H	62.55400	60.48180	72.94690	-1113.47260	-2283.51931	-1855.78678	1
8994	C	62.74300	58.45280	73.65390	-412.71609	-249.10353	773.99216	1
8995	H	62.41300	57.69680	72.95690	-618.05730	2898.96796	-1054.61660	1
8996	C	64.26900	58.73380	73.87290	-728.96113	259.56186	482.38398	1
8997	H	64.76100	57.78280	74.17290	901.55280	931.36218	-2866.70425	1
8998	H	64.35500	59.49580	74.67690	-1452.49062	-2621.83855	956.27393	1
8999	S	64.98900	59.21680	72.26490	-194.13488	-76.32355	517.39441	1
9000	H	64.69800	60.50780	72.31790	-681.37477	-1452.89683	2706.11261	1
9001	C	62.19100	57.92080	74.99590	116.85271	739.49730	-520.51915	1
9002	O	61.86400	56.75380	75.16990	182.68119	593.14954	488.29135	1
9003	N	62.14600	58.80680	76.01990	45.70287	804.95113	-250.27427	1
9004	H	62.48500	59.73680	75.89890	-674.89009	-2327.51731	-2006.34313	1
9005	C	61.69700	58.38880	77.38590	-740.98950	-479.25022	-229.57526	1
9006	H	62.07100	57.41880	77.67990	-2645.96527	1517.62944	770.64577	1
9007	C	62.30100	59.29480	78.44190	757.50892	468.49620	-195.30118	1
9008	H	61.96400	58.85080	79.40290	2406.12827	1321.26137	-1537.21872	1
9009	H	61.85500	60.29480	78.25690	2782.91557	1102.01246	969.11076	1
9010	C	63.83700	59.35180	78.28390	-803.14102	140.99230	408.08906	1
9011	C	64.38900	60.56680	77.83490	569.90361	535.86548	-468.51795	1
9012	H	63.80300	61.43580	77.57490	901.26748	2307.51083	1939.41664	1
9013	C	65.78200	60.60780	77.65190	-37.77197	-597.50180	-687.76150	1
9014	H	66.16600	61.51380	77.20790	-904.88168	1353.36004	2692.17978	1
9015	C	66.60500	59.53580	77.92290	-817.15962	-16.96333	-404.24424	1
9016	O	67.97300	59.58680	77.66090	-653.44068	-391.55089	208.15958	1
9017	H	68.15200	60.22280	76.96390	1760.09192	-2576.95817	-399.48619	1
9018	C	64.61200	58.27280	78.57190	-385.75690	437.13966	701.10737	1
9019	H	64.11800	57.43480	79.04090	2260.45440	-996.47659	1948.23164	1
9020	C	66.01500	58.33080	78.34490	-476.74657	-368.24947	684.51153	1
9021	H	66.62900	57.44280	78.37690	958.68698	-2912.64048	-704.03901	1
9022	C	60.22600	58.36380	77.44290	40.66128	834.47524	-365.30637	1
9023	O	59.63100	57.65280	78.25890	-322.55860	526.28303	-492.55391	1
9024	N	59.50100	59.13780	76.59090	188.73066	-563.22900	-599.85508	1
9025	H	59.91300	59.78880	75.95890	-2203.55087	1691.57533	1476.87599	1
9026	C	58.09000	58.99580	76.38390	-901.54697	-95.99147	97.20962	1
9027	H	57.66200	59.15280	77.36290	1913.20878	-2197.06582	1187.75425	1
9028	C	57.49900	60.00280	75.39790	-3.91098	-816.22786	406.45762	1
9029	H	57.89000	60.99280	75.71490	-1932.81911	-1896.28298	-1602.04474	1
9030	H	57.90100	59.81880	74.37790	730.76234	-3020.63486	489.87516	1
9031	S	55.72300	60.08580	75.22290	-8.62032	-298.44196	471.24165	1
9032	H	55.62900	59.09380	74.34990	-2337.76039	1913.19876	879.07513	1
9033	C	57.68600	57.57480	75.97290	-725.82512	212.06652	-509.56519	1
9034	O	56.79800	56.98380	76.56690	-675.41180	-371.42640	-171.72231	1
9035	N	58.36000	56.95880	75.04090	12.16073	-815.10765	-219.37167	1
9036	H	58.91300	57.53180	74.44090	-727.88212	2445.23033	1840.99497	1
9037	C	58.10400	55.59180	74.61790	-590.94656	130.60970	682.03685	1
9038	H	57.05600	55.50580	74.37190	1979.92371	-2441.04385	-139.40326	1
9039	C	58.88400	55.19280	73.32890	626.26332	-583.85032	-313.63045	1
9040	H	59.96700	55.39580	73.47690	-2093.11751	1786.25521	-1525.24674	1
9041	C	58.75700	53.70380	73.07890	-704.92997	108.48903	568.11519	1
9042	H	59.12800	53.48880	72.05390	2482.17114	1404.67173	-1328.13778	1
9043	H	59.29400	53.04680	73.79590	2783.72384	-1395.70830	-448.44861	1
9044	H	57.68400	53.41180	73.07590	2819.67443	1395.41107	22.14147	1
9045	C	58.35700	55.95380	72.10590	625.30349	-64.59327	-660.51060	1

9046	H	57.42400	55.51380	71.69390	1383.39231	2825.00579	-61.59749	1
9047	H	58.03500	56.99480	72.32590	2392.04041	2043.19427	41.54653	1
9048	C	59.39500	56.11680	70.97890	697.09019	-527.59108	-259.16004	1
9049	H	59.93700	55.16780	70.78090	1909.84300	-1424.44627	2054.67242	1
9050	H	59.03200	56.60880	70.05190	1920.85389	178.12630	2485.32042	1
9051	H	60.04100	56.97780	71.25290	2526.20734	1579.75436	1010.38550	1
9052	C	58.48800	54.59080	75.69290	-672.90234	35.56105	-614.31983	1
9053	O	57.74000	53.60180	75.90990	-478.48117	-400.52770	-484.00470	1
9054	N	59.64700	54.78980	76.37390	-594.65392	-518.80353	-299.83646	1
9055	H	59.99800	55.71780	76.27190	-2801.41960	-1160.56416	838.66875	1
9056	C	60.34200	53.84080	77.29690	-465.92880	-632.01678	-463.59049	1
9057	H	60.57700	52.90980	76.80290	2104.64880	-1398.78162	-1874.05700	1
9058	C	61.81500	54.30380	77.78890	563.73452	-478.79226	533.30326	1
9059	H	61.72400	55.38780	78.01790	-180.62567	2661.80876	-1667.44557	1
9060	C	62.20200	53.43880	79.01190	-735.72828	495.54516	211.16321	1
9061	H	62.13300	52.35980	78.75490	1744.68210	1919.39457	1780.51539	1
9062	H	63.25500	53.63080	79.30990	-2455.01550	-1863.10778	-632.41956	1
9063	H	61.54700	53.49980	79.90690	-3074.15489	510.41792	-432.74879	1
9064	C	62.82100	54.15980	76.66190	-535.57079	392.91337	-624.68714	1
9065	H	62.32800	54.42880	75.70290	2535.16225	-1816.52634	-414.01766	1
9066	H	63.23200	53.13380	76.55490	637.95677	-2996.20685	-716.92531	1
9067	C	64.08400	54.91880	76.90390	-180.83755	852.62476	267.91753	1
9068	H	63.83200	55.97580	77.13390	-2162.95064	-237.77774	-2272.29675	1
9069	H	64.72100	54.56480	77.74290	-681.95603	-2936.95997	-898.57017	1
9070	H	64.80100	54.81880	76.06190	-102.88974	-380.35460	-3121.37314	1
9071	C	59.39500	53.38480	78.45890	365.42209	-771.75666	319.85834	1
9072	O	59.23700	52.19880	78.85690	-130.96376	-582.10112	-517.33356	1
9073	N	58.74100	54.39080	79.02790	-580.04826	-497.83537	358.29632	1
9074	H	58.82900	55.33080	78.70690	-2465.17050	1949.98831	136.77065	1
9075	C	57.95400	54.24980	80.20890	552.93237	-538.66922	485.33727	1
9076	H	58.55600	53.66780	80.89190	-1936.24275	1681.77355	1822.31390	1
9077	C	57.67700	55.58980	80.88790	-544.96510	524.50920	-509.26825	1
9078	H	57.07200	55.33580	81.78590	2316.46170	-1887.20468	-985.23598	1
9079	C	58.98100	56.16480	81.44990	634.75023	581.47036	300.72474	1
9080	H	58.79600	57.04280	82.10490	2074.77167	-1603.44444	1738.53809	1
9081	H	59.55900	55.40180	82.01390	-3027.53279	730.20764	-446.17064	1
9082	H	59.56000	56.60080	80.60790	492.25962	-3013.89594	756.53021	1
9083	C	56.89100	56.57580	80.03690	-735.50513	-67.82815	-534.67985	1
9084	H	57.59600	57.08480	79.34490	-2011.17990	2111.92388	1180.32164	1
9085	H	56.23000	55.99780	79.35490	-1755.26170	1810.64938	1881.17820	1
9086	C	56.10400	57.58680	80.84990	614.68626	74.55363	669.36803	1
9087	H	55.43400	57.04080	81.54790	2510.66828	1886.50010	189.44233	1
9088	H	55.39900	58.12580	80.18290	-12.55402	61.42276	-3145.51997	1
9089	H	56.80600	58.30380	81.32690	2078.87938	-1735.19968	1601.73931	1
9090	C	56.78400	53.35880	80.02290	-743.53414	511.49723	-130.30185	1
9091	O	56.23600	52.76380	80.96890	588.39911	524.92125	43.25962	1
9092	N	56.27700	53.27880	78.79190	13.28607	588.62638	604.99153	1
9093	H	56.73500	53.86180	78.12490	946.06818	-1978.89572	2255.47178	1
9094	C	55.13000	52.49880	78.47790	-295.89285	791.67877	-342.26182	1
9095	H	54.47900	52.42980	79.33690	843.43458	1701.42202	2508.38742	1
9096	C	54.26500	53.22480	77.40490	754.02901	511.08116	-41.07688	1
9097	H	53.70300	54.02080	77.93790	-1909.60232	-2485.84722	268.71691	1
9098	H	53.51500	52.55080	76.93890	-2511.76953	-1578.68953	1047.36786	1
9099	O	55.06400	53.77880	76.36790	-400.51945	635.55216	-243.48482	1
9100	H	55.77900	53.17280	76.16290	126.75732	3123.91475	351.16297	1
9101	C	55.34500	51.08080	78.13790	729.63697	-446.46594	315.83076	1
9102	O	54.38400	50.33480	77.74290	442.93773	-651.90520	-49.52781	1
9103	N	56.56600	50.60580	78.30390	-107.75884	-765.91461	338.28262	1
9104	H	57.18900	51.23380	78.76590	-203.77245	1794.70073	-2575.99540	1
9105	C	56.93000	49.22180	78.07690	649.67172	-639.82059	2.69468	1
9106	H	56.17700	48.60980	78.54990	-1683.53299	-2008.38757	1740.78209	1
9107	C	56.90500	48.80080	76.58590	550.37529	503.16102	524.75426	1

9108	H	55.84500	48.89880	76.26890	-1913.41416	2467.82422	383.29633	1
9109	H	57.16400	47.73180	76.43290	1246.14911	2688.02245	1058.24095	1
9110	C	57.61500	49.74880	75.55590	-524.85807	656.88756	352.80837	1
9111	H	58.66700	49.92380	75.86590	53.68440	-3097.36282	-549.26111	1
9112	H	57.07500	50.71580	75.64090	813.94205	1730.01573	-2498.55361	1
9113	C	57.50000	49.15880	74.14190	-220.05618	494.47871	733.83724	1
9114	H	58.09000	49.79580	73.44890	-2571.25717	-1811.98947	59.64017	1
9115	H	58.01800	48.17680	74.12790	2258.20433	443.46897	-2145.24468	1
9116	C	56.08000	49.16180	73.63190	570.19697	-673.94438	228.30983	1
9117	H	55.39300	48.50380	74.20690	1472.61415	-1731.58635	-2175.14195	1
9118	H	55.70700	50.20880	73.64390	2314.10831	134.62230	-2127.20610	1
9119	N	56.00100	48.71280	72.26790	-364.77716	-342.77374	-679.79120	1
9120	H	56.26500	49.45680	71.59090	165.10505	-2618.56232	1736.11575	1
9121	H	55.01000	48.47780	72.05990	1485.64317	2105.19406	1805.33891	1
9122	H	56.61600	47.89280	72.09290	2555.77940	-661.07959	-1711.48814	1
9123	C	58.25800	48.62980	78.70690	530.68986	545.42282	502.32780	1
9124	O	58.67000	47.50480	78.41790	-483.71484	-550.91079	293.50382	1
9125	N	58.87400	49.39780	79.67090	-9.30974	-840.03168	83.26103	1
9126	H	58.55300	50.33080	79.81490	2297.01815	2051.55425	-642.69667	1
9127	C	60.05300	49.01480	80.43090	-738.17546	52.50969	532.72011	1
9128	H	60.85900	48.83280	79.73490	-210.22144	1446.03697	2786.21791	1
9129	C	60.48400	50.11080	81.40890	-591.45373	419.26880	-553.03451	1
9130	H	60.55300	51.07380	80.85790	-1981.72135	-900.86016	2271.44396	1
9131	H	59.62900	50.22680	82.10890	-1607.70201	-1667.68815	-2128.92854	1
9132	C	61.81200	49.86180	82.09690	-16.13933	55.14233	910.02739	1
9133	H	61.77700	48.88480	82.62590	487.95653	2621.51135	1669.67149	1
9134	C	62.94700	50.01980	81.06690	705.18292	-576.44655	-43.32926	1
9135	H	62.97300	51.01480	80.57190	-2305.40820	1828.95797	1112.75874	1
9136	H	62.94200	49.14980	80.37590	-378.26055	-366.92465	-3101.69494	1
9137	H	63.86500	49.83680	81.66490	2805.76968	1332.24762	-500.99800	1
9138	C	61.98100	50.95380	83.20990	-529.26154	-527.10529	-522.96582	1
9139	H	61.11500	50.89480	83.90290	-2600.06500	-10.89578	1771.37503	1
9140	H	62.95000	50.78680	83.72690	-2857.22398	-1163.83868	-616.42263	1
9141	H	62.00600	51.98380	82.79390	-1978.21852	-1094.01348	2188.15270	1
9142	C	59.83400	47.69080	81.19690	29.37427	590.26214	-694.39093	1
9143	O	60.73700	46.80980	81.21890	-395.33304	-155.10882	665.79296	1
9144	N	58.64700	47.46780	81.86090	190.50952	-793.34384	-216.75786	1
9145	H	57.93700	48.16280	81.93990	-2342.89876	-2093.71748	159.36980	1
9146	C	58.32400	46.20480	82.43990	-697.54255	580.86657	-86.48359	1
9147	H	59.16000	45.72380	82.92390	-135.59744	-1219.89506	2896.84235	1
9148	C	57.25300	46.40580	83.55490	439.01971	-366.94824	709.97302	1
9149	H	56.46500	47.09480	83.18390	-2983.55025	-793.80366	-605.41709	1
9150	H	56.84700	45.42880	83.89290	-1528.44556	2391.22976	-1357.97666	1
9151	O	57.79400	47.05480	84.72390	-58.33021	-271.59339	-739.23058	1
9152	H	58.33600	46.39680	85.16390	-3067.75475	-104.94495	689.99534	1
9153	C	57.74300	45.15880	81.47690	-760.62354	368.20265	-342.53415	1
9154	O	57.44700	44.02980	81.86390	658.98494	-55.19269	-431.64782	1
9155	N	57.64000	45.44880	80.18090	-27.63665	-200.09890	-819.67612	1
9156	H	57.87600	46.33480	79.79090	-2405.58554	1968.51410	486.14470	1
9157	C	57.07300	44.51080	79.22090	223.58277	529.74666	-707.69359	1
9158	H	56.64100	43.64980	79.70890	-2194.21227	2069.53962	894.79860	1
9159	C	55.93600	45.12680	78.34290	-518.88023	-145.33223	735.59014	1
9160	H	56.29600	45.99180	77.74590	2184.72905	100.66614	2261.64797	1
9161	H	55.54800	44.49680	77.51490	1248.43424	-602.57619	-2824.27692	1
9162	N	53.71900	46.31980	78.70290	-450.62011	535.76950	-471.76779	1
9163	H	53.67500	46.71180	77.78490	2145.22324	692.26068	-2194.77074	1
9164	C	54.76900	45.59380	79.19390	747.60014	320.33242	412.22830	1
9165	C	52.84700	46.50780	79.73890	-653.78111	361.98540	522.48238	1
9166	H	51.89400	47.02380	79.61890	821.71042	-3004.28058	-444.20312	1
9167	N	53.29900	45.96080	80.86590	-521.14493	-363.93868	555.54378	1
9168	C	54.52600	45.35480	80.48390	151.03952	173.87420	882.27310	1
9169	H	55.14700	44.83680	81.20490	-1933.72550	1915.08321	1578.41320	1

9170	C	58.04800	44.00880	78.19490	737.17950	260.16697	469.39380	1
9171	O	57.88200	42.94680	77.55890	260.74621	-502.24469	550.80751	1
9172	N	59.14200	44.76280	78.02990	-229.19614	-767.26064	-267.30605	1
9173	H	59.21600	45.65280	78.47390	2722.75767	-1531.41429	-373.61368	1
9174	C	60.37000	44.45780	77.32690	475.53858	-634.38824	450.40607	1
9175	H	60.06600	43.86780	76.47490	1926.73388	-1447.61399	-2022.45804	1
9176	C	61.19700	45.73880	76.87590	-753.09062	-29.10756	513.28186	1
9177	H	62.10800	45.47580	76.29590	-203.08343	-2886.69370	1234.49700	1
9178	H	61.43300	46.19080	77.86290	-2217.83936	860.91246	-2058.69972	1
9179	O	60.39300	46.65880	76.10090	299.48177	657.88616	317.99952	1
9180	H	59.93500	47.30180	76.64590	-931.22968	1921.92466	2310.24742	1
9181	C	61.25600	43.57680	78.15690	-178.70763	-160.85079	879.56899	1
9182	O	61.74400	44.02380	79.23190	668.96290	409.43745	92.06977	1
9183	O	61.55900	42.43480	77.70390	607.49542	-496.86289	-87.77135	1
9184	N	68.09800	39.69880	83.86190	571.61285	349.91433	513.31374	1
9185	H	68.31400	38.85080	84.42290	910.08563	2169.10908	2089.24296	1
9186	H	68.24600	39.59180	82.83790	1776.01328	-2241.62595	1311.15071	1
9187	H	67.12500	40.02180	84.03590	1021.37160	1012.12330	-2798.32677	1
9188	C	68.95200	40.75780	84.30590	777.55891	146.67247	453.14493	1
9189	H	68.94300	40.82480	85.38390	1946.09249	226.04804	2461.67677	1
9190	C	70.47100	40.56280	83.91090	-111.61165	613.31428	665.46182	1
9191	H	70.98000	41.53880	84.06090	2031.28577	2399.19909	-126.28571	1
9192	H	70.47900	40.45980	82.80490	230.72473	-2499.99811	-1896.04900	1
9193	C	71.15500	39.33080	84.51890	-126.72152	-755.37306	494.77692	1
9194	H	72.17500	39.10180	84.14190	2817.21167	-1316.06727	479.07368	1
9195	H	70.62200	38.43880	84.12690	2586.76849	178.09807	-1781.89115	1
9196	C	71.32300	39.38980	86.03290	463.17499	681.60177	-390.30625	1
9197	H	70.30800	39.45380	86.48090	140.17274	-556.15974	-3093.42273	1
9198	H	71.82700	40.34380	86.29990	-1194.98471	1307.19899	2600.28240	1
9199	C	71.99000	38.13380	86.56490	192.57395	-856.97157	244.87956	1
9200	H	71.54000	37.18180	86.20890	2223.30287	-2111.73266	704.08501	1
9201	H	73.02200	38.05280	86.16090	-2223.17803	-1828.22959	1270.15048	1
9202	N	72.01700	38.08680	88.06190	-231.46637	312.51116	749.28792	1
9203	H	72.40100	38.94980	88.49690	-1219.09390	2187.79300	-1904.10033	1
9204	H	71.06600	37.95380	88.46190	-1435.97863	-1999.74162	-1958.88362	1
9205	H	72.60700	37.30680	88.41590	2885.33725	1136.02598	-531.50744	1
9206	C	68.42100	42.10180	83.76190	-828.88752	-98.95561	366.88455	1
9207	O	67.82500	42.17680	82.71690	-522.37256	-577.22668	-132.52735	1
9208	N	68.61900	43.27580	84.43490	-646.96390	541.01008	-37.65773	1
9209	H	69.20800	43.27780	85.23890	2269.17026	2048.11863	744.51504	1
9210	C	67.99400	44.54780	83.99690	242.27881	241.13978	-845.34229	1
9211	H	68.34000	44.71780	82.98890	859.63306	-1423.90944	-2670.53162	1
9212	H	66.91700	44.46680	83.96490	-771.66451	-605.82432	-2989.27031	1
9213	C	68.37200	45.68480	84.92590	184.66813	-321.36860	833.10918	1
9214	O	68.20000	46.83880	84.64490	-682.82653	-368.19143	147.68288	1
9215	N	68.83800	45.43480	86.17690	-151.80695	593.35009	-581.00139	1
9216	H	69.14100	44.52880	86.46290	2037.25410	2010.44992	1306.10606	1
9217	C	69.04600	46.53980	87.06590	-543.62316	-345.00075	-645.67743	1
9218	H	68.12300	47.09580	87.14390	66.33524	-2802.41070	1428.39775	1
9219	C	69.42500	45.95680	88.48290	-272.01223	-709.62501	-503.87766	1
9220	H	69.61000	46.79780	89.18490	-409.90894	2764.32361	-1445.23903	1
9221	H	70.26400	45.23680	88.37490	2379.73334	927.90655	1836.86822	1
9222	N	68.12900	45.25980	90.58990	460.74564	311.05029	-635.32154	1
9223	H	68.44200	46.05880	91.10290	-330.13030	2963.30336	1004.02859	1
9224	C	68.28000	45.18480	89.23290	519.54692	329.33351	-673.09839	1
9225	C	67.11100	44.45380	90.92790	644.40650	-337.95750	549.52342	1
9226	H	66.88800	44.18780	91.96090	1809.78404	2565.69366	-200.30982	1
9227	N	66.50500	43.97780	89.88790	-540.84101	466.07973	-450.48082	1
9228	C	67.24500	44.40280	88.80090	233.82681	632.05969	614.22844	1
9229	H	67.06100	44.12980	87.76890	2200.32966	771.33471	-2112.30168	1
9230	C	70.13100	47.50080	86.71590	173.45819	439.65766	-779.78484	1
9231	O	69.95600	48.68880	86.84090	222.39656	-627.13672	425.28406	1

9232	N	71.22300	46.97380	86.14590	204.60913	810.01953	121.14355	1
9233	H	71.30800	45.98380	86.05590	1395.58742	-1035.56346	2622.62660	1
9234	C	72.34500	47.79380	85.73390	660.80815	628.31392	2.28335	1
9235	H	72.45100	48.61880	86.42290	-1545.53051	576.21836	-2679.09202	1
9236	C	73.65200	47.05680	85.70090	-425.79057	48.13732	804.88272	1
9237	H	73.55600	46.00080	85.36790	3039.25537	630.53926	-513.39387	1
9238	H	74.35000	47.50180	84.95990	-1972.72698	1038.17948	-2220.08060	1
9239	C	74.30700	47.04680	87.09390	480.53013	151.83766	759.92574	1
9240	H	74.48500	48.04780	87.54190	2370.68197	2029.45804	-399.24092	1
9241	H	75.34400	46.64680	87.06490	1467.22559	-1259.41518	2481.80352	1
9242	C	73.53900	46.29480	88.22990	58.71735	865.85843	279.80790	1
9243	O	73.14300	46.94180	89.21590	700.56881	-336.87543	-139.08814	1
9244	N	73.26100	44.98580	88.05190	-505.79474	159.24044	-656.87629	1
9245	H	73.59700	44.45680	87.27190	3144.97068	8.48997	-85.51932	1
9246	H	72.71800	44.56680	88.77890	2893.42752	214.46368	-1216.67940	1
9247	C	72.00600	48.49580	84.37690	-652.05618	177.10620	-612.29661	1
9248	O	72.38900	49.64980	84.14890	350.99120	170.81571	-686.47971	1
9249	N	71.16500	47.88080	83.49290	-302.53106	-766.33903	-184.04277	1
9250	H	70.90700	46.92780	83.63290	364.44118	-1764.43515	2579.18155	1
9251	C	70.59400	48.62080	82.36290	-862.50171	-289.28886	-62.07866	1
9252	H	71.41900	49.01280	81.78590	1036.01167	2208.48577	-1986.83081	1
9253	C	69.70100	47.63480	81.51590	-164.55527	-344.16843	-828.20327	1
9254	H	69.09700	47.05380	82.24590	658.45871	-2145.97582	2204.41515	1
9255	H	69.01800	48.11480	80.78390	2985.10277	-664.84523	738.49069	1
9256	C	70.56200	46.67680	80.62690	283.54917	211.53191	840.41961	1
9257	H	71.33500	46.24680	81.29890	-1916.84059	822.55660	-2355.28109	1
9258	H	71.11300	47.16180	79.79190	-944.70943	-446.17113	2967.60537	1
9259	C	69.74500	45.52780	80.02090	524.29088	-391.76342	634.89487	1
9260	H	69.31500	44.92580	80.84990	-1229.57383	1844.48205	2232.54572	1
9261	H	70.38800	44.89380	79.37490	1015.63131	-780.23833	-2873.66446	1
9262	C	68.59400	45.99380	79.11190	-663.46686	-12.73768	-625.38027	1
9263	H	67.85700	46.48980	79.77890	2253.08905	-497.15486	-2138.84385	1
9264	H	68.97400	46.63180	78.28490	916.62625	-2520.24030	1645.11743	1
9265	N	68.02900	44.78280	78.47990	-646.67135	411.61989	353.63473	1
9266	H	67.98800	44.08980	79.25490	456.55696	-1691.11499	2613.41005	1
9267	H	67.10500	44.86980	78.00990	1932.75723	1360.21106	2076.65635	1
9268	H	68.67200	44.54580	77.69790	417.66651	2948.47236	1015.03285	1
9269	C	69.71700	49.79980	82.79390	-617.67290	-324.69073	586.94729	1
9270	O	69.79800	50.86580	82.22390	540.16093	474.80293	-326.21401	1
9271	N	68.85600	49.66080	83.84290	594.48378	432.66991	-414.79883	1
9272	H	68.79800	48.77280	84.29290	-978.53363	2663.26302	-1359.31167	1
9273	C	68.00000	50.77580	84.28590	715.14807	-556.17579	103.35727	1
9274	H	67.57400	51.25780	83.41790	2428.98298	1120.09530	1656.39803	1
9275	C	66.81200	50.11480	85.12790	-332.12868	-304.81920	792.60759	1
9276	H	67.22400	49.50880	85.96190	-139.30877	1651.25559	-2674.35493	1
9277	H	66.27300	50.96480	85.59790	-1694.81756	919.65983	2485.96972	1
9278	C	65.87200	49.30880	84.17590	395.52658	651.74012	-500.24449	1
9279	H	66.45800	48.61780	83.53290	-1809.92321	376.01599	2545.78400	1
9280	H	65.40700	50.13980	83.60490	-2338.21175	-441.51441	-2058.16838	1
9281	C	64.58100	48.69080	84.76490	226.48407	674.72310	570.00413	1
9282	H	63.91200	48.26980	83.98490	-2066.60647	-2145.83371	-1011.31678	1
9283	H	64.00700	49.44380	85.34690	2912.66198	1184.58333	106.71804	1
9284	N	64.98200	47.51680	85.61290	-664.91099	244.64166	-459.03826	1
9285	H	64.97100	46.61780	85.17490	-2236.99295	368.58991	2181.33680	1
9286	C	64.91300	47.44980	86.91190	515.92537	620.47959	-424.59050	1
9287	N	65.22000	46.31280	87.50190	290.27672	-635.12157	-474.37570	1
9288	H	65.23700	45.48880	86.93590	-2931.03971	-12.51396	1143.27417	1
9289	H	64.79200	46.14780	88.39090	-219.68945	1131.84790	2927.26546	1
9290	N	64.55700	48.39180	87.74590	366.70747	732.70913	203.31074	1
9291	H	64.32200	49.30080	87.40390	1717.53574	-1465.36163	2191.12129	1
9292	H	64.48300	48.15980	88.71590	896.89385	606.79751	2953.91341	1
9293	C	68.76300	51.77380	85.17190	-285.50188	631.16787	-592.93069	1

9294	O	68.31700	52.89480	85.38790	455.07951	-469.12633	-443.22720	1
9295	N	69.99200	51.44480	85.66490	3.21938	-338.54617	773.33590	1
9296	H	70.22400	50.48180	85.78290	-2461.25588	946.01213	-1716.24788	1
9297	C	71.03900	52.33780	86.14090	-581.44329	507.81909	485.27773	1
9298	H	70.60600	52.99280	86.88290	-1990.57360	-1242.27221	-2095.85370	1
9299	C	72.06500	51.49980	86.96290	573.91930	-554.52735	441.09757	1
9300	H	72.56500	50.79680	86.26290	-1932.81945	2229.60763	-1091.46003	1
9301	H	71.46100	50.99980	87.75090	560.37078	3084.03253	-270.10028	1
9302	C	73.17300	52.34480	87.63990	60.06995	701.82141	-579.04172	1
9303	H	73.64300	52.97080	86.85090	1255.68737	-183.46375	2878.85681	1
9304	H	74.04000	51.75980	88.01390	319.95097	2014.62973	2395.22956	1
9305	C	72.66500	53.24480	88.79790	-478.15527	563.67583	533.93642	1
9306	H	72.29600	54.16380	88.29490	-1899.60117	-2176.04413	1246.82540	1
9307	H	71.81600	52.78380	89.34490	-611.93222	2480.08668	-1836.55526	1
9308	C	73.72900	53.65480	89.76990	779.41680	-154.22984	447.40765	1
9309	H	74.54200	54.24280	89.29390	-2182.45431	-1070.66177	1997.19874	1
9310	H	74.15700	52.71680	90.18490	-258.53165	184.47061	3130.07319	1
9311	N	73.08500	54.51480	90.80690	-312.61414	-447.45925	643.99139	1
9312	H	72.42900	53.95380	91.38690	1690.89145	-1863.86110	-1888.15628	1
9313	H	72.53100	55.23180	90.29690	245.16499	3099.80847	478.86093	1
9314	H	73.73600	55.06480	91.40390	2155.19886	-2109.17509	897.06441	1
9315	C	71.68500	53.15880	85.00390	623.75668	-425.37872	-511.30378	1
9316	O	71.94000	54.39380	85.13790	210.32796	-64.02608	758.47877	1
9317	N	72.06400	52.55680	83.85790	-512.68802	-561.07426	367.44925	1
9318	H	72.02800	51.56080	83.83890	-1340.09802	-2231.07034	-1767.67889	1
9319	C	72.45900	53.18580	82.59290	272.44450	717.63508	492.16348	1
9320	H	73.31700	53.82280	82.75190	-2566.36552	740.82608	-1662.27885	1
9321	C	72.73700	52.17980	81.49090	-525.34461	-458.00046	587.96226	1
9322	H	73.16400	52.69180	80.60190	-869.76759	-2305.19100	-1956.48282	1
9323	H	73.43100	51.39180	81.85490	1353.06864	498.04678	-2796.31559	1
9324	H	71.81100	51.66480	81.15690	-241.38724	2448.10649	-1961.30901	1
9325	C	71.42300	54.10280	82.09390	-689.97708	-585.91715	109.92600	1
9326	O	71.72400	55.20980	81.62890	-552.83839	-246.67264	507.09915	1
9327	N	70.15100	53.68580	82.18190	-342.29331	458.75259	-620.52691	1
9328	H	69.93300	52.74080	82.41190	-2053.05600	-911.11173	2202.96680	1
9329	C	69.05200	54.61880	81.81290	-661.84217	377.23300	501.10998	1
9330	H	69.27300	54.93580	80.80490	2243.27517	930.64832	-1999.95911	1
9331	C	67.72000	53.76380	81.88590	639.20273	-551.70776	344.22291	1
9332	H	67.86000	52.87180	81.23890	-2063.73426	-2288.81104	632.90689	1
9333	H	67.52600	53.54180	82.95690	-1559.68592	-2705.88566	379.19502	1
9334	C	66.42000	54.44080	81.37090	430.20625	-46.35091	-802.63639	1
9335	H	66.26400	55.30580	82.05090	-681.97645	-583.37952	3015.42744	1
9336	C	66.51600	54.88780	79.91790	-173.14037	-434.96732	782.48121	1
9337	H	67.34800	55.61980	79.84090	-803.72996	-2374.21637	-1901.40501	1
9338	H	66.83700	54.05780	79.25390	1898.90846	2069.68757	-1417.30952	1
9339	H	65.61300	55.35880	79.47290	-1667.41036	-79.12497	2666.77861	1
9340	C	65.08700	53.64980	81.60090	-731.35607	301.24535	-453.67448	1
9341	H	64.19400	54.26480	81.35690	-2511.54906	1572.20663	1057.59817	1
9342	H	65.13500	52.68680	81.04990	-595.74175	-3073.77495	-308.58642	1
9343	H	65.04700	53.31080	82.65790	-2822.71283	-1352.70024	317.36508	1
9344	C	68.94000	55.86580	82.65390	-70.47272	-828.70885	373.79973	1
9345	O	68.94800	56.97480	82.06590	-446.80757	137.32904	636.49899	1
9346	N	68.95500	55.70480	84.03490	279.57794	-554.94538	571.44036	1
9347	H	68.90000	54.78480	84.41390	1046.08587	-532.20686	2919.02149	1
9348	C	69.01700	56.76980	84.97390	-534.55167	-434.10288	597.71247	1
9349	H	68.18000	57.41880	84.76190	-1645.94003	-1799.36271	-1987.81324	1
9350	C	68.98700	56.10080	86.37390	385.92827	769.98546	-299.38731	1
9351	H	67.97000	55.65380	86.34790	1889.06635	1409.96097	2083.66615	1
9352	H	69.84200	55.41280	86.55090	-1619.21534	815.70040	2571.18664	1
9353	C	69.01600	57.12980	87.55390	-623.59984	585.04799	316.69085	1
9354	H	68.64300	58.10980	87.18590	2090.21703	-1164.78809	-2042.66681	1
9355	H	70.04000	57.51080	87.75690	2155.28233	1395.29939	-1818.27499	1

9356	C	68.28500	56.64680	88.80690	-56.65648	-649.82734	-637.15420	1
9357	H	67.27800	56.32580	88.46590	-516.46076	-2477.12087	-1869.58998	1
9358	H	68.78000	55.77180	89.27990	-2708.29037	-130.47564	1595.73357	1
9359	C	68.18300	57.76180	89.88990	-301.37460	-720.47852	470.67511	1
9360	H	67.70500	58.60680	89.34890	-1411.07974	-1846.54891	2120.69265	1
9361	H	69.18300	58.07080	90.26390	2505.33603	-21.34407	1902.90884	1
9362	N	67.28600	57.24180	90.94090	-427.52308	-725.09425	-64.30115	1
9363	H	67.23400	57.85680	91.77790	-2217.36352	404.32433	-2195.00503	1
9364	H	66.34800	56.94180	90.60490	2024.90662	1892.46171	-1488.81432	1
9365	H	67.76700	56.37380	91.25190	2451.35277	-664.42586	1856.78058	1
9366	C	70.26400	57.65280	84.87290	243.27956	-474.74816	-739.51352	1
9367	O	70.14300	58.87780	84.98790	-350.36558	642.74227	-296.23228	1
9368	N	71.49100	57.15780	84.71690	525.38516	-576.92895	322.17342	1
9369	H	71.63100	56.17080	84.69590	192.96560	-1746.91109	-2609.46204	1
9370	C	72.71900	57.94580	84.52690	-330.22362	621.77168	579.48541	1
9371	H	72.79500	58.56780	85.40690	-1952.93453	2422.54589	-464.26757	1
9372	C	74.01800	57.10780	84.51390	-88.98608	856.89754	298.76258	1
9373	H	74.13900	56.57280	83.54790	1097.55944	-2284.88143	-1863.57355	1
9374	O	74.08600	56.29880	85.65490	-367.30544	-694.24777	82.06081	1
9375	H	73.52300	55.52680	85.55590	2455.66144	-868.21927	-1764.69500	1
9376	C	75.19200	58.07780	84.76890	20.29836	-909.46653	-62.52683	1
9377	H	75.21200	58.81580	83.93790	3118.96169	66.95838	-407.21098	1
9378	H	76.17100	57.55180	84.75690	2081.85373	-2327.17554	-385.18214	1
9379	H	75.14700	58.74180	85.65790	1243.13381	322.57344	-2872.07085	1
9380	C	72.59200	58.81480	83.22690	-330.46249	261.44679	-808.63534	1
9381	O	73.01500	59.98280	83.18890	-340.56796	-20.52919	-712.19326	1
9382	N	72.00200	58.27580	82.17390	268.31858	-474.22387	-644.81715	1
9383	H	71.78800	57.30480	82.23390	1714.59334	745.53730	-2530.33002	1
9384	C	71.67800	58.96180	80.92490	197.77714	-849.81669	-264.85240	1
9385	H	72.62500	59.27280	80.50790	164.43913	870.78194	3018.76213	1
9386	C	71.09500	58.12480	79.80190	-407.85511	-507.48595	-638.40678	1
9387	H	70.05700	57.80880	80.03990	-2605.82938	1041.61792	1422.29096	1
9388	O	71.89200	56.91180	79.71290	480.89195	457.24105	428.13641	1
9389	H	71.56000	56.30780	80.38190	-2278.15747	2128.42482	-421.93905	1
9390	C	71.17200	58.81080	78.46790	509.30657	20.67635	756.06237	1
9391	H	72.19700	59.09080	78.14290	1932.07419	920.80895	2305.95456	1
9392	H	70.51100	59.70180	78.53390	-407.85607	3061.21716	600.69058	1
9393	H	70.87600	58.20880	77.58290	637.30372	-1572.87634	-2649.17538	1
9394	C	70.83300	60.20580	81.08790	-909.86007	-35.78903	-48.21613	1
9395	O	71.24500	61.35880	80.80990	298.18598	-476.17007	554.95443	1
9396	N	69.70300	59.95480	81.76090	-226.13355	-415.64329	699.12557	1
9397	H	69.43500	59.01180	81.94290	-1315.49295	1570.02918	2388.03537	1
9398	C	68.79200	60.93480	82.26090	-456.02518	37.45616	-788.72624	1
9399	H	68.27700	61.41580	81.44290	-286.12146	1164.47398	2908.66999	1
9400	C	67.64800	60.18880	82.90290	570.37181	-682.81244	-199.73525	1
9401	H	68.05500	59.43180	83.60690	-1276.19407	2174.53921	1881.73700	1
9402	C	66.77000	61.10180	83.78390	326.57539	660.06675	-537.69081	1
9403	H	65.86900	60.56480	84.14890	2409.09134	642.70293	1918.70740	1
9404	H	66.36600	61.97780	83.23390	-1844.74327	2366.54682	-945.83543	1
9405	H	67.30500	61.44380	84.69590	-2707.66627	1602.04970	-14.36530	1
9406	C	66.87700	59.43380	81.79990	-552.19502	-579.97955	-436.06809	1
9407	H	65.98800	58.91880	82.22390	1821.96405	-2564.38861	50.83576	1
9408	H	67.56900	58.76680	81.24290	2706.18772	-1097.80482	-1170.29860	1
9409	H	66.48400	60.21480	81.11490	1610.79832	-15.96195	-2702.46188	1
9410	C	69.33700	61.96280	83.14390	171.94929	749.49115	-490.04842	1
9411	O	69.12900	63.14880	82.91090	-217.41480	-646.23898	398.41338	1
9412	N	70.16800	61.60980	84.15190	639.72837	-179.72673	520.69012	1
9413	H	70.42600	60.68180	84.41090	574.47676	-1720.67927	2570.49908	1
9414	C	70.81100	62.52780	85.05990	765.64765	-88.77459	487.18964	1
9415	H	70.02500	63.10980	85.51790	-1690.19238	-1785.53545	-1962.99238	1
9416	C	71.57800	61.78180	86.15290	-646.68575	67.45467	639.29524	1
9417	H	72.12500	60.95180	85.65690	-2582.64648	1101.73039	-1419.27923	1

9418	C	72.63700	62.69880	86.91090	509.85807	454.90297	-603.78725	1
9419	H	73.14200	62.11380	87.70790	-1397.43705	-1333.21994	2483.52985	1
9420	H	72.14800	63.58180	87.37590	-35.65275	3117.99305	-418.41898	1
9421	H	73.44600	62.89480	86.17490	-1420.38108	-1983.24603	-1986.82636	1
9422	C	70.63500	61.17080	87.20590	553.34893	534.02336	489.97451	1
9423	H	69.64800	60.89180	86.77890	-1578.04832	140.24373	2718.14669	1
9424	H	70.45800	61.96580	87.96190	2868.32007	896.40040	931.36058	1
9425	C	71.26700	59.95680	87.91890	85.39618	-811.05417	-407.85981	1
9426	H	70.48700	59.54080	88.59190	-1870.51271	-1676.22946	-1894.64066	1
9427	H	71.59500	59.21580	87.15890	-1924.64270	-1979.66680	1508.27586	1
9428	H	72.13800	60.22880	88.55390	-2473.46250	-76.71059	1942.76220	1
9429	C	71.66200	63.52580	84.35490	438.07441	633.69871	-487.81940	1
9430	O	71.52800	64.71780	84.59990	-443.34025	-349.46283	552.22494	1
9431	N	72.44000	63.06280	83.35390	-624.40211	557.05801	-111.71691	1
9432	H	72.41000	62.08380	83.16990	386.38993	-135.32627	3119.39351	1
9433	C	73.23300	63.90780	82.52590	365.35043	-426.39720	718.43962	1
9434	H	73.88400	64.42880	83.21190	550.96647	1392.34146	2766.95635	1
9435	C	74.22100	63.07780	81.65290	-146.04760	808.90844	-394.70019	1
9436	H	73.76600	62.28180	81.02690	-2505.44589	-11.68796	1902.84800	1
9437	H	74.79000	62.50380	82.41590	2273.04631	-1218.22742	1802.05678	1
9438	C	75.19500	63.90380	80.72890	-542.81902	264.10424	683.40871	1
9439	H	74.55500	64.48980	80.03390	-767.21379	2580.81773	1627.57152	1
9440	C	76.09000	64.93880	81.32490	14.20169	-878.17541	-245.06582	1
9441	H	76.90300	64.44380	81.89790	1439.76558	-2322.83709	1558.75886	1
9442	H	75.62900	65.65480	82.03890	-739.09741	2217.17861	2106.20043	1
9443	H	76.67100	65.48180	80.54890	-1948.68896	-2390.62720	621.07902	1
9444	C	76.03300	62.90280	79.89590	-458.99115	-255.15187	745.43655	1
9445	H	76.48300	62.22980	80.65690	2600.30754	1525.48479	-899.73501	1
9446	H	76.84200	63.38880	79.30890	1497.07460	-1397.33276	2388.40010	1
9447	H	75.43400	62.30680	79.17490	2301.56355	-2144.06834	-63.26486	1
9448	C	72.43700	64.90980	81.66490	-222.19629	779.00499	418.60606	1
9449	O	72.81300	66.08780	81.57690	-433.56174	-600.34748	-274.28881	1
9450	N	71.36300	64.44380	80.99590	-324.41239	573.49571	527.76089	1
9451	H	71.19000	63.46780	81.10790	1198.28039	1442.96826	2525.90438	1
9452	C	70.42600	65.14580	80.24290	-623.76666	556.66821	363.98716	1
9453	H	71.03900	65.71780	79.56190	-2613.07726	-1465.26358	-960.75809	1
9454	C	69.50000	64.18580	79.47790	248.39544	-8.29385	877.31518	1
9455	H	69.27400	63.33580	80.15590	17.57965	1064.64299	-2960.48180	1
9456	C	68.14600	64.84580	79.02290	719.99373	-206.78992	-519.90188	1
9457	H	67.51200	65.16380	79.87790	860.76847	-3026.02063	22.42768	1
9458	H	67.58600	64.15180	78.35890	-522.75864	2584.60160	-1716.03735	1
9459	H	68.45800	65.75480	78.46590	-660.30959	-2856.39409	1141.59112	1
9460	C	70.28000	63.43880	78.39190	-471.10765	-680.19178	383.20717	1
9461	H	70.44600	64.25280	77.65390	-148.63059	2023.65396	-2404.36266	1
9462	H	71.27200	63.03780	78.69290	-1939.54892	2067.38678	-1364.65679	1
9463	C	69.41000	62.39680	77.58790	27.87344	617.60138	670.25563	1
9464	H	68.96100	61.73580	78.35990	-2867.19630	554.91047	-1170.25039	1
9465	H	68.57700	62.83380	76.99690	977.52840	-2604.20158	1469.96550	1
9466	H	70.16900	61.86880	76.97190	-1503.18671	-2078.04153	-1822.19629	1
9467	C	69.70600	66.19980	80.98090	615.56666	-32.45129	-671.91935	1
9468	O	69.55800	67.36380	80.51690	444.73037	316.86583	570.47189	1
9469	N	69.14000	65.92480	82.22190	-560.34921	575.99168	258.67863	1
9470	H	69.22700	64.99080	82.55990	-2543.67384	-1684.65722	-768.03624	1
9471	C	68.75000	66.92180	83.19690	-549.25090	-557.48047	467.96364	1
9472	H	67.89500	67.41080	82.75390	-1202.66214	2108.85369	2001.14120	1
9473	C	68.34200	66.10180	84.47590	406.38210	-489.19738	653.44511	1
9474	H	68.06800	66.67780	85.38590	743.46099	-750.85036	-2963.39598	1
9475	H	69.24300	65.50480	84.73090	-2010.00971	-2073.72596	-1248.09769	1
9476	C	67.11800	65.15880	84.29590	-81.02934	-73.17877	-905.27903	1
9477	H	67.27600	64.54180	83.38490	-1070.74360	-2563.83302	-1475.97244	1
9478	C	67.17400	64.17980	85.52090	463.14448	-513.33840	-594.50137	1
9479	H	66.20600	63.64480	85.41390	2399.23451	1929.74753	-646.50944	1

9480	H	67.27400	64.75380	86.46590	-2867.84577	1245.42519	-350.14706	1
9481	H	68.06800	63.52580	85.43190	1296.50617	-786.12915	-2756.68260	1
9482	C	65.84000	65.91780	84.21390	870.64524	268.71178	-34.95503	1
9483	H	65.86700	66.56680	83.31290	2138.08734	-2069.27399	-1022.21029	1
9484	H	64.97100	65.22780	84.18490	2231.15667	-824.78726	-2059.09983	1
9485	H	65.68500	66.60280	85.07490	-1727.56287	-1803.47867	-1913.43080	1
9486	C	69.78900	67.93480	83.58990	-666.59651	591.10016	-194.16668	1
9487	O	69.52000	69.15080	83.59590	-327.14884	-500.18694	516.15297	1
9488	N	71.02500	67.45980	83.92190	-668.40418	452.16205	-247.90648	1
9489	H	71.29900	66.50280	83.86090	1266.76997	2405.96981	1582.66527	1
9490	C	72.04000	68.25880	84.44690	15.43303	422.10510	808.10897	1
9491	H	71.72900	68.65180	85.40390	-1702.36420	688.91380	2554.52151	1
9492	C	73.35000	67.44380	84.73490	-744.59771	-367.26277	377.01897	1
9493	H	74.10400	68.14980	85.14490	2988.90615	-697.01464	-691.98039	1
9494	H	73.20500	66.70780	85.55390	-703.87624	-2780.78880	1292.28406	1
9495	H	73.77200	66.98480	83.81490	2028.40491	-2216.74908	932.64316	1
9496	C	72.37500	69.33780	83.44090	-762.43527	-335.32620	-371.07923	1
9497	O	72.35400	70.52480	83.71590	535.09965	467.64694	344.38631	1
9498	N	72.52600	68.93380	82.15690	567.82762	-253.64860	570.88218	1
9499	H	72.48400	67.96680	81.91890	-311.17023	2478.09920	-1913.22338	1
9500	C	72.88600	69.73780	81.06290	281.76155	528.84857	-687.29951	1
9501	H	73.82700	70.20980	81.30690	-2876.31137	100.50283	-1270.81010	1
9502	C	73.15900	68.74380	79.88290	38.65303	903.87174	-113.89831	1
9503	H	72.24600	68.13780	79.70290	2003.80494	-786.29881	-2294.49911	1
9504	H	74.00200	68.08380	80.18090	-1457.38086	2589.07619	-1034.86797	1
9505	C	73.42400	69.35880	78.57890	807.67268	-421.78101	-34.88021	1
9506	C	74.73300	69.62180	78.20490	-887.19590	-172.55521	120.66125	1
9507	H	75.61300	69.41980	78.79790	514.38192	-2657.95822	1602.77746	1
9508	C	74.94800	70.16980	76.88990	506.85242	-148.00777	743.40119	1
9509	H	75.94500	70.40780	76.54990	-2057.27705	-762.85986	-2254.74659	1
9510	C	73.86900	70.43680	76.05490	-115.11739	-903.73521	-38.23159	1
9511	H	74.11800	70.79380	75.06590	-810.10216	2960.38401	-691.43851	1
9512	C	72.34100	69.62080	77.69590	-637.40370	-2.52272	-652.04384	1
9513	H	71.31700	69.47980	78.01090	-913.71889	1686.08332	2494.08641	1
9514	C	72.56000	70.16080	76.43590	-547.91257	-660.70685	-307.74874	1
9515	H	71.70500	70.39580	75.81990	-2798.21263	423.81403	1374.26851	1
9516	C	71.85900	70.76280	80.73490	361.91530	-606.37613	-576.86767	1
9517	O	72.02600	71.98080	80.52490	251.12941	291.83528	689.48779	1
9518	N	70.56600	70.38080	80.67190	-574.94779	539.68619	-301.40694	1
9519	H	70.32800	69.41380	80.71090	1729.56689	2048.77939	-1646.00352	1
9520	C	69.44000	71.27380	80.50690	-831.09200	347.37310	-141.66520	1
9521	H	69.51600	71.89380	79.62590	-663.10323	-2419.00002	-1899.19963	1
9522	C	68.15900	70.43480	80.33790	507.21461	-180.16149	736.02051	1
9523	H	67.91400	69.83780	81.24290	-1462.49686	1425.98534	2392.88424	1
9524	H	68.37400	69.74180	79.49790	1822.66047	2229.26481	-1267.48312	1
9525	C	66.92100	71.17580	80.05790	-383.58289	-227.95308	-795.20599	1
9526	C	66.57200	71.44880	78.74590	-795.50275	442.43117	-53.67529	1
9527	H	67.31800	71.24980	77.98990	982.27208	1484.92119	2593.91150	1
9528	C	65.36200	72.05980	78.40290	-424.62679	560.01409	-580.97100	1
9529	H	65.06300	72.19480	77.37390	2881.47047	177.74285	1250.50455	1
9530	C	64.52500	72.43380	79.47390	287.06335	-522.43045	690.00874	1
9531	H	63.62600	73.01480	79.32790	-1612.45005	2071.34543	1734.28924	1
9532	C	66.02700	71.52980	81.08290	-416.92943	-447.70391	676.15239	1
9533	H	66.30100	71.35380	82.11290	-3035.20177	-817.83505	-130.08575	1
9534	C	64.89600	72.27080	80.79890	306.78485	561.44746	-649.70055	1
9535	H	64.14400	72.56780	81.51590	2267.31498	-343.02556	-2154.02936	1
9536	C	69.33500	72.26180	81.71990	787.55063	-102.23205	-448.06654	1
9537	O	69.08000	73.41680	81.52690	-372.56696	694.58838	48.66286	1
9538	N	69.63000	71.85980	82.96790	433.03109	-325.42850	647.49722	1
9539	H	69.70200	70.91080	83.26390	-1650.72846	-2672.16063	-181.32662	1
9540	C	69.74000	72.75980	84.02890	-875.54912	-117.10418	-226.16667	1
9541	H	68.80600	73.27580	84.19490	2218.07323	-1064.37813	1960.98867	1

9542	C	69.97200	71.99480	85.34890	-255.79290	521.70126	702.74376	1
9543	H	69.16700	71.24180	85.48590	1967.09899	1790.97782	-1679.62681	1
9544	H	70.95100	71.47480	85.41890	-258.16526	-3132.40923	-139.96202	1
9545	H	69.93600	72.73580	86.17590	-1650.24808	1788.44499	1994.08426	1
9546	C	70.81600	73.85580	83.78590	299.93807	614.64045	603.07982	1
9547	O	70.62400	75.02280	84.15090	-635.12172	-331.96871	-331.72942	1
9548	N	71.92800	73.46580	83.15890	219.79269	688.33212	-436.53449	1
9549	H	71.88900	72.59580	82.67490	-2318.58861	-1320.12745	-1667.22423	1
9550	C	73.00100	74.43080	82.80690	-56.28492	505.89737	-756.53874	1
9551	H	73.28100	74.87180	83.75190	560.35807	-260.08162	3084.89588	1
9552	C	74.19600	73.61780	82.23390	-178.32623	-426.60590	-785.91231	1
9553	H	74.96200	74.36980	81.94790	-90.42995	2301.01560	-2143.68278	1
9554	H	73.88900	73.19180	81.25490	-2496.61376	281.72810	-1893.61433	1
9555	S	74.87400	72.35080	83.38990	-391.10506	304.14548	-256.40390	1
9556	H	73.67600	71.91480	83.75190	2085.04461	-1803.58698	1515.87902	1
9557	C	72.62400	75.52980	81.86190	-616.08198	158.70291	653.22843	1
9558	O	72.81800	76.70480	82.13490	782.67298	-104.30276	13.08299	1
9559	N	71.91800	75.07780	80.72890	-223.12259	-529.41462	-618.55376	1
9560	H	71.92300	74.09580	80.55290	-2078.71397	-2344.42619	-284.32429	1
9561	C	71.54200	75.91280	79.63390	160.71277	284.92917	-851.13911	1
9562	H	72.31800	76.64380	79.46390	687.85511	2637.49308	1571.21349	1
9563	C	71.62200	74.98880	78.37290	-14.87462	-544.45953	-731.29581	1
9564	H	71.04500	75.42080	77.52690	546.99020	792.51684	2995.15359	1
9565	H	71.17500	73.99780	78.60090	1747.68890	-1667.58371	-2015.68209	1
9566	C	73.02200	74.78780	77.81290	67.32814	600.59950	682.78706	1
9567	C	73.70700	73.56580	77.87990	108.14474	662.31673	-617.32671	1
9568	H	73.23900	72.61380	78.08190	2252.51218	599.02628	2113.19251	1
9569	N	74.94100	73.72080	77.23790	664.40130	-435.37845	-285.81253	1
9570	H	75.57100	73.04880	76.91690	-2958.82831	-154.63791	-1058.13439	1
9571	C	75.03800	74.99780	76.86390	318.30645	-448.54322	727.28329	1
9572	C	73.88500	75.72880	77.20590	101.30690	-666.07712	-614.43403	1
9573	C	73.84600	77.15180	77.05090	602.07279	-458.97011	508.23793	1
9574	H	72.96800	77.73480	77.28890	-102.26161	3138.63819	191.62225	1
9575	C	74.99200	77.74080	76.45190	-384.88471	-657.20590	-501.39323	1
9576	H	74.97600	78.77380	76.13690	2077.72398	2362.45752	-9.15197	1
9577	C	76.13500	75.64780	76.26290	273.95214	365.00384	-789.41334	1
9578	H	77.00800	75.08280	75.96990	-1844.42720	-2080.93541	-1471.74127	1
9579	C	76.07400	77.02980	76.04390	265.68115	714.65104	500.13841	1
9580	H	76.95300	77.55880	75.70590	-2227.71763	1240.99214	-1842.67167	1
9581	C	70.21200	76.64580	79.76090	-791.09693	346.49207	292.50624	1
9582	O	70.11700	77.79280	79.22390	-397.74122	-250.32718	634.63805	1
9583	N	69.22300	76.15280	80.47990	-738.81374	392.55939	112.79924	1
9584	H	69.32500	75.27080	80.93290	-2383.06337	1963.14052	604.41252	1
9585	C	67.91700	76.79680	80.50690	-228.98232	-612.60296	635.40201	1
9586	H	67.50100	76.72480	79.51290	-2652.48398	586.45764	1587.01682	1
9587	C	67.04200	75.89380	81.32190	253.12686	-868.38801	-115.23913	1
9588	H	67.50300	75.63980	82.29990	1794.50829	-2443.81903	-840.06832	1
9589	H	67.00500	74.91080	80.80590	2392.61939	1490.38827	1397.26214	1
9590	C	65.64000	76.49380	81.61290	-712.02831	-496.01506	280.06384	1
9591	H	65.63400	77.50380	82.07590	-2855.05416	-392.98280	1261.92571	1
9592	C	64.73900	76.55180	80.32490	-185.66717	-392.15166	801.99488	1
9593	H	64.91700	75.65380	79.69490	2031.57726	-631.98670	2317.65245	1
9594	H	63.67100	76.57880	80.62790	-3050.89579	-760.90833	-106.20553	1
9595	H	64.89500	77.50380	79.77390	1268.44632	2145.45816	1919.96860	1
9596	C	64.90600	75.60280	82.61490	217.91727	481.57359	-743.00063	1
9597	H	65.60700	75.23780	83.39590	-1776.92534	1897.96495	1771.57885	1
9598	H	64.05500	76.15680	83.06690	1742.36489	-1253.92117	-2300.01577	1
9599	H	64.60100	74.61180	82.21590	1329.07292	-1922.97514	2105.69656	1
9600	C	67.88300	78.25880	80.97990	-721.79164	-420.42846	-365.66070	1
9601	O	67.19700	79.02380	80.29190	491.88635	473.02935	397.38934	1
9602	N	68.52100	78.78280	82.02490	-50.66107	833.81815	-121.87301	1
9603	C	69.31500	77.97980	82.97190	-774.94738	288.15534	384.54396	1

9604	H	68.96900	76.92580	83.03290	-430.51626	2323.24255	-2077.36036	1
9605	H	70.36000	78.03480	82.59890	-123.70575	-1711.17270	2637.19759	1
9606	C	68.47200	80.19080	82.39590	123.65519	-846.88794	-314.54923	1
9607	H	67.44000	80.42380	82.61490	-718.05829	-2317.42853	-2003.03358	1
9608	C	69.25900	80.17180	83.75390	-400.17499	590.16441	-568.34580	1
9609	H	68.88300	80.87580	84.52690	2876.13069	1213.09254	393.07118	1
9610	H	70.32300	80.40280	83.53390	1018.20321	2831.75888	-917.94886	1
9611	C	69.11600	78.74880	84.28590	826.15565	200.65177	329.63118	1
9612	H	69.94800	78.54280	84.99390	2720.23055	1575.50067	-127.94379	1
9613	H	68.10900	78.61380	84.73490	1975.53506	-1680.30383	1781.02962	1
9614	C	69.05500	81.12380	81.23090	627.27813	121.76532	650.49701	1
9615	O	68.57200	82.24780	81.04590	358.18926	669.48263	217.07301	1
9616	N	70.09900	80.67380	80.54090	-757.99160	-237.76688	285.63601	1
9617	H	70.39500	79.77580	80.85690	1831.42459	-1978.30896	-1621.85199	1
9618	C	70.60700	81.42980	79.40390	-215.14607	876.68391	128.79633	1
9619	H	70.77000	82.44380	79.73990	-1946.65767	-2362.23219	727.05515	1
9620	C	71.94100	80.76680	78.92290	439.12220	-738.99675	-304.14882	1
9621	H	71.86800	79.65880	78.87490	1433.13192	865.53009	-2663.68481	1
9622	H	72.71000	80.96280	79.70090	2497.91656	-1128.30750	1544.52622	1
9623	C	72.44600	81.21980	77.54890	551.45682	363.65370	-628.57169	1
9624	C	73.03200	82.49780	77.40790	126.03326	887.00283	-169.68381	1
9625	H	73.19700	83.12680	78.26990	2997.77976	-929.91023	-216.35544	1
9626	C	73.38000	82.91680	76.12890	-268.62169	687.00284	536.02284	1
9627	H	73.80300	83.90780	76.04790	286.85084	3044.91548	737.85674	1
9628	C	73.21100	82.08580	74.99290	-484.43244	-749.27995	188.03130	1
9629	O	73.66500	82.54480	73.75290	658.54087	-314.36535	-301.87013	1
9630	H	74.19700	83.33680	73.85990	-741.21548	2282.44509	2034.51966	1
9631	C	72.14500	80.45680	76.39290	-380.39147	-828.65090	-9.54060	1
9632	H	71.53000	79.57280	76.46990	-237.42891	-3112.42521	-393.27223	1
9633	C	72.59800	80.86680	75.14790	360.82114	-783.09724	-296.67797	1
9634	H	72.46700	80.20280	74.30690	2569.56100	-1632.10586	-794.86662	1
9635	C	69.60500	81.53480	78.26890	-278.55029	-734.90649	462.35613	1
9636	O	69.34000	82.63880	77.79490	698.00129	-336.44272	152.40644	1
9637	N	68.89900	80.39980	77.87590	717.85149	441.77882	46.82945	1
9638	H	69.15900	79.51980	78.26490	-1642.63553	-2014.54850	-1772.44720	1
9639	C	67.79400	80.35980	76.99690	794.35812	-98.70473	-436.69619	1
9640	H	68.02800	80.90180	76.09190	-809.75792	-1680.34789	-2533.56455	1
9641	C	67.37900	78.88380	76.66290	784.30748	152.04994	-439.53793	1
9642	H	67.35800	78.20080	77.53890	2473.25549	1467.80879	1275.44927	1
9643	H	66.31400	78.74980	76.37590	1805.91656	-974.83447	-2384.65707	1
9644	C	68.31100	78.32080	75.65290	-698.59298	500.17537	-305.35791	1
9645	C	68.11000	78.68280	74.28590	540.67500	540.67818	-496.77827	1
9646	H	67.23800	79.29980	74.12290	1016.32147	2082.23211	2128.29188	1
9647	C	68.99100	78.15880	73.25190	212.00214	-690.14627	556.95980	1
9648	H	68.92600	78.57780	72.25790	-1771.57840	-172.91884	2594.19260	1
9649	C	69.92600	77.15880	73.58790	-488.10877	111.40820	762.09517	1
9650	O	70.77300	76.70680	72.57590	624.88106	256.11046	-409.33888	1
9651	H	70.57700	77.24380	71.80390	-2369.74769	-1734.43725	1128.82661	1
9652	C	69.24800	77.30080	75.92290	399.94764	-446.97378	686.80953	1
9653	H	69.32500	76.81380	76.88390	2438.68726	1984.75587	-108.51194	1
9654	C	70.03300	76.73280	74.90990	274.87732	481.77146	-723.73318	1
9655	H	70.81500	76.02580	75.14390	1698.21567	2136.86009	1564.64652	1
9656	C	66.60900	81.16880	77.39390	-503.59349	535.04360	539.97494	1
9657	O	66.03000	81.91280	76.59390	-555.71653	-31.06093	-560.21566	1
9658	N	66.26200	81.14380	78.69490	-423.91051	460.76442	-566.27583	1
9659	H	66.72900	80.59280	79.38290	231.56496	-420.20322	-3109.34610	1
9660	C	65.22400	82.07880	79.20490	673.00490	-614.10019	-37.36801	1
9661	H	64.38800	81.88480	78.54990	-2063.42445	-1517.23627	-1827.15623	1
9662	C	64.68300	81.72780	80.60790	-832.15514	-43.89968	-370.19135	1
9663	H	65.60700	81.77480	81.22190	-1925.12662	1278.53341	2134.82225	1
9664	C	63.60600	82.80080	81.01090	505.36527	-397.43725	646.60697	1
9665	H	62.70300	82.86080	80.36690	-2007.05635	1127.90983	2144.24123	1

9666	H	63.25600	82.57980	82.04190	-2206.49127	-827.25388	2084.53196	1
9667	H	64.00900	83.83280	81.09290	-2810.47507	-735.62911	-1207.60337	1
9668	C	64.11400	80.29080	80.63890	612.56915	-593.56585	322.31913	1
9669	H	63.25500	80.13980	79.95190	2849.58568	596.58090	-1192.55142	1
9670	H	64.84000	79.61680	80.13490	-1849.77837	-2543.24136	-92.03029	1
9671	C	63.65900	79.83980	81.99690	532.32684	449.11009	-588.53994	1
9672	H	64.50200	79.89380	82.71890	2476.88810	-656.72205	-1825.36783	1
9673	H	63.43900	78.75180	81.95090	2383.43696	-183.50493	2045.42916	1
9674	H	62.80200	80.44580	82.35890	-734.01996	2926.88786	890.37542	1
9675	C	65.58000	83.61280	79.03390	-662.43462	-189.91493	597.12955	1
9676	O	64.77400	84.26080	78.37690	-448.56273	-99.99674	642.19884	1
9677	N	66.82900	84.06580	79.36490	-665.14497	222.68035	-469.75304	1
9678	H	67.45400	83.43180	79.81190	-2950.53399	-175.34435	1077.88206	1
9679	C	67.13807	85.37603	79.01349	-145.16289	748.18281	975.57355	1
9680	H	66.30427	86.08032	79.35173	4025.27172	-1397.97570	198.41499	1
9681	H	68.12015	85.42546	79.52849	2332.84745	1845.68102	475.26894	1
9682	C	67.20112	85.68521	77.40237	-582.54134	485.37805	205.31967	1
9683	O	66.77357	86.78251	77.06833	-160.76338	-234.36112	228.58727	1
9684	N	67.89100	84.89680	76.61290	356.73523	-663.28731	381.39508	1
9685	H	68.32900	84.14080	77.09390	888.15468	2662.37180	1421.68347	1
9686	C	67.92599	85.12474	75.16463	76.61114	-973.33100	-168.67840	1
9687	H	68.44977	86.09948	75.15724	2540.35559	-51.91251	2952.87404	1
9688	C	68.53600	83.92580	74.53290	-676.89647	-545.29416	-275.52940	1
9689	H	68.10500	82.98380	74.93690	-1566.49989	1817.76903	-2034.70393	1
9690	C	68.34900	83.93880	73.05490	-859.83284	287.47088	97.46273	1
9691	H	67.38300	83.53880	72.67890	559.45597	-3034.42126	614.42889	1
9692	H	68.68700	84.91880	72.65490	-2379.23533	1914.79470	755.66312	1
9693	H	69.02400	83.17980	72.60690	2573.12642	-623.55059	-1699.53856	1
9694	C	70.05800	83.94780	74.75490	-859.47197	15.31935	304.17799	1
9695	H	70.56200	83.01280	74.42890	-557.06634	2791.46622	1340.00734	1
9696	H	70.17300	83.76380	75.84390	1858.38971	1313.36782	-2172.48219	1
9697	C	70.97024	85.17591	74.37880	761.68664	527.09125	-432.72830	1
9698	H	70.49517	86.03336	74.79007	-1435.08936	-647.68095	329.40645	1
9699	H	72.05058	85.08970	74.67081	1093.48795	209.70895	269.01653	1
9700	H	70.99847	85.38734	73.26199	-1793.80546	927.45615	989.55924	1
9701	C	66.28413	85.23771	74.63271	-159.88434	1510.72331	-442.89339	1
9702	O	66.06694	86.07690	73.80062	1005.83234	-986.34171	254.76712	1
9703	N	65.47600	84.30180	75.09290	-415.11655	435.25446	-592.37158	1
9704	H	65.70400	83.60980	75.77290	-77.01283	-2431.77744	1994.68136	1
9705	C	64.05600	84.33580	74.67990	-310.60242	222.51014	-827.92897	1
9706	H	64.10600	84.16680	73.61490	-2580.20351	-1213.99403	-1329.28347	1
9707	C	63.18100	83.19080	75.19690	304.73127	-482.89879	710.91393	1
9708	H	62.22600	83.07180	74.64190	2747.40308	654.17390	1386.38344	1
9709	H	63.77500	82.27180	75.00590	524.28411	-1982.39564	-2386.09722	1
9710	O	62.80900	83.14980	76.55590	289.23783	159.36988	717.33531	1
9711	H	63.47300	83.61580	77.06990	2995.73456	32.18442	-960.60649	1
9712	C	63.41789	85.77856	75.07775	-37.02953	357.67220	-406.15693	1
9713	O	62.75386	86.39214	74.28077	276.67969	115.20960	139.45494	1
9714	N	63.74022	86.10250	76.34170	351.99098	-141.11059	-477.43725	1
9715	H	64.37467	85.37819	76.87004	-643.70623	-493.26336	-1251.03018	1
9716	C	63.29891	87.38045	76.84813	-209.81531	304.84739	-416.09804	1
9717	H	62.16935	87.38724	76.71596	2022.38225	-695.05992	-873.32911	1
9718	C	63.67626	87.42624	78.35543	-1465.27561	656.90762	748.17226	1
9719	H	64.41447	86.55667	78.41150	66.39797	1045.43419	-3249.44613	1
9720	C	64.40250	88.67339	78.65424	-35.04159	159.65254	260.10558	1
9721	H	65.03135	88.98374	77.76207	657.77752	-596.04961	1281.35102	1
9722	H	64.98852	88.48801	79.57987	-3638.57596	319.95908	1987.35030	1
9723	H	63.72601	89.54204	78.80433	-1080.78520	1648.13621	73.94533	1
9724	C	62.48818	87.22482	79.29149	-736.96122	-786.29087	-459.17666	1
9725	H	61.86889	88.14460	79.35243	-1529.01402	-219.25327	2112.90188	1
9726	H	62.82459	87.03401	80.30079	523.04493	854.40546	91.72906	1
9727	C	61.63049	85.98136	78.78236	-733.83151	342.62272	67.69959	1

9728	H	62.02004	85.03657	79.19996	-1321.73762	957.54379	1315.02670	1
9729	H	60.52716	86.05181	79.01161	-1174.28326	191.20071	1563.13050	1
9730	H	61.64467	85.76539	77.71167	863.77335	4679.72460	-302.73039	1
9731	C	63.85224	88.55864	75.83177	485.08124	254.65374	-236.17860	1
9732	O	63.21389	89.56170	75.63380	57.38119	357.67811	-591.90075	1
9733	N	65.09138	88.31881	75.34339	514.24866	-603.21481	-1246.78729	1
9734	H	65.56809	87.45035	75.65693	-1348.94711	-2484.95825	-2831.20384	1
9735	C	65.81708	89.14912	74.49147	234.35969	119.82682	-377.60953	1
9736	H	65.49124	90.13369	74.91595	-202.00921	-1467.13838	-827.35639	1
9737	C	67.32865	88.72980	74.61218	337.19381	740.56566	333.78828	1
9738	H	67.47344	87.76215	74.09087	-479.54416	2774.05527	-1167.42475	1
9739	H	67.60901	88.49528	75.63449	1763.75535	496.74803	-382.28551	1
9740	C	68.35586	89.75592	73.90606	-141.10611	305.19398	-86.59275	1
9741	O	69.53983	89.25793	73.86973	47.19698	-55.15700	-108.08150	1
9742	O	68.15997	90.98714	73.69724	-390.66956	231.00651	-384.65926	1
9743	C	65.45128	88.76560	72.91395	265.75831	407.16911	330.07622	1
9744	O	66.09327	89.41925	72.09730	382.97414	90.70325	513.88163	1
9745	N	64.59051	87.79263	72.73147	594.89187	59.65662	362.85871	1
9746	H	64.25127	87.22258	73.52866	-2218.21229	545.65859	-1246.59406	1
9747	C	64.09058	87.63544	71.39389	562.78958	233.84269	-182.50600	1
9748	H	64.84270	87.95652	70.63243	2718.37688	-761.72524	887.22843	1
9749	C	63.89785	86.02855	71.22189	869.63114	-245.38233	-465.39967	1
9750	H	63.35997	85.82217	72.18420	-777.22885	-1902.55231	1174.93062	1
9751	H	63.15553	85.80828	70.40289	-1924.82706	-416.41039	-2388.02584	1
9752	O	65.06158	85.27787	70.82229	-298.14420	361.58504	391.45734	1
9753	H	65.50923	85.25251	71.74329	541.61830	-1445.28577	332.13362	1
9754	C	62.65094	88.32956	71.35360	147.97608	-948.12547	1008.74046	1
9755	O	62.18257	88.63823	70.26708	304.03513	-921.04026	-284.38693	1
9756	N	61.99790	88.26780	72.52193	-364.21661	246.32173	-203.87587	1
9757	H	62.42815	87.79650	73.34892	-1925.27246	-905.22466	-1163.69422	1
9758	C	60.82873	89.03797	72.70381	346.35445	-241.88210	-361.96002	1
9759	H	60.13354	88.74160	71.82312	96.86448	-2536.91141	-524.12372	1
9760	C	60.21517	88.56592	74.07243	223.36283	-184.40945	-271.62387	1
9761	H	59.28275	89.05645	74.23705	1717.24492	-1310.49104	1016.10539	1
9762	H	60.82341	88.73746	74.90173	-98.29847	649.65087	-704.04383	1
9763	C	59.93268	86.98761	74.05330	719.32016	-222.66040	-931.48472	1
9764	C	59.64322	86.22067	72.88988	211.54056	184.20985	4.06718	1
9765	H	59.72782	86.58949	71.82073	636.32109	-327.31585	1543.80549	1
9766	C	59.30100	84.85880	73.12290	25.30453	-618.46486	669.56098	1
9767	H	59.12100	84.20580	72.28090	1154.23989	2424.67675	1639.17636	1
9768	C	59.18800	84.30980	74.35190	550.80277	-533.65806	493.23056	1
9769	H	59.20900	83.23180	74.40590	-120.72906	-1414.18726	-2807.79720	1
9770	C	59.88705	86.43922	75.32462	-320.63477	558.04307	-222.27591	1
9771	H	60.33016	86.96588	76.14573	3520.67086	953.23777	-4008.12697	1
9772	C	59.40636	85.11008	75.50301	-521.98044	-721.83692	-220.74932	1
9773	H	59.40800	84.60080	76.43090	499.78648	3074.09538	445.39565	1
9774	C	61.23538	90.63985	72.52264	-986.45445	515.03105	522.72210	1
9775	O	60.29713	91.41348	72.47531	-103.58257	-514.62661	847.19247	1
9776	N	62.53706	90.79413	72.48841	348.42162	59.50774	-375.00233	1
9777	H	63.05203	89.95387	72.69410	1012.57794	-658.24410	-2328.66676	1
9778	C	63.12423	92.02100	72.06402	-451.04346	-603.54150	-145.43760	1
9779	H	62.13654	92.54610	71.98878	1763.82467	321.91835	-237.57450	1
9780	C	64.02722	92.55750	73.28806	405.50878	-414.70406	575.28475	1
9781	H	63.59059	92.24823	74.28967	3809.35317	-1257.68097	-278.82120	1
9782	C	65.57427	92.13381	73.32592	-390.74006	-570.78715	149.54890	1
9783	H	66.21358	92.59478	72.53781	1553.03618	-4089.22502	-1938.51013	1
9784	H	66.07477	92.34832	74.27803	-526.90687	4165.98304	2378.27717	1
9785	H	65.63201	91.00895	73.16707	4305.26599	-732.92882	206.78830	1
9786	C	64.16059	94.09245	73.05477	-695.25206	-947.51702	798.41248	1
9787	H	63.24044	94.61921	72.70955	3750.07462	5809.04974	-496.69218	1
9788	H	64.97480	94.37185	72.40678	548.47303	-72.55208	690.92797	1
9789	C	64.46027	94.60422	74.54250	687.27026	-864.37035	317.17314	1

9790	H	63.71236	94.44247	75.38065	-3234.98094	-72.63199	1599.61320	1
9791	H	64.55619	95.69763	74.55247	78.56136	-655.51675	2940.37802	1
9792	H	65.37249	94.11496	74.84845	626.61540	-714.31574	-2685.05947	1
9793	C	64.22793	91.96591	70.84920	-320.95819	-1168.67827	294.96096	1
9794	O	64.94483	92.92792	70.66441	-128.56324	-116.02316	216.46314	1
9795	N	64.18892	90.83324	70.17779	-231.88388	716.03453	292.24796	1
9796	H	63.47877	90.11102	70.39524	177.36323	-432.52144	-5526.70670	1
9797	C	65.03159	90.77575	69.00045	228.09582	-562.36408	-1183.76956	1
9798	H	65.40974	91.80397	68.87249	-2274.91165	5068.70767	1153.08431	1
9799	C	66.15556	89.65385	69.26705	48.71869	-415.49540	669.80509	1
9800	H	65.63432	88.69442	69.10626	955.00711	1310.76044	250.43060	1
9801	H	66.41036	89.44346	70.37168	1795.79057	-1484.78343	47.11881	1
9802	C	67.42210	89.72350	68.46238	1134.53145	-105.96650	418.20001	1
9803	H	67.47273	90.66674	67.86005	1516.26425	2315.12213	-567.84850	1
9804	C	68.60486	89.83611	69.41656	115.57490	-617.80950	-80.77482	1
9805	H	68.61053	90.81298	69.95965	-1793.68961	1944.91970	4507.90449	1
9806	H	69.55186	89.73516	68.87339	-3122.33335	1464.62980	-411.66400	1
9807	H	68.59185	89.07360	70.22700	941.23375	-975.75450	-1013.46899	1
9808	C	67.57531	88.44674	67.62620	344.24517	-244.45227	111.72822	1
9809	H	68.43572	88.39465	66.93954	391.94103	-668.56059	2221.92373	1
9810	H	67.62287	87.55836	68.29162	404.67180	1217.50658	1054.89916	1
9811	H	66.63269	88.33839	67.02236	2330.74642	2293.24011	-854.15303	1
9812	C	64.13459	90.37992	67.74764	571.02208	195.19476	21.68154	1
9813	O	64.37291	91.03606	66.75512	-113.66400	-207.52953	-200.30929	1
9814	N	63.35050	89.28533	67.93583	-600.18841	199.35312	11.37239	1
9815	H	63.25304	88.72200	68.80774	-1789.09723	483.46980	235.63464	1
9816	C	62.11616	89.37645	67.24508	483.54063	-317.37824	-62.70057	1
9817	H	62.42813	89.44045	66.15221	2679.90086	-90.82520	-652.19242	1
9818	C	61.15253	88.11988	67.71737	115.45424	-319.17787	514.41803	1
9819	H	60.72597	88.43242	68.68745	-77.58130	490.00161	1504.06313	1
9820	H	61.79733	87.24232	67.94087	1292.42454	-133.07468	-2203.84493	1
9821	C	60.07377	87.79175	66.74725	306.21110	411.02618	234.37817	1
9822	H	59.40265	88.63586	66.72003	88.81591	1213.20938	-126.47820	1
9823	C	60.59093	87.32465	65.39974	362.30700	-456.99037	424.10211	1
9824	H	61.38696	88.01930	65.02002	-1903.82099	3881.42382	259.21223	1
9825	H	59.67322	87.27311	64.70556	532.19668	-1014.81457	748.60574	1
9826	H	61.03585	86.34611	65.51773	1671.69261	657.86432	-351.90016	1
9827	C	59.23704	86.61309	67.26162	887.64891	139.65467	277.73760	1
9828	H	59.63428	85.60376	67.00081	-2180.29460	-1499.47873	871.96541	1
9829	H	58.99066	86.68193	68.39686	-215.66185	-253.07333	-2049.21248	1
9830	H	58.21262	86.76957	66.82979	510.38671	-632.98503	1428.11057	1
9831	C	61.31674	90.76998	67.55378	-758.91755	-216.29404	-711.18781	1
9832	O	60.44397	91.06778	66.72595	510.40957	1017.28348	306.81837	1
9833	N	61.49132	91.31726	68.77344	326.77270	971.87749	-885.31510	1
9834	H	62.03531	90.71465	69.31937	548.88185	1419.44796	2838.07652	1
9835	C	61.35892	92.67586	68.98393	-604.58472	-385.49053	401.38489	1
9836	H	61.94610	92.63358	69.99956	1409.08709	-2012.99696	-56.32654	1
9837	C	62.00603	93.55333	67.86916	-711.11655	-97.98535	-227.29602	1
9838	H	62.22162	92.88282	67.00098	2076.93127	-1711.47439	-405.18808	1
9839	H	61.35078	94.39402	67.43804	-1979.92397	1701.72476	2710.27250	1
9840	C	63.23701	94.15686	68.58959	-277.36563	-484.54081	72.45925	1
9841	H	63.76352	93.20948	68.97709	-3806.08153	1393.56596	1248.12340	1
9842	H	62.90673	94.74931	69.50685	-159.09579	-1212.10593	1747.03665	1
9843	C	64.15747	95.06567	67.67124	397.64876	482.04976	-56.08122	1
9844	O	64.42873	94.54482	66.39365	-903.45219	-415.34398	320.07636	1
9845	O	64.65091	96.06402	68.11123	-303.99946	588.58407	-231.39307	1
9846	C	59.77233	93.19039	69.09418	1032.54786	-1022.91936	-646.79863	1
9847	O	59.42802	93.99359	68.27679	-833.16977	544.42067	704.12390	1
9848	N	59.12297	92.70077	70.11217	535.27025	-119.28431	-246.10206	1
9849	H	59.62100	91.98649	70.68464	-824.97425	2054.75152	-1368.81545	1
9850	C	57.86975	93.15156	70.63129	418.59829	-807.17651	-458.47624	1
9851	H	57.21387	93.67205	69.86412	2019.35565	-2570.27052	-1988.48432	1

9852	C	57.14173	91.96092	71.27752	-902.00020	177.86152	34.85372	1
9853	H	57.69452	91.52233	72.17658	-1913.05360	-2831.08048	-257.96470	1
9854	C	55.86697	92.44183	71.87277	-361.94258	-158.31817	-826.23386	1
9855	H	55.59766	93.47604	71.37518	-567.92893	-261.83381	2069.16425	1
9856	H	54.95080	91.79685	71.99245	-1331.79305	-3804.74487	229.91937	1
9857	H	56.13379	92.81749	72.92223	158.18612	2029.54822	682.58865	1
9858	C	56.94545	90.85965	70.23753	372.28374	-7.34158	-83.95498	1
9859	H	56.99054	91.34543	69.22426	1076.38010	-1163.27875	-1483.71971	1
9860	H	55.90776	90.47159	70.36346	1164.57174	-730.47923	-1315.98868	1
9861	C	58.05329	89.74193	70.39136	356.75657	-118.86218	742.60126	1
9862	H	58.03996	89.17331	71.38066	9.31454	-525.14709	1694.00181	1
9863	H	58.11630	88.98685	69.53461	-2168.15811	524.02121	-1204.45935	1
9864	H	58.93696	90.35361	70.29380	2241.29756	1326.12738	-255.26516	1
9865	C	58.08763	94.40689	71.72449	604.62233	47.57693	324.63428	1
9866	O	57.12443	94.87542	72.26776	30.46376	-750.62364	-93.95145	1
9867	N	59.36933	94.45872	72.11488	-747.85266	-485.98463	257.58212	1
9868	H	59.91690	93.84244	71.50386	1089.90441	-870.17558	499.61839	1
9869	C	60.01439	95.67587	72.55358	48.69392	600.23365	123.03204	1
9870	H	59.32671	96.50082	72.70160	-1462.99490	736.93476	-2058.40037	1
9871	C	60.69194	95.42670	73.88898	118.52449	-633.04241	89.10250	1
9872	H	61.48864	94.70816	73.70519	2303.31175	-1463.41492	1180.93043	1
9873	C	61.30006	96.63908	74.52696	484.35049	-551.12141	169.65275	1
9874	H	60.52860	97.34850	75.02686	3187.80144	-1787.97707	-1448.69028	1
9875	H	61.97965	96.27565	75.31816	-1356.76092	-2854.68769	1325.84251	1
9876	H	61.81517	97.13931	73.74501	618.44371	-1894.32154	2395.47721	1
9877	C	59.89388	94.69230	74.93545	346.13949	101.08204	1139.48084	1
9878	H	58.97280	95.34884	75.00518	-3472.54180	-985.34811	-898.51779	1
9879	H	60.35542	94.76251	75.93379	-719.45876	-3236.52044	-478.96876	1
9880	C	59.80859	93.18495	74.43774	116.21627	985.02463	612.93833	1
9881	H	59.52119	92.92690	73.44831	-742.00135	2469.26437	-299.64254	1
9882	H	59.07830	92.59446	75.00843	1215.06940	-410.66089	-3025.04585	1
9883	H	60.80280	92.60232	74.59436	-360.05226	-842.83632	966.48273	1
9884	C	61.32219	95.77639	71.48897	112.72394	58.59136	410.68333	1
9885	O	61.72237	94.76428	70.96773	-215.73413	571.03565	543.78808	1
9886	N	61.88157	96.99414	71.45030	126.69569	435.35844	-270.80720	1
9887	H	61.33511	97.64960	72.00637	-1214.95321	-1744.58214	-293.19743	1
9888	C	62.89815	97.27585	70.50671	-193.61601	-1055.02075	470.16962	1
9889	H	63.21730	96.25753	70.01322	4132.86307	-972.18964	2308.40050	1
9890	C	62.14869	98.26975	69.53946	152.38444	-394.85333	13.93860	1
9891	H	62.71841	98.38626	68.56954	806.37853	-299.52493	-4418.01670	1
9892	H	62.35466	99.25356	70.04467	-3661.35480	-1766.31108	-328.85221	1
9893	C	60.65851	97.91613	69.18296	904.67663	876.38801	-136.27097	1
9894	H	59.99104	97.72849	70.05533	399.57143	1829.62954	2022.38961	1
9895	H	60.20574	98.79670	68.67974	-303.73371	5297.21280	128.23457	1
9896	C	60.87072	96.65449	68.28698	98.78659	-105.59070	-966.17177	1
9897	H	59.86310	96.33170	67.83147	497.37643	-835.07542	-414.08552	1
9898	H	61.14948	95.75482	68.90497	1878.17343	1907.92208	149.47909	1
9899	C	61.74070	96.80486	66.98781	-556.84854	256.24391	131.38427	1
9900	H	62.85198	96.94782	67.15463	500.59234	3767.83219	-102.90506	1
9901	H	61.56118	97.70848	66.34683	-3060.79338	604.18465	671.64300	1
9902	N	61.50682	95.59490	66.22128	234.07694	852.01966	581.27639	1
9903	H	65.25373	95.00038	66.05408	375.55070	-1054.42186	287.08960	1
9904	H	62.23838	95.14376	65.69984	-930.53513	2495.64234	320.33443	1
9905	H	60.95507	95.90964	65.42150	-3321.66590	2171.52042	934.71093	1
9906	C	64.14095	98.06059	71.31299	-297.47754	-6.26424	-130.55523	1
9907	O	63.81536	98.78262	72.27944	-660.21812	673.21761	2.09021	1
9908	N	65.27490	97.88169	70.68713	860.03506	-1387.47584	23.83353	1
9909	H	65.29215	97.40757	69.76977	-1178.44959	-574.86707	-2535.89735	1
9910	C	66.43858	98.63246	71.07537	-13.96787	-803.69793	247.84556	1
9911	H	66.27253	99.73481	70.83453	1543.37411	-960.69912	1638.97174	1
9912	C	66.57075	98.19154	72.57335	669.16095	-251.12629	224.47952	1
9913	H	66.39613	97.08203	72.71958	1265.68671	-228.81686	-1204.49055	1

9914	H	65.69087	98.52691	73.16911	-242.12068	-690.49952	-1536.19908	1
9915	C	67.86603	98.53255	73.37085	-292.07218	-298.52361	161.93862	1
9916	H	67.79200	98.10709	74.40223	-1310.16054	1173.25061	-2378.55467	1
9917	H	68.77794	98.16432	72.87449	-389.11007	1354.24309	1313.82201	1
9918	C	67.97478	100.09999	73.40663	-567.00123	638.76378	392.71990	1
9919	O	67.45511	100.73455	72.53175	80.67964	-316.55334	32.93704	1
9920	N	68.55415	100.49938	74.57313	231.98878	-445.79302	-199.03204	1
9921	H	68.96020	99.80218	75.20934	-1.01304	-3244.72167	-747.83586	1
9922	H	68.92957	101.43503	74.78781	1216.85490	1624.11566	-642.90536	1
9923	C	67.69249	98.02281	70.22566	-155.54066	1145.98434	-1197.10991	1
9924	O	67.65028	96.95487	69.55674	425.65436	-800.01944	230.76179	1
9925	N	68.74812	98.79614	70.33765	1353.71810	-477.38105	-214.30757	1
9926	H	68.63290	99.69033	70.72568	516.35340	-379.51149	-44.47599	1
9927	C	69.97330	98.26259	69.80589	-240.72456	380.21236	961.98917	1
9928	H	70.62884	99.12448	69.60864	-2695.81817	3456.88578	2151.96436	1
9929	H	69.54764	97.63026	68.95981	-1851.11482	-1324.90581	-961.19888	1
9930	C	70.69635	97.40518	70.95156	494.49416	196.13111	-26.44998	1
9931	O	70.68594	97.58152	72.19700	-41.13427	242.66362	-626.58813	1
9932	N	71.54707	96.58189	70.34821	350.60011	-80.59609	-24.14305	1
9933	H	71.54740	96.53959	69.20457	-1370.98996	-1245.23123	-1023.20584	1
9934	C	71.94079	95.38617	71.09614	-919.05640	-482.40096	-138.94817	1
9935	H	71.04930	95.14403	71.67508	733.60444	2889.43833	-3392.02220	1
9936	C	72.40987	94.14277	70.27090	-320.70375	-1043.48215	-203.90122	1
9937	H	72.51444	93.25873	70.93239	869.56417	1671.40700	-233.22339	1
9938	H	73.45431	94.59975	70.04990	2932.29892	2034.10289	-3455.41203	1
9939	S	71.44622	93.68142	68.76806	318.80910	527.23757	238.69761	1
9940	C	73.28337	95.75294	71.95541	-1070.66068	-264.72799	920.31830	1
9941	O	73.62406	94.88239	72.77194	63.11268	500.66760	-494.71587	1
9942	N	73.91630	96.84176	71.54564	-4.21475	-133.56001	-138.60011	1
9943	H	73.33909	97.31238	70.82594	524.64017	485.92635	-428.40466	1
9944	C	74.97925	97.52741	72.30079	-137.05313	1376.43974	-468.20252	1
9945	H	75.50559	96.74727	72.73910	-1400.56638	921.12450	-1062.62998	1
9946	C	75.76436	98.33396	71.20638	-601.98744	630.46797	364.85837	1
9947	H	75.18844	99.08341	70.54477	61.07108	2545.44834	2859.04655	1
9948	H	76.28562	97.55329	70.62165	-2590.71635	375.37052	-1760.87508	1
9949	C	76.94195	99.05765	71.90440	-528.41260	-159.99751	104.81608	1
9950	H	76.57042	99.75652	72.72641	3242.63204	-2561.24374	-3111.15653	1
9951	H	77.70068	98.33860	72.48097	-2425.57339	2288.92010	1509.60605	1
9952	C	77.75788	99.96386	70.88807	1030.14550	-656.14241	-340.15491	1
9953	O	78.44377	100.80396	71.53527	360.16900	-56.84818	-1082.17803	1
9954	O	77.68656	99.83240	69.64135	951.69989	835.58919	543.96979	1
9955	C	74.43347	98.52172	73.46029	609.20291	-436.52936	-602.63452	1
9956	O	75.14903	98.94235	74.33442	99.28608	-179.43249	298.99500	1
9957	N	73.17307	98.89239	73.25040	856.39143	164.07836	79.50453	1
9958	H	72.63140	98.46977	72.46743	3169.74915	-2797.64493	1836.14063	1
9959	C	72.53149	99.60331	74.31006	-71.81494	194.03836	296.18491	1
9960	H	73.33184	100.15483	74.84687	2259.20478	2150.33507	-1360.29179	1
9961	C	71.43727	100.50522	73.65552	-1280.03412	390.05268	-266.59308	1
9962	H	70.62490	99.99200	73.10723	1848.80090	1673.43931	1049.15964	1
9963	H	70.94236	101.08249	74.45181	-2165.97658	-1671.47354	-14.79403	1
9964	C	71.93868	101.48007	72.55415	703.21830	274.84375	-90.08745	1
9965	C	70.91269	102.26547	72.04327	485.97957	-346.76991	494.20007	1
9966	H	69.85818	102.18918	72.46294	-3167.25672	767.14248	1051.93869	1
9967	C	71.28707	103.05806	70.88184	-165.61662	-221.00323	100.75159	1
9968	H	70.52333	103.60394	70.24985	-1329.05462	2288.98636	409.90141	1
9969	C	72.56309	102.95566	70.31512	971.09963	477.44492	-371.05631	1
9970	H	72.73813	103.60983	69.43864	-2669.76795	474.45120	68.64315	1
9971	C	73.25280	101.30134	72.01204	819.35413	-546.78554	-195.77998	1
9972	H	73.99654	100.53112	72.33057	1909.48786	-130.62959	-1010.81112	1
9973	C	73.58596	102.14207	70.97728	-206.14305	-636.28364	10.58559	1
9974	H	74.67555	102.11568	70.60792	3558.95520	-1474.92325	1363.96967	1
9975	C	71.79154	98.43878	75.27135	-398.34888	-273.58293	537.53229	1

9976	O	71.03303	98.84582	76.14250	-107.52158	-33.66238	-149.62687	1
9977	N	72.21789	97.18368	75.04484	180.72904	385.78730	-741.15441	1
9978	H	72.95992	97.04829	74.29390	-474.68504	-2043.04418	1373.29608	1
9979	C	71.48633	96.09191	75.51456	663.98374	255.90921	-549.81777	1
9980	H	70.93535	96.59728	76.33317	443.83790	1497.78863	4203.80457	1
9981	C	70.49994	95.62364	74.33342	-759.07324	593.56999	-631.74854	1
9982	H	70.43993	96.39021	73.49679	-704.20522	-2776.84228	-843.64346	1
9983	H	70.94309	94.68776	73.91257	-118.30465	931.32963	466.76216	1
9984	C	69.13804	95.44186	74.98080	-293.52531	-143.36955	66.68041	1
9985	H	68.90033	96.43074	75.37183	2664.74230	994.05036	-2649.80926	1
9986	H	69.10970	94.86113	75.88097	-799.70671	-1401.03272	689.18493	1
9987	C	68.08763	94.98994	73.82394	326.41536	-270.04349	-88.07534	1
9988	O	66.98473	95.46469	73.98881	113.16828	59.40745	529.28644	1
9989	O	68.55415	94.48592	72.74064	210.85808	-127.65623	662.35524	1
9990	C	72.47357	94.89030	76.00047	-77.93688	-510.50852	-519.84728	1
9991	O	71.97198	93.78276	76.16446	-72.11583	86.74543	-561.08604	1
9992	N	73.68704	95.31956	76.32994	989.51925	-387.01803	184.41745	1
9993	H	73.91750	96.32965	76.21428	-1031.84881	682.27823	1169.37947	1
9994	C	74.31641	94.76273	77.50518	70.12308	1121.63507	1340.29377	1
9995	H	74.28533	93.65020	77.30646	-239.48857	582.09073	1346.52144	1
9996	C	75.67434	95.49884	77.63771	-859.09035	-724.62495	52.63778	1
9997	H	75.48029	96.45346	78.19150	-63.34558	-1336.00087	310.57625	1
9998	H	76.02558	95.78788	76.65673	-3003.38651	-1496.14878	3774.27811	1
9999	C	76.68915	94.56981	78.45936	73.08675	-485.32222	563.87031	1
10000	O	76.79796	94.45963	79.66761	217.60098	-844.26943	-49.96385	1
10001	N	77.38601	93.86645	77.53490	-648.62752	-38.68335	-659.46535	1
10002	H	77.12859	93.87793	76.46610	-177.37408	149.05705	-1881.16967	1
10003	H	78.13352	93.17685	77.70036	1565.66922	2672.06589	-1309.16192	1
10004	C	73.32186	94.85450	78.82812	-147.90512	88.81739	623.67386	1
10005	O	73.68659	94.15882	79.81005	440.46313	-124.15006	-358.77213	1
10006	N	72.37142	95.71814	78.68600	512.93203	-113.79004	87.93041	1
10007	H	72.57850	96.25935	77.83925	293.65865	-1022.55157	507.60021	1
10008	C	71.25861	95.85237	79.60744	-422.18093	492.80856	-152.67275	1
10009	H	71.80490	96.24015	80.41229	3310.03925	2621.72084	-241.27921	1
10010	C	70.22369	96.93283	79.16584	296.88890	-52.48756	-486.31045	1
10011	H	69.96420	96.91667	78.08811	-2462.51949	-1265.29572	2330.94017	1
10012	O	70.71988	98.65659	79.06951	414.57147	246.84402	-413.82545	1
10013	H	70.68333	98.79334	78.06380	499.80539	-331.08964	341.02393	1
10014	C	68.93989	96.98414	79.96566	-217.21508	157.75152	-60.76841	1
10015	H	68.97927	97.16283	81.07886	-258.10750	-1094.51101	2466.78661	1
10016	H	68.34336	96.10792	79.58913	735.19760	-1244.29217	-3073.74201	1
10017	H	68.46587	97.88935	79.59498	1934.42255	2878.04240	3960.96038	1
10018	C	70.54556	94.39206	79.84041	248.70050	336.49201	251.73759	1
10019	O	70.01025	94.24577	80.92715	252.78980	413.80624	-168.19478	1
10020	N	70.19143	93.81138	78.66492	-53.71518	-380.34790	138.14796	1
10021	H	70.77904	94.21204	77.92824	2481.81472	-2427.77006	41.46128	1
10022	C	69.68061	92.51108	78.86156	-506.16848	243.64948	-438.74344	1
10023	H	69.09760	92.57062	79.78844	424.19732	300.55754	-985.46694	1
10024	C	68.61395	92.17789	77.70943	551.44821	669.61619	177.92436	1
10025	H	67.96735	93.05432	77.84155	2188.31683	-1342.41076	1807.88263	1
10026	C	69.17858	92.31466	76.23895	14.48752	1123.09166	-618.40457	1
10027	H	69.76833	93.25289	76.09736	1082.61464	-93.44337	-2469.61315	1
10028	H	69.82658	91.46315	75.92951	-582.45539	3044.23458	-4122.78788	1
10029	H	68.37367	92.39334	75.50506	-2133.38739	-543.81992	3918.50888	1
10030	C	67.84052	90.80769	77.91591	-251.88644	-303.59140	-71.49415	1
10031	H	68.26280	90.23025	78.75797	-3735.74222	1080.39412	2036.56083	1
10032	H	66.75658	90.86379	78.01981	-2098.21349	846.16282	-2307.36378	1
10033	H	68.11500	90.17805	77.02592	1805.78157	-1395.77645	1464.69016	1
10034	C	71.07270	91.62558	79.08055	-68.43727	508.95749	401.90213	1
10035	O	71.08281	90.78508	79.96737	-115.35187	548.14984	350.39374	1
10036	N	71.96785	91.88318	78.19242	-310.72095	183.47830	440.23673	1
10037	H	71.86391	92.67171	77.49824	-2035.20177	-1202.80300	2243.27304	1

10038	C	72.83805	90.81592	77.72205	-607.77111	546.51520	-14.95702	1
10039	H	72.18879	89.98764	77.32138	-440.79057	1350.32800	-1462.07315	1
10040	C	73.58756	91.30982	76.42693	-781.00549	-172.10699	992.63788	1
10041	H	74.05874	92.25103	76.71115	811.83320	-2618.49257	392.71405	1
10042	H	72.82870	91.62271	75.61487	2184.94135	-392.61170	-2570.86849	1
10043	N	74.31026	89.16955	75.22369	-668.17235	-176.19505	379.16912	1
10044	C	74.60536	90.25935	75.93331	-886.50459	-617.77793	300.20998	1
10045	C	75.45640	88.51335	74.99371	-435.04340	474.53371	-919.71923	1
10046	H	75.62975	87.55118	74.36536	281.30114	1272.93224	103.08550	1
10047	N	76.44086	89.19396	75.60870	292.66494	1213.88294	413.60258	1
10048	H	77.42719	88.95289	75.64782	-212.16053	1110.03407	-2191.94327	1
10049	C	76.02797	90.25271	76.21654	-48.74832	1281.48332	-159.18407	1
10050	H	76.65324	90.90680	76.80259	512.40585	887.96780	205.10528	1
10051	C	73.75236	90.32455	78.96270	261.16174	-820.85552	-595.45704	1
10052	O	74.07106	89.13718	79.15441	-249.60399	-41.13591	486.49510	1
10053	N	74.09786	91.40494	79.72276	-978.08913	418.50211	-731.45134	1
10054	H	73.73408	92.33285	79.40125	-1735.66425	551.74896	1015.50160	1
10055	C	75.01830	91.10332	80.89680	952.69769	845.84917	163.21656	1
10056	H	76.06991	91.04482	80.44727	-32.31767	933.31010	3411.09613	1
10057	C	75.23677	92.36315	81.78342	-102.59628	303.36276	-25.59182	1
10058	H	75.48047	93.25126	81.16575	180.05457	-1526.41776	397.72645	1
10059	H	76.10866	92.10283	82.42688	2736.75837	2023.91290	-2383.18922	1
10060	C	74.01038	93.03868	82.58337	1309.02406	-287.19164	-203.48326	1
10061	H	73.29836	93.32365	81.76387	1678.02529	-1543.18412	69.64231	1
10062	H	73.50934	92.25268	83.12308	-596.53667	3866.17659	907.51634	1
10063	C	74.23874	94.06745	83.73161	-890.22308	553.68793	-41.35986	1
10064	H	75.02746	93.83398	84.52924	-2338.92533	-1601.70774	-312.41162	1
10065	H	73.22229	94.18168	84.17854	3078.22622	900.68237	1149.33746	1
10066	C	74.68309	95.39858	82.95663	153.73651	-319.55946	-655.39007	1
10067	H	75.64285	95.31126	82.38993	1964.55502	-491.22489	-1172.18308	1
10068	H	73.88564	95.82873	82.22556	-645.93408	1496.27794	-3388.20742	1
10069	N	74.97505	96.35099	83.97358	108.86118	529.86728	-214.52370	1
10070	H	71.67773	98.33897	79.25112	1341.98329	-1449.11221	880.65007	1
10071	H	76.00008	96.40753	84.33096	-2600.14453	-1422.43327	-3821.37410	1
10072	H	74.83166	97.27434	83.58403	-238.63527	-217.70600	1541.45590	1
10073	C	74.61329	89.80638	81.72016	-808.37130	-464.39677	482.94124	1
10074	O	75.41903	89.03210	82.31397	403.22398	-599.70681	-161.87689	1
10075	N	73.27065	89.79276	81.84805	485.02297	-239.01016	227.43622	1
10076	H	72.60473	90.39317	81.33970	-1306.60131	1767.54474	-2039.13431	1
10077	C	72.68767	88.80869	82.67790	35.31011	-284.37965	371.12589	1
10078	H	73.30950	88.85657	83.53654	-1151.42648	-1015.69098	1303.81933	1
10079	C	71.11630	89.14214	82.88691	-209.78735	199.12675	141.45485	1
10080	H	70.63131	88.31238	83.53087	-455.74384	-1381.97126	1519.79200	1
10081	H	70.61079	89.20514	81.85150	667.78168	-2330.25998	-993.28299	1
10082	C	71.09430	90.50190	83.60445	502.78738	878.71077	-287.95863	1
10083	C	71.16161	91.71619	82.89868	-74.83655	-105.73975	-174.36674	1
10084	H	71.27761	91.94668	81.82277	53.34608	-1653.97686	-1355.76328	1
10085	N	71.03744	92.73761	83.76379	148.97665	412.60054	-345.06205	1
10086	H	70.78043	93.64487	83.39837	-3446.15726	1565.71782	-2182.15891	1
10087	C	70.89852	92.39654	85.09651	283.92582	663.98126	367.14658	1
10088	C	70.82066	90.89109	84.98244	-195.77891	-745.93078	-844.89218	1
10089	C	70.75346	90.21359	86.27718	-791.31439	-290.90686	470.26880	1
10090	H	70.49850	89.14488	86.36874	534.43351	-275.68153	288.50112	1
10091	C	70.83137	91.06239	87.39620	339.57979	-342.47404	-516.48886	1
10092	H	70.77259	90.49185	88.29094	1530.65103	957.57408	-244.87734	1
10093	C	70.82011	93.25193	86.21534	433.75305	43.94395	-195.98890	1
10094	H	70.74342	94.36949	86.11664	-314.34117	-165.07496	-3885.16509	1
10095	C	70.93027	92.48550	87.44564	-48.93512	200.94220	237.26997	1
10096	H	70.96505	93.01689	88.37645	-1433.99429	-229.88895	1630.77583	1
10097	C	72.71202	87.28086	82.07536	-212.75393	-495.57790	313.72865	1
10098	O	72.81066	86.33673	82.87698	144.65193	-428.47920	64.35651	1
10099	N	72.54635	87.34063	80.78247	-394.90825	-541.40479	278.69029	1

10100	H	72.42301	88.33353	80.53972	-278.33121	-531.54260	303.52228	1
10101	C	72.73300	86.30149	79.77878	-233.92911	-177.14281	109.24532	1
10102	H	72.20621	85.35367	80.13902	525.70929	1066.03925	1648.45311	1
10103	C	71.97447	86.77100	78.53151	717.59227	-15.12702	-483.57714	1
10104	H	72.20133	87.83800	78.35019	-554.44231	1599.50206	2813.46788	1
10105	C	72.50364	86.05697	77.32311	-65.21880	258.02027	-1103.21566	1
10106	H	72.35166	84.94608	77.35115	-734.66701	-801.34230	871.54667	1
10107	H	73.62062	86.12922	77.04715	-1940.07946	2388.08039	-2109.78893	1
10108	H	71.91582	86.45492	76.40465	981.14673	3718.32329	-1806.10460	1
10109	C	70.49452	86.58241	78.75624	-265.03888	-18.94700	76.64556	1
10110	H	70.19869	86.95565	79.78250	-433.27957	2832.83897	885.32865	1
10111	H	70.22309	85.49811	78.59594	2651.42653	-1943.82524	2195.07024	1
10112	C	69.84878	87.55586	77.66871	351.71781	622.36750	-937.77993	1
10113	H	70.48173	88.48771	77.55751	2716.02403	1619.70664	1169.84938	1
10114	H	69.71735	87.08447	76.63670	752.16414	273.55038	18.77905	1
10115	H	68.82668	87.83534	77.97423	-781.66124	1035.88973	3383.76025	1
10116	C	74.33736	85.94036	79.64042	386.60010	535.11501	-344.63536	1
10117	O	74.59756	84.77530	79.35306	-823.78752	523.85983	-8.43557	1
10118	N	75.13213	86.96005	79.92987	-609.89381	-8.23272	-215.55303	1
10119	H	74.79146	87.88298	80.15060	35.04609	-2700.55186	917.46703	1
10120	C	76.50541	86.76085	80.07400	689.03548	94.63375	92.83832	1
10121	H	76.70564	86.02579	79.24811	1375.61145	-2028.32092	-1274.08124	1
10122	C	77.29548	88.15509	79.86829	90.46501	-71.65253	-401.03512	1
10123	H	76.87266	88.51470	78.93285	566.08714	2816.29975	-451.33514	1
10124	H	76.97576	88.89494	80.66192	-962.59119	1357.50600	233.74271	1
10125	O	78.79659	88.07624	79.86640	160.35459	-19.40604	249.87168	1
10126	H	79.02681	87.98059	78.95051	1453.90615	-990.61654	1903.20650	1
10127	C	76.78641	85.91902	81.48766	-67.44770	-327.39450	24.01874	1
10128	O	77.43417	84.88620	81.41477	306.33380	-512.27228	-550.30985	1
10129	N	76.30325	86.46737	82.59958	-554.18276	184.67916	-101.58002	1
10130	H	75.56927	87.22615	82.40961	-22.50058	355.87641	-1725.42667	1
10131	C	76.52118	85.65070	83.78095	-563.51053	-124.09815	-269.14511	1
10132	H	77.57811	85.57124	83.60259	3697.66994	526.09950	-2511.98191	1
10133	C	76.14330	86.53417	85.04671	1109.38245	254.90959	642.15319	1
10134	H	75.16786	87.04117	84.93913	1901.94974	-319.38326	1129.15073	1
10135	C	76.20943	85.55094	86.28163	38.38924	8.03827	870.10261	1
10136	H	76.14139	86.05800	87.27010	209.08342	3067.17723	648.64037	1
10137	H	75.51400	84.69780	86.20590	-1205.53578	-2376.94491	1671.83810	1
10138	H	77.24434	85.09025	86.17427	2677.06579	-909.89260	602.30615	1
10139	C	77.16679	87.67978	85.36549	-170.85863	-550.82497	239.49524	1
10140	H	76.55183	88.53986	85.78446	-2005.98925	-1101.64423	2587.48865	1
10141	H	77.77239	87.34233	86.20456	1044.26193	593.86091	1081.15150	1
10142	C	78.10665	88.12310	84.16422	607.61427	147.74255	699.08388	1
10143	H	77.48841	88.34443	83.26781	1440.70146	-2321.39830	-797.18665	1
10144	H	78.87519	87.32013	83.85906	-435.46422	-417.59811	-3204.16467	1
10145	H	78.66620	89.11181	84.35780	-1479.97154	1066.49847	-3668.37496	1
10146	C	75.78700	84.21280	83.67290	785.59210	-41.69588	-461.03959	1
10147	O	76.22800	83.19180	84.17690	-760.26374	-47.55351	208.24251	1
10148	N	74.61500	84.11980	83.04490	568.63411	-188.08241	-594.93911	1
10149	H	74.13500	84.95480	82.78790	-339.13717	2869.24803	-1245.24213	1
10150	C	73.91400	82.81280	82.88690	-714.12081	390.46939	411.11572	1
10151	H	74.00400	82.22380	83.78790	627.52040	2153.46706	-2206.13327	1
10152	C	72.40500	82.98880	82.63790	728.78165	-305.49799	-454.97175	1
10153	H	71.80800	82.06780	82.46190	-1939.59620	-1719.67361	1782.95134	1
10154	O	72.05500	83.93480	81.60190	-711.95499	-76.44498	333.02175	1
10155	H	72.41500	84.72780	82.00590	2028.88158	-1577.80108	-1814.49979	1
10156	C	71.88900	83.50080	83.95390	610.30246	-359.87625	573.99564	1
10157	H	72.21200	84.53380	84.20790	2197.15808	-1938.77183	-1145.37609	1
10158	H	72.03100	82.81280	84.81390	1808.91683	84.80891	-2572.71327	1
10159	H	70.78500	83.62080	83.92590	-1622.85904	-2138.11175	-1641.04629	1
10160	C	74.57400	81.90580	81.81590	620.58496	-666.18084	50.28313	1
10161	O	74.51000	80.70880	81.83790	-641.08760	129.02499	442.70360	1

10162	N	75.20800	82.54480	80.80190	479.05021	677.55215	155.26194	1
10163	H	75.17800	83.52780	80.63590	-837.16039	-1004.73959	2861.44842	1
10164	C	76.14000	81.91880	79.89590	163.53308	867.18234	229.57076	1
10165	H	75.54400	81.19980	79.35290	2581.68508	1356.24594	-1180.56144	1
10166	C	76.52300	82.92480	78.72290	281.23824	729.14528	-469.79061	1
10167	H	75.62500	83.11680	78.09690	2071.08828	-1560.73574	-1781.27019	1
10168	H	76.66500	83.94280	79.14390	2175.09361	-2265.87376	-181.68689	1
10169	C	77.84600	82.66780	77.99590	-611.28743	136.94309	662.58982	1
10170	H	77.88700	81.63180	77.59590	-1864.58453	2010.47920	-1542.57063	1
10171	H	78.72200	82.60580	78.67690	3008.43310	-858.42995	332.64770	1
10172	C	78.18500	83.71880	76.95690	-100.08441	-888.55719	178.60636	1
10173	O	77.71100	83.55580	75.80090	695.97028	2.01554	373.16019	1
10174	O	78.82900	84.76080	77.27790	526.81165	293.53919	509.83473	1
10175	C	77.35300	81.31380	80.52590	123.66998	725.30763	538.59594	1
10176	O	77.70100	80.15980	80.26390	-47.60118	737.08425	-279.40682	1
10177	N	77.95800	82.09480	81.38790	501.09383	643.90192	-216.72006	1
10178	H	77.75900	83.05180	81.58290	-1879.33957	-2215.99323	-1206.51688	1
10179	C	79.11300	81.64780	82.15290	-452.63025	499.63369	-613.95687	1
10180	H	79.84000	81.34180	81.41590	786.17076	-2556.41567	-1656.77418	1
10181	C	79.73600	82.80780	82.92590	554.46504	-703.14981	172.04613	1
10182	H	79.00500	83.27380	83.62090	2004.73176	-30.22616	2424.53360	1
10183	H	80.07200	83.58180	82.20390	1772.73343	-1970.85715	1694.51011	1
10184	H	80.64900	82.46280	83.45690	2.80618	2331.74634	-2112.14993	1
10185	C	78.82700	80.48580	83.13890	-364.78748	-599.64303	-582.07331	1
10186	O	79.55900	79.51980	83.22390	155.80951	287.15421	718.95277	1
10187	N	77.64800	80.51980	83.78290	449.33258	348.72806	623.82791	1
10188	H	77.05800	81.29980	83.58990	1784.10871	2072.15124	-1556.07570	1
10189	C	77.12500	79.38880	84.44290	-295.09981	-726.39276	465.53266	1
10190	H	77.86300	79.04080	85.15090	-2727.53363	-1206.29691	-1001.81550	1
10191	C	75.91800	79.80180	85.39390	-757.97348	-220.69563	-456.31201	1
10192	H	75.08100	80.21480	84.79090	1548.95543	-1156.06598	2482.43323	1
10193	H	75.49200	78.90680	85.89490	1945.07207	1925.55312	-1551.50444	1
10194	C	76.28200	80.82580	86.48490	-429.60876	81.85717	800.11669	1
10195	H	76.98000	81.55880	86.02790	3043.05091	527.76234	-599.61179	1
10196	C	74.98200	81.56780	86.85190	-739.86855	-312.57104	-431.67682	1
10197	H	75.18900	82.57080	87.28190	-2660.18509	-1222.97732	-1151.50683	1
10198	H	74.37200	80.96780	87.56090	447.33926	-2204.42072	2199.69159	1
10199	H	74.21300	81.76580	86.07590	-2694.53847	-1171.12975	-1125.23053	1
10200	C	77.11200	80.14080	87.64290	469.81814	-361.58067	-692.80686	1
10201	H	78.19900	80.15580	87.41590	-732.39479	-2433.87245	-1854.20845	1
10202	H	76.72400	79.10680	87.76490	765.36022	-721.81661	-2965.03469	1
10203	H	77.02300	80.76480	88.55790	-1923.97086	-2479.18462	224.06694	1
10204	C	76.81200	78.16480	83.60190	-22.31535	583.42087	700.40925	1
10205	O	76.88800	77.02780	84.09590	685.45654	-368.42810	-134.30301	1
10206	N	76.40900	78.34580	82.33290	119.54106	-327.95053	-768.65511	1
10207	H	76.25200	79.28280	82.02990	-478.66696	1307.72408	-2821.16322	1
10208	C	76.00000	77.24280	81.44990	226.40760	-710.74026	524.44150	1
10209	H	75.30300	76.60780	81.97590	-1972.63729	1232.05443	2118.71901	1
10210	C	75.34000	77.71080	80.16190	-746.49746	356.20258	-383.81280	1
10211	H	74.36600	78.17280	80.43090	-560.59934	2524.15006	-1792.37861	1
10212	H	76.02600	78.35680	79.57290	2904.65159	-1130.66475	427.57756	1
10213	H	75.07000	76.89780	79.45490	-1751.90925	-2497.87211	767.90308	1
10214	C	77.21500	76.45580	81.18090	254.29364	646.04355	591.11207	1
10215	O	77.05800	75.22780	81.01690	85.78053	472.65664	626.78914	1
10216	N	78.42600	76.99280	81.18490	358.51261	-73.79128	760.72061	1
10217	H	78.51000	77.98480	81.24190	2131.35755	-951.09259	2109.73081	1
10218	C	79.72500	76.37280	80.94990	790.95648	-213.49684	400.32231	1
10219	H	79.67100	75.84580	80.00890	-2579.11328	-1694.61832	-612.10266	1
10220	C	80.84500	77.40480	80.87490	-626.90113	612.71879	-251.04114	1
10221	H	81.81300	76.89780	80.67290	1830.89959	-2197.76584	-1309.90773	1
10222	H	80.83100	77.90280	81.86790	-790.79718	1507.55025	2645.78122	1
10223	C	80.72800	78.48680	79.85590	479.70328	135.08583	-763.60172	1

10224	C	79.79900	78.45180	78.78390	-183.74456	-156.55681	-879.30592	1
10225	H	79.19800	77.57480	78.59390	1926.01378	2015.95197	1457.61271	1
10226	C	79.71500	79.51180	77.92990	-489.63198	-675.39204	368.18083	1
10227	H	78.93100	79.51880	77.18690	-2290.19744	314.94731	2134.01736	1
10228	C	80.60300	80.61280	78.00890	-880.95828	130.84427	195.55891	1
10229	H	80.63700	81.41480	77.28690	-1401.23023	-534.01084	-2765.79328	1
10230	C	81.56500	79.61080	80.03390	-30.08665	719.81308	558.94089	1
10231	H	82.29100	79.66680	80.83190	-3115.34577	373.38735	231.14680	1
10232	C	81.49000	80.62980	79.09190	-431.76577	-325.69810	-734.13219	1
10233	H	82.21500	81.42980	79.14390	989.86037	1265.28560	-2705.07949	1
10234	C	80.06500	75.30780	81.89290	31.90069	-619.47539	-668.34391	1
10235	O	80.91900	74.45080	81.59690	674.12057	393.73415	119.00462	1
10236	N	79.44000	75.24380	83.07190	604.30545	-486.62010	-332.69820	1
10237	H	78.65900	75.82680	83.28190	105.38128	2691.56887	1625.60081	1
10238	C	79.63100	74.13880	83.98890	-66.99465	63.58043	907.14952	1
10239	H	80.68900	74.07380	84.19190	2817.10129	-1089.75806	880.11018	1
10240	C	78.87000	74.41180	85.37190	-411.44980	-610.69340	-537.78586	1
10241	H	78.83600	73.47280	85.96590	-1799.52483	-1148.24537	-2311.16187	1
10242	H	77.82200	74.75780	85.24390	738.91547	2930.71442	873.58066	1
10243	C	79.70500	75.33080	86.30090	16.30274	410.88287	813.85533	1
10244	C	79.44800	76.73280	86.29990	328.68061	-573.89021	-627.75002	1
10245	H	78.60500	77.12880	85.75290	2073.69103	1839.07786	1488.56453	1
10246	C	80.18400	77.60480	87.17890	-239.16738	833.38714	-282.33993	1
10247	H	79.91800	78.64980	87.23690	-69.32709	882.12279	-3019.15209	1
10248	C	81.22300	77.03480	87.99790	-586.87850	17.73531	-697.64610	1
10249	H	81.76900	77.73080	88.61790	22.20190	-2098.03390	2344.35216	1
10250	C	80.73400	74.83380	87.05290	-299.66440	445.90339	-736.76483	1
10251	H	80.89600	73.77180	87.15890	-2127.09584	-1154.87293	-2009.96469	1
10252	C	81.50200	75.61880	87.92690	-213.40335	885.98350	30.71242	1
10253	H	82.33500	75.21480	88.48390	-441.49341	2000.91161	-2387.39660	1
10254	C	79.16300	72.79280	83.47990	-512.18341	551.44290	-514.81054	1
10255	O	79.55200	71.72080	84.04290	546.98955	-434.99900	-367.70305	1
10256	N	78.30700	72.68380	82.44790	-838.63012	80.80121	53.31956	1
10257	H	77.94400	73.50180	82.00890	1039.05760	-615.25822	2905.17518	1
10258	C	78.01100	71.39980	81.79690	-309.55387	391.59378	-763.07386	1
10259	H	77.51000	70.87580	82.59890	1354.97506	1384.02390	-2479.26333	1
10260	C	77.14300	71.47680	80.57290	-596.12525	-477.18205	498.38036	1
10261	H	76.78100	70.46380	80.29490	-985.45094	-236.74442	-2978.43327	1
10262	H	76.21100	71.97380	80.91690	-387.48183	-1088.87301	2926.16466	1
10263	N	77.72300	73.44280	79.04490	341.93191	-771.55333	-21.45493	1
10264	H	77.43600	74.19280	79.63990	-1938.80414	-1989.10208	-1477.40910	1
10265	C	77.73900	72.10080	79.28290	344.02764	657.14981	530.33019	1
10266	C	78.21500	73.63280	77.79190	-501.13935	-650.85986	-395.84316	1
10267	H	78.09200	74.62580	77.35890	2928.43007	-608.88172	975.59552	1
10268	N	78.44100	72.46680	77.21390	490.42239	-384.41680	-569.54534	1
10269	C	78.16100	71.51680	78.14890	-688.54299	-588.20201	106.66745	1
10270	H	78.36500	70.47680	77.92590	1216.27355	1923.67520	-2172.18291	1
10271	C	79.20000	70.61280	81.39290	735.05954	475.77954	254.50403	1
10272	O	79.29400	69.44680	81.75690	-83.43832	41.34332	-784.19131	1
10273	N	80.23700	71.24080	80.70990	572.91786	430.53569	-446.17982	1
10274	H	80.12400	72.15080	80.31990	-1145.03920	-2406.47985	-1672.11428	1
10275	C	81.53600	70.68980	80.37790	262.62537	-782.51813	-387.48458	1
10276	H	81.30400	69.88380	79.69790	319.28447	-2656.90068	-1654.43720	1
10277	C	82.43700	71.71380	79.66390	595.61793	253.45936	-642.22165	1
10278	H	82.58700	72.59480	80.32390	637.66042	936.40154	2935.09243	1
10279	H	83.49300	71.39880	79.52090	1359.47320	-2172.67367	-1824.70490	1
10280	S	81.70000	72.38080	78.16590	99.41861	-448.52625	316.46604	1
10281	H	80.97600	71.33580	77.79290	1224.90468	-1566.27297	2438.15991	1
10282	C	82.28600	70.13480	81.59390	-536.82951	549.70559	491.00799	1
10283	O	82.97200	69.12480	81.49390	-432.37493	390.92855	532.77952	1
10284	N	82.03700	70.65580	82.81090	10.04037	-152.43001	830.26295	1
10285	H	81.50900	71.49380	82.92690	-1332.28925	1918.42969	2107.80908	1

10286	C	82.76200	70.16280	84.01490	-508.81131	510.36718	-558.64783	1
10287	H	83.68700	69.72280	83.67190	2442.91795	1691.13637	-1034.61871	1
10288	C	82.99500	71.37380	84.95390	747.48769	-516.64910	76.07140	1
10289	H	83.61300	70.98680	85.79290	-2661.14238	1489.24911	773.74709	1
10290	H	82.07200	71.89880	85.27890	-560.36490	-2073.15394	-2299.18467	1
10291	S	83.97900	72.63280	84.11290	-393.35366	170.28612	357.05201	1
10292	H	85.18200	72.12980	84.34390	-934.84142	706.51112	-2919.78420	1
10293	C	81.93800	69.10780	84.71990	-663.17384	500.13723	376.18375	1
10294	O	82.51800	68.29280	85.42290	-489.82023	-377.73486	-490.93762	1
10295	N	80.65300	69.10580	84.45990	620.55471	-132.67695	556.75935	1
10296	H	80.19800	69.73580	83.83490	-2555.32480	-1828.15402	-162.46305	1
10297	C	79.68700	68.14480	85.04490	-411.87352	253.31633	-773.07312	1
10298	H	80.05800	67.92580	86.03490	-1436.50210	-2775.98866	-358.57345	1
10299	C	78.28300	68.75380	85.06290	-345.68825	763.58357	359.01361	1
10300	H	77.45500	68.03180	85.23190	2182.10346	2181.03833	616.21628	1
10301	H	78.09100	69.16680	84.04990	1968.74098	-958.03083	-2259.30567	1
10302	C	78.00400	69.82480	86.20890	21.66441	198.75540	889.65046	1
10303	H	78.90500	70.47180	86.14290	-1124.67544	653.13390	-2864.74213	1
10304	C	76.81100	70.73680	85.85990	-442.51807	603.47208	521.00884	1
10305	H	76.67900	71.41480	86.72990	-1424.58125	2302.51876	-1602.24900	1
10306	H	77.14500	71.31780	84.97290	-1675.25388	735.45172	-2559.46507	1
10307	H	75.93600	70.06580	85.72890	2457.59394	1188.55643	1563.90277	1
10308	C	77.83700	69.07980	87.51390	259.07306	560.55749	670.90048	1
10309	H	76.86500	68.54180	87.53190	2630.65550	885.60610	1481.07384	1
10310	H	77.89600	69.81380	88.34590	1042.12469	-1661.88916	-2459.74120	1
10311	H	78.56200	68.26680	87.73190	100.03453	2293.77046	2151.00823	1
10312	C	79.65200	66.80780	84.29190	-497.04322	-497.78045	580.18417	1
10313	O	79.37600	65.74280	84.89590	483.03343	-539.98788	-314.19584	1
10314	N	79.98800	66.80280	82.99990	630.53445	-66.55911	557.37642	1
10315	H	80.13000	67.65680	82.50490	1403.00927	-2147.30901	-1821.77255	1
10316	C	80.27200	65.57980	82.21990	348.30010	-448.08950	-713.69030	1
10317	H	79.38000	64.97580	82.30090	1653.53871	1518.54351	-2204.10108	1
10318	C	80.25600	65.98080	80.69390	-330.36906	570.92528	629.56462	1
10319	H	80.91000	66.86380	80.53090	2649.74001	-536.50494	1609.11980	1
10320	H	79.24200	66.28180	80.35290	28.02504	-800.85526	-3042.37928	1
10321	C	80.67100	64.84780	79.76590	95.16582	863.10047	278.30207	1
10322	O	80.29900	63.70080	79.96890	494.90230	508.91229	345.98732	1
10323	N	81.33000	65.20580	78.66090	438.82548	-590.04873	-414.66491	1
10324	H	81.30100	66.17680	78.42390	-88.44591	2770.89819	-1487.45648	1
10325	H	81.92300	64.53680	78.21290	-1620.76387	-664.79494	2613.31177	1
10326	C	81.38000	64.62380	82.85090	827.58549	-12.68046	382.61268	1
10327	O	81.10700	63.45380	83.05790	-128.54851	778.97455	-17.35391	1
10328	N	82.53700	65.11480	83.31390	-336.41963	-722.01654	279.61803	1
10329	C	83.22100	66.26080	82.69590	545.21241	-111.42309	722.34294	1
10330	H	82.94100	67.16080	83.28390	1549.02701	-2008.63643	1861.21499	1
10331	H	82.92800	66.49280	81.64990	909.45614	-1204.18131	-2760.62730	1
10332	C	83.43800	64.25680	84.07790	-238.07708	-339.70476	-812.01661	1
10333	H	83.55400	63.29780	83.59490	2126.73239	-1230.34476	1965.06675	1
10334	C	84.69700	65.12580	84.13990	-794.25120	-125.86467	429.85360	1
10335	H	85.61200	64.50480	84.24490	2282.02598	693.88454	2051.61105	1
10336	H	84.61000	65.77680	85.03590	-1598.53836	-1253.88925	2402.22045	1
10337	C	84.69800	65.91280	82.85790	-745.90164	-524.29326	-14.08283	1
10338	H	85.34200	66.81680	82.82290	1915.70789	-1911.19203	-1604.87836	1
10339	H	85.02000	65.31480	81.97890	2196.43781	-1270.72493	1859.87777	1
10340	C	82.95000	63.89680	85.48290	699.85510	-16.64032	-584.27471	1
10341	O	83.29800	62.85680	86.07890	430.43769	-589.05475	-302.26665	1
10342	N	82.18500	64.85480	86.18890	647.91516	-462.28353	281.37551	1
10343	H	82.04200	65.79680	85.89690	-1847.35312	-2155.36681	-1356.43157	1
10344	C	81.67900	64.58180	87.53990	887.62622	204.82628	40.21058	1
10345	H	82.46700	64.31080	88.22590	1310.86746	1453.57780	-2463.12085	1
10346	C	80.99100	65.83580	88.13590	-474.95018	757.05842	-180.93058	1
10347	H	80.39700	66.35780	87.35590	2521.47463	1877.07192	130.35679	1

10348	C	80.07500	65.51980	89.33090	-484.17800	742.03202	215.43246	1
10349	H	79.23600	64.80180	89.20790	-1420.43333	-679.00593	2723.88442	1
10350	H	79.60200	66.50280	89.53890	-348.43063	1610.18341	-2680.32306	1
10351	H	80.59200	65.06380	90.20190	-2652.82464	1246.87961	1142.82060	1
10352	C	82.10400	66.82480	88.54790	342.79674	752.15329	384.97640	1
10353	H	82.94700	66.77280	87.82690	1060.16392	253.18339	2951.30088	1
10354	H	82.54800	66.39380	89.46990	211.16541	-1465.18218	2776.12618	1
10355	C	81.75600	68.27980	88.67090	768.55745	474.63903	-124.45175	1
10356	H	81.18400	68.37880	89.61690	-1083.06842	-2623.20134	1357.94100	1
10357	H	82.69900	68.86180	88.75190	-1627.98157	-1946.31068	1860.04758	1
10358	H	81.16100	68.59880	87.78890	-1718.41937	-506.04212	2586.34539	1
10359	C	80.71800	63.40580	87.53890	685.09411	526.56062	291.25758	1
10360	O	80.75900	62.52280	88.33690	-297.37391	285.74901	-673.45637	1
10361	N	79.82600	63.35580	86.53090	-564.81906	398.55425	-484.56808	1
10362	H	79.63700	64.12880	85.92890	1420.45157	-2166.26829	-1785.44820	1
10363	C	78.94800	62.20480	86.22690	3.46571	435.45703	-801.13430	1
10364	H	78.49300	61.75780	87.09790	1788.16026	-1479.33231	2124.21398	1
10365	C	77.77100	62.67180	85.34990	-247.32046	-653.19514	-586.19084	1
10366	H	78.14500	63.09380	84.39290	-1169.14294	2061.70156	2068.98953	1
10367	H	77.13300	61.79380	85.11490	2696.87489	115.39037	1616.09935	1
10368	C	76.80000	63.71180	86.07290	-89.35583	-902.76136	92.13284	1
10369	H	77.33300	64.63980	86.37290	241.23475	258.76471	-3126.19143	1
10370	C	75.74100	64.25280	85.11390	508.89365	-686.87176	-317.30970	1
10371	H	76.09600	64.59780	84.11990	1290.22365	-2286.51655	-1733.60642	1
10372	H	74.99800	63.47780	84.82990	-1470.30461	176.98919	-2775.80717	1
10373	H	75.09800	65.00780	85.61490	2434.08427	-1731.40928	987.76611	1
10374	C	76.08600	63.16980	87.28090	-698.92658	-473.00164	-345.28551	1
10375	H	75.75700	62.14180	87.01690	-444.39435	-2545.30035	1795.04485	1
10376	H	76.70900	63.27280	88.19590	1112.26189	2060.49673	2101.29792	1
10377	H	75.17000	63.75080	87.51990	-1081.19711	-1744.84542	2384.27211	1
10378	C	79.71000	61.03980	85.48290	407.63862	567.41295	-585.93883	1
10379	O	79.10700	60.24680	84.78490	-160.11677	548.56613	545.03674	1
10380	N	81.05000	60.89580	85.67690	535.16889	-564.79892	-327.51905	1
10381	H	81.56300	61.63580	86.10390	1084.70637	-1558.34142	2508.62718	1
10382	C	81.67900	59.58380	85.48290	568.02070	-235.90330	673.16649	1
10383	H	80.94000	58.86180	85.16790	-1777.96583	935.53677	2421.12261	1
10384	C	82.84300	59.77880	84.44790	539.89634	-555.84947	480.61868	1
10385	H	83.72900	59.14880	84.67490	1893.32725	1319.30710	2138.44966	1
10386	H	83.19000	60.83380	84.42090	1060.88305	2829.74290	874.81911	1
10387	C	82.46800	59.21580	83.06090	638.82962	-68.15783	-647.07204	1
10388	C	82.09700	57.87180	82.98090	-614.41689	664.29035	-112.52206	1
10389	H	82.06500	57.29180	83.89090	-1039.31101	257.72386	-2958.31663	1
10390	C	81.76000	57.32380	81.74990	-200.07316	-400.13889	794.55057	1
10391	H	81.57400	56.26280	81.67190	1132.54480	2819.76813	-815.15411	1
10392	C	81.73300	58.12080	80.62590	794.88340	-446.15328	-23.63556	1
10393	O	81.35100	57.56780	79.39290	474.27188	613.47937	-149.45392	1
10394	H	80.98200	56.68280	79.44890	-2193.12138	-319.55392	-2233.00921	1
10395	C	82.57200	59.98580	81.93490	662.44523	-600.59580	-178.61133	1
10396	H	82.88300	61.01080	82.07090	2145.09316	-1742.62567	-1503.34871	1
10397	C	82.18800	59.43480	80.71690	-585.85399	-486.28005	-501.75474	1
10398	H	82.27300	60.00980	79.80690	-2931.97802	-993.46169	561.03920	1
10399	C	82.20300	59.06980	86.83590	541.32979	112.43807	725.10050	1
10400	O	82.67700	57.91880	86.94890	332.09874	31.53896	715.78136	1
10401	N	82.03300	59.88880	87.89690	-705.35059	-270.74143	-376.63232	1
10402	H	81.63800	60.79980	87.80690	-2286.10306	230.95421	2149.09730	1
10403	C	82.49000	59.51680	89.18790	-428.60429	-658.60830	-462.58456	1
10404	H	83.47100	59.07480	89.09290	-656.54819	-2944.77325	891.89752	1
10405	C	82.64400	60.75380	90.06890	594.76028	562.03824	-402.27382	1
10406	H	83.36700	60.50080	90.87390	1955.73995	-1226.39319	2137.58443	1
10407	H	81.69200	61.08180	90.53790	2705.22946	-863.29827	1354.50209	1
10408	H	83.13700	61.58380	89.51890	-2831.04941	-1372.20502	-20.94952	1
10409	C	81.62000	58.45680	89.91790	690.61544	503.73551	317.41432	1

10410	O	80.36400	58.52880	89.88090	473.31981	534.42028	-337.62487	1
10411	N	82.22900	57.62180	90.79390	-74.95390	-710.43364	449.82023	1
10412	H	83.21700	57.48780	90.80390	-2531.29487	1335.52380	1306.57900	1
10413	C	81.49200	56.95580	91.86190	-485.07052	583.70129	505.42101	1
10414	H	82.21900	56.51580	92.52890	415.96401	-2019.59418	-2376.22379	1
10415	C	80.59000	57.87080	92.75390	-491.30625	-658.90044	394.86630	1
10416	H	79.86600	58.38380	92.08590	1816.04908	1152.37066	2296.13454	1
10417	H	80.09300	57.24080	93.52290	2201.76944	-1700.96961	-1468.72051	1
10418	C	81.46100	58.86380	93.52190	-583.73211	606.76237	-350.06750	1
10419	C	82.52500	58.47380	94.32090	-97.74378	-758.65384	496.32802	1
10420	H	82.86400	57.44780	94.30990	2840.28852	-959.12381	954.49927	1
10421	C	83.30600	59.40880	95.01490	402.20585	465.13548	673.29818	1
10422	H	84.13400	59.10480	95.63690	2263.76029	-1687.84156	-1387.37393	1
10423	C	82.96400	60.78380	94.84590	562.69367	510.87950	503.81442	1
10424	H	83.47000	61.57380	95.38290	2290.66345	1104.58151	1852.29232	1
10425	C	81.16500	60.24680	93.35090	630.27321	595.89160	281.28258	1
10426	H	80.29800	60.48480	92.75290	-1224.04756	2160.53694	-1931.84211	1
10427	C	81.88600	61.18680	94.02290	-516.25570	734.96358	157.35180	1
10428	H	81.69100	62.24580	93.93990	-141.20022	-1686.02368	2652.47297	1
10429	C	80.76400	55.70980	91.43490	-500.67091	191.22002	-737.70899	1
10430	O	79.70800	55.31080	91.95290	-20.76668	609.16259	502.11245	1
10431	N	81.30300	54.90280	90.49790	-613.53821	139.25076	-562.89642	1
10432	H	82.18100	55.22180	90.14890	-1239.73952	2117.27393	1969.37129	1
10433	C	80.71900	53.68480	89.94390	612.00407	597.23992	-316.55411	1
10434	H	79.65100	53.83680	89.97990	2833.75944	-1174.44528	-699.07934	1
10435	C	81.27100	53.31280	88.53290	-560.37603	454.47798	-557.56567	1
10436	H	80.83700	52.33080	88.24890	1578.57404	-2692.15327	398.29759	1
10437	H	82.36400	53.11580	88.57390	1257.69372	-2241.60671	-1814.28556	1
10438	C	80.98500	54.38180	87.51690	-841.99760	349.42617	19.80891	1
10439	H	81.51500	55.32680	87.76390	2395.44139	-729.31323	-1904.78056	1
10440	C	81.53700	54.10480	86.08490	671.95339	-472.07004	396.33259	1
10441	H	81.59600	55.10380	85.60390	-965.80976	2726.10573	1238.46084	1
10442	H	82.55700	53.69280	86.23790	-2210.97216	-2224.80784	-245.06818	1
10443	H	81.03200	53.33780	85.45890	-1644.81482	-2509.38904	946.45502	1
10444	C	79.54200	54.65580	87.23390	-438.41855	552.71613	-577.70672	1
10445	H	79.04100	54.79480	88.21590	-1489.29346	-1960.43075	-1958.81150	1
10446	H	79.34300	55.38180	86.41690	-2620.30005	1269.85404	1191.52198	1
10447	H	79.14800	53.69780	86.83090	-875.74175	-2192.85269	2079.11032	1
10448	C	80.97300	52.63780	90.95190	-295.42717	226.19485	832.47203	1
10449	O	82.06500	52.10580	91.11790	-627.35600	133.17096	460.77888	1
10450	N	79.89800	52.16980	91.66690	699.98022	-390.63673	264.76956	1
10451	H	78.97800	52.45280	91.40590	-682.54242	2389.00221	-1930.03381	1
10452	C	80.08900	51.23780	92.72590	-238.89617	603.03427	640.88165	1
10453	H	79.15000	50.75680	92.95390	2214.23644	-2229.66527	-154.84179	1
10454	H	80.83200	50.52280	92.40490	-1666.71564	2604.77001	-579.18770	1
10455	C	80.71500	51.67880	93.95290	774.96208	-244.92028	-413.39912	1
10456	O	81.35700	50.96780	94.71090	241.13544	-647.48386	382.42068	1
10457	N	80.54900	52.96080	94.25390	210.37923	-723.05530	381.58078	1
10458	H	80.17900	53.60180	93.58590	2801.91022	231.30967	1412.09814	1
10459	C	81.11800	53.58680	95.39990	-687.52660	598.73800	16.46173	1
10460	H	82.06300	53.10980	95.61590	-2114.34932	-2272.06003	515.26344	1
10461	C	81.44900	55.05980	95.20090	14.46586	-473.49130	779.13268	1
10462	H	82.12800	55.25980	94.34390	-3143.66611	68.32620	104.50435	1
10463	H	80.47800	55.52680	94.93090	1235.10165	-2883.76761	237.98003	1
10464	H	81.73900	55.58780	96.13490	-2909.47399	-1185.33090	-167.86302	1
10465	C	80.21700	53.42580	96.59890	723.55233	-554.90228	-2.54632	1
10466	O	79.01700	53.23880	96.46890	631.29480	-307.86580	360.98858	1
10467	N	80.81200	53.47280	97.79790	-256.05364	543.33727	593.20607	1
10468	H	81.79700	53.59180	97.89590	-556.24216	1897.09413	2447.41798	1
10469	C	80.10400	53.53380	99.00590	-86.72511	664.13658	618.75064	1
10470	H	79.05200	53.39680	98.80390	-475.19793	2330.06184	-2059.90897	1
10471	C	80.72100	52.50880	100.05290	230.36682	-429.05876	-770.90253	1

10472	H	81.81400	52.47280	99.85790	1869.39229	-1429.11700	-2088.35420	1
10473	H	80.40300	52.62580	101.11090	2229.68911	-1199.15006	1867.82008	1
10474	C	80.28200	51.06780	99.72490	737.32720	385.05736	373.53773	1
10475	H	80.89900	50.69980	98.87790	-910.52263	-2102.76751	-2155.81621	1
10476	H	80.52600	50.40280	100.58090	1206.09344	-2445.06171	1570.10765	1
10477	C	78.78400	50.94080	99.35690	-220.94944	-409.60827	-784.12589	1
10478	H	78.65100	51.25080	98.29890	592.24843	643.37699	-3022.17373	1
10479	H	78.23800	51.66280	100.00090	-865.79467	1998.83832	2270.08175	1
10480	C	78.18400	49.58980	99.52590	655.94020	477.55902	-416.08993	1
10481	H	78.30600	49.19080	100.55490	2211.02539	2206.23220	-377.00458	1
10482	H	78.65300	48.87980	98.81090	2548.99670	-723.66099	1696.21839	1
10483	N	76.74200	49.65680	99.25790	416.26646	494.79098	542.74894	1
10484	H	76.66100	49.91580	98.25390	-1361.29987	743.28023	2737.26568	1
10485	H	76.41300	50.36980	99.93990	2244.37531	-1615.88694	1499.97171	1
10486	H	76.27200	48.73580	99.36890	-544.92497	471.79777	3062.46467	1
10487	C	80.22600	54.95980	99.62690	-378.19203	-96.29545	-824.10495	1
10488	O	81.26600	55.62880	99.55690	-515.08317	-299.62246	-518.21129	1
10489	N	79.06500	55.53180	100.15290	70.80141	-566.95695	-621.46542	1
10490	H	78.24600	54.96680	100.20890	2164.26931	2075.14709	952.85317	1
10491	C	78.96600	56.92180	100.51590	-589.40826	-553.58529	-421.41694	1
10492	H	79.79100	57.47180	100.08790	-1675.87924	-833.15247	-2528.93495	1
10493	C	77.72400	57.53680	99.83390	623.27081	199.74475	-634.89096	1
10494	H	76.80700	57.08980	100.27490	1411.86485	-2624.29912	-1008.91922	1
10495	H	77.67100	58.59880	100.15690	-2148.84816	713.62940	-2184.35595	1
10496	C	77.84300	57.42380	98.31090	-242.60111	-876.89297	60.45187	1
10497	C	78.61700	58.35580	97.58790	105.34580	-787.70608	447.07090	1
10498	H	79.29400	59.02580	98.09690	-525.39720	2291.80635	-2090.40849	1
10499	C	78.64100	58.25080	96.16690	851.10042	-138.40312	-296.51924	1
10500	H	79.20400	58.96380	95.58290	-2920.42460	1090.93755	423.32218	1
10501	C	77.93600	57.23580	95.50590	-630.03242	-493.47572	437.02616	1
10502	H	78.04600	57.12480	94.43790	1998.86955	251.13034	-2416.54305	1
10503	C	77.15700	56.45480	97.64590	577.85381	-618.90545	338.36670	1
10504	H	76.68800	55.65580	98.20190	-267.36934	-1292.25015	2856.01635	1
10505	C	77.20800	56.31680	96.28190	561.30100	446.83096	-562.79151	1
10506	H	76.74300	55.47580	95.78890	-2001.23461	2387.81635	437.74347	1
10507	C	78.97800	57.25380	102.00090	-768.63764	349.27438	344.46275	1
10508	O	79.06900	58.41480	102.47090	125.32698	449.02694	637.41289	1
10509	N	78.95100	56.16180	102.83090	540.14932	-557.66368	-331.54521	1
10510	H	78.58300	55.30280	102.48390	-2360.81145	1736.90962	-1143.65227	1
10511	C	78.88800	56.33080	104.26790	675.31176	-597.84226	-134.12552	1
10512	H	78.72600	57.37580	104.48790	2697.96271	376.01024	1574.11554	1
10513	C	77.73800	55.52780	104.91990	583.94266	-608.02770	-347.51156	1
10514	H	77.73700	55.67180	106.02190	-2152.12641	2287.11714	188.87393	1
10515	H	78.02200	54.47280	104.71790	854.06480	-2371.74791	-1882.44824	1
10516	C	76.39500	56.07880	104.37490	-387.71609	-456.11444	-687.81310	1
10517	H	76.33400	56.03080	103.26590	2421.74602	-1977.78675	-348.90118	1
10518	H	76.43600	57.17880	104.52490	2443.08952	841.08750	1795.02413	1
10519	C	75.12500	55.41780	105.00790	97.14733	-453.00127	-785.36823	1
10520	H	74.21200	55.89580	104.59090	-829.78562	-2235.84412	-2051.99492	1
10521	H	75.24900	55.59280	106.09790	-2546.31834	-786.16770	-1672.25282	1
10522	C	75.05000	53.89580	104.84890	-167.98973	-550.29803	-707.39136	1
10523	H	75.91600	53.36880	105.30390	2465.04029	-386.94185	-1916.26684	1
10524	H	74.88900	53.64780	103.77790	-1773.59602	2596.47137	104.49781	1
10525	N	73.87300	53.41980	105.56690	-551.26435	350.18367	-534.93112	1
10526	H	74.07600	53.58480	106.57290	2814.68176	-460.90583	-1327.91516	1
10527	H	73.01100	53.99980	105.60990	-241.20627	2579.86855	-1784.46744	1
10528	H	73.73800	52.42180	105.30890	1431.47478	1835.82938	2116.32622	1
10529	C	80.16700	55.94380	104.98190	-566.28741	-635.08442	327.77637	1
10530	O	80.39300	56.21780	106.18890	-474.92593	-350.84747	-524.38406	1
10531	N	81.09000	55.32780	104.18990	-623.65888	50.73588	566.69900	1
10532	H	80.83000	54.95680	103.30190	-1478.77195	1668.88869	2219.52028	1
10533	C	82.53200	55.16980	104.40690	222.09073	827.13953	312.99667	1

10534	H	82.59600	54.28380	105.02190	-3144.52774	-72.28619	70.32920	1
10535	C	83.29300	54.91580	103.09090	63.11093	744.29227	-522.96944	1
10536	H	82.81500	54.08480	102.53090	-1224.14638	-2204.00011	1882.04021	1
10537	O	84.67700	54.54080	103.24590	-725.06844	-109.93823	-292.94466	1
10538	H	84.78500	53.96080	104.00290	-304.29553	-2261.69628	-2165.72399	1
10539	C	83.23200	56.06680	102.10790	-556.50453	-374.31243	617.77335	1
10540	H	83.45200	55.63380	101.10790	-1792.42401	-2551.05235	421.39563	1
10541	H	83.82700	56.93980	102.45090	-1821.08005	-628.06650	2487.45375	1
10542	H	82.23100	56.54280	102.03790	1180.34726	2425.35769	-1619.45875	1
10543	C	83.20700	56.25880	105.24790	-485.58654	578.43675	-510.94779	1
10544	O	83.00500	57.44880	105.00190	547.13124	-567.29965	-49.45441	1
10545	N	83.99000	55.88980	106.24490	529.58547	240.29309	-611.94015	1
10546	H	84.16600	54.94980	106.52790	88.04386	-84.20542	3143.78497	1
10547	C	84.73700	56.88680	106.99290	821.10572	-384.26135	-97.87550	1
10548	H	84.96900	57.66880	106.28490	-2004.76628	1616.49215	-1807.23311	1
10549	C	83.91500	57.42980	108.20490	901.59265	121.77557	-61.25690	1
10550	H	84.21500	58.48080	108.40390	58.48733	-2968.54791	1040.44643	1
10551	H	82.85200	57.49980	107.89190	1198.21386	1397.51495	2551.36468	1
10552	O	83.89700	56.69080	109.40790	-31.33697	777.03860	137.31799	1
10553	H	83.44200	57.18580	110.09290	1292.49466	1810.80216	2224.56272	1
10554	C	86.04500	56.31880	107.48390	910.25559	-53.67074	2.28316	1
10555	O	86.23700	55.11080	107.49890	224.73168	386.38818	-651.02003	1
10556	N	86.96200	57.19680	107.92490	592.41732	-115.38395	-590.25465	1
10557	H	86.55800	58.10780	107.88190	-196.95547	-3017.49164	868.43480	1
10558	C	88.24100	56.92680	108.44490	-44.60705	39.58217	-909.88706	1
10559	H	88.79900	56.31480	107.75190	-2313.53670	-391.48440	2095.83257	1
10560	C	88.99900	58.27680	108.62790	528.28372	275.33553	-690.33156	1
10561	H	88.48300	58.99280	109.30190	1616.71985	2514.68091	980.21583	1
10562	H	90.03800	57.98680	108.89590	2278.22391	-1515.91739	-1552.39059	1
10563	H	89.10200	58.71980	107.61390	-2193.15855	-1988.53404	1064.90103	1
10564	C	88.23700	56.08880	109.70490	636.87901	275.86417	591.38404	1
10565	O	89.01500	55.11480	109.84290	668.78163	-409.00382	95.25881	1
10566	N	87.28400	56.41280	110.61790	542.61366	463.04814	-451.47439	1
10567	H	86.91200	57.33580	110.56290	2022.12249	-1412.01961	1953.31705	1
10568	C	86.97200	55.47480	111.74990	-589.19915	-411.36289	-561.31626	1
10569	H	87.90700	55.26180	112.24790	2295.20594	491.90314	-2094.82391	1
10570	C	85.97400	56.15380	112.70390	-440.56961	335.32811	724.50292	1
10571	H	85.55200	55.42080	113.42490	-2658.59194	-436.23655	1624.75006	1
10572	H	85.16200	56.58080	112.07790	1386.42037	-1331.91514	2490.39492	1
10573	C	86.51500	57.41880	113.51390	-524.96174	589.96805	455.85510	1
10574	H	85.63700	57.75580	114.10590	-403.58530	-2866.71174	-1231.79094	1
10575	H	86.86800	58.20880	112.81690	3080.02555	295.04673	569.75107	1
10576	C	87.65700	56.97980	114.46190	-379.69386	543.51629	-625.99810	1
10577	O	87.51800	56.06080	115.23690	-568.76345	-231.43650	-496.56068	1
10578	N	88.78900	57.67580	114.32290	105.92758	837.51450	-4.59422	1
10579	H	88.76800	58.52780	113.79990	-1547.03354	-1699.33908	2148.75782	1
10580	H	89.56800	57.40480	114.88790	25.26782	-2350.18093	-2091.46775	1
10581	C	86.38100	54.13380	111.32290	180.00555	27.32998	-893.47752	1
10582	O	86.84900	53.05580	111.69790	-204.81051	-507.76855	569.07907	1
10583	N	85.41700	54.13580	110.31590	-576.83895	-497.44063	-363.98067	1
10584	H	85.05700	54.93680	109.84490	1266.94635	-2491.28727	1444.49330	1
10585	C	84.85500	52.81180	109.85490	416.52979	487.10829	-648.59807	1
10586	H	84.53200	52.34680	110.77490	299.29514	-727.32019	-3046.25245	1
10587	C	83.70500	53.01180	108.93090	-15.29436	-675.26288	-612.56601	1
10588	H	84.01300	53.65080	108.07590	1428.91896	-2800.76377	-110.17758	1
10589	H	83.34100	52.09480	108.41990	2239.82015	-1322.46097	-1769.89517	1
10590	N	82.20500	53.38680	110.95190	-135.16195	-113.48893	-825.54455	1
10591	H	82.76300	52.85980	111.59290	2109.15876	335.39947	-2310.23435	1
10592	C	82.52300	53.64980	109.61990	-546.29797	-362.55731	633.68899	1
10593	C	81.11100	54.09780	111.23090	-452.77879	119.68693	782.37932	1
10594	H	80.61100	53.96480	112.18990	515.65026	-1085.65638	-2907.52150	1
10595	N	80.67200	54.79180	110.20390	-672.10464	-496.37782	120.65113	1

10596	C	81.57800	54.50080	109.14890	-415.10380	170.73927	793.71780	1
10597	H	81.39700	54.85780	108.14190	-2409.73621	-1633.57327	1192.82690	1
10598	C	85.90800	51.89980	109.19590	-57.11934	500.76370	759.88427	1
10599	O	85.88900	50.70180	109.38790	747.08667	-254.89254	-22.77120	1
10600	N	86.82900	52.50780	108.42890	434.81749	-696.92036	194.69990	1
10601	H	86.68300	53.45680	108.15990	2062.99251	-2373.89735	-83.06334	1
10602	C	88.02200	51.87180	107.84890	682.44651	538.86219	-274.49097	1
10603	H	87.57200	51.13580	107.19990	-1843.79418	-2538.43053	234.56273	1
10604	C	88.70700	52.92580	106.97790	-743.15574	-519.11314	98.44841	1
10605	H	89.07900	53.71380	107.66690	1482.52963	-2243.39052	-1633.25781	1
10606	H	88.02500	53.45380	106.27890	1598.24750	-2654.66864	544.57836	1
10607	H	89.64100	52.60980	106.46590	-670.78534	1167.49753	2843.45262	1
10608	C	88.99100	51.29980	108.85590	656.08552	-500.36518	-388.12045	1
10609	O	89.45100	50.19180	108.67390	-267.34786	-76.77617	-739.09253	1
10610	N	89.27600	51.98380	109.97890	-430.61950	-549.47687	474.67284	1
10611	H	88.76800	52.80380	110.22890	-911.04899	-2824.16187	1045.14387	1
10612	C	90.10100	51.42580	111.06990	-685.54544	552.14713	237.93275	1
10613	H	91.01100	51.07180	110.60790	-937.79610	2652.29756	-1408.57459	1
10614	C	90.26000	52.46080	112.19890	-150.36184	-552.95767	-709.28142	1
10615	H	90.54900	51.99480	113.16490	-2813.47406	1355.73689	380.22020	1
10616	H	89.29800	53.00080	112.32690	-1967.51298	1885.96383	1571.70587	1
10617	C	91.46800	53.42280	111.91590	547.78928	-534.48686	495.68306	1
10618	H	91.24700	53.92980	110.95190	945.15212	-928.87648	2853.43690	1
10619	C	91.52600	54.66780	112.80790	-324.36065	-543.92493	656.03875	1
10620	H	91.94300	54.47580	113.81990	-1370.29770	-1637.02729	-2310.98510	1
10621	H	92.19500	55.45480	112.39790	-1482.15837	2656.29835	-803.43753	1
10622	H	90.49100	55.02780	112.99190	-1680.46250	1661.10919	-2077.25499	1
10623	C	92.83900	52.70780	111.87190	-401.11306	622.08389	-532.51380	1
10624	H	92.94400	52.02380	111.00290	-152.06164	-2008.65723	2416.69188	1
10625	H	93.60500	53.51180	111.82990	2247.42890	2158.53128	433.62692	1
10626	H	93.04000	52.07480	112.76290	1888.77528	1844.73379	-1711.05564	1
10627	C	89.46100	50.19980	111.71690	-554.61851	177.36824	701.70494	1
10628	O	90.15700	49.23380	112.03990	-668.38767	417.15757	-53.52294	1
10629	N	88.19500	50.21680	112.07190	504.38531	-570.37054	364.61650	1
10630	H	87.72300	51.07580	111.88590	-1725.82391	1957.80252	-1756.91984	1
10631	C	87.47100	49.11180	112.69890	394.57747	402.03212	717.02845	1
10632	H	88.04300	48.79080	113.55590	-2404.20558	-1920.06895	656.77771	1
10633	C	86.10000	49.48680	113.13590	601.96840	-204.01925	-653.80516	1
10634	H	85.43700	48.61080	113.30090	-2440.18554	-196.75757	-1976.10911	1
10635	O	85.50100	50.38680	112.30590	203.56133	657.91341	386.44529	1
10636	H	85.67800	50.08280	111.41290	-2043.42410	390.47843	-2360.12092	1
10637	C	86.15600	50.20880	114.52090	-427.06329	239.43245	-769.24642	1
10638	H	85.14000	50.56980	114.78890	-2914.04759	63.16303	-1184.29867	1
10639	H	86.84200	51.06980	114.37390	-874.83740	-2997.72464	382.79595	1
10640	H	86.58700	49.54880	115.30390	-2521.49096	-1567.58855	-1040.66119	1
10641	C	87.33200	47.86380	111.81290	737.98452	-530.38323	74.32013	1
10642	O	87.28100	47.98280	110.59890	396.32778	-502.71341	462.41837	1
10643	N	87.22900	46.69980	112.39890	-249.40738	613.04579	-524.06403	1
10644	H	87.31500	46.64780	113.38990	1722.25761	-1493.91079	-2168.01418	1
10645	C	87.00800	45.43480	111.73590	786.20236	-460.38551	37.17575	1
10646	H	87.60700	45.49580	110.83890	767.49152	2902.13019	-941.71299	1
10647	C	87.63800	44.22280	112.49690	-387.94917	-654.79188	502.18925	1
10648	H	87.57500	43.32580	111.84390	-1412.57714	-1579.46339	-2325.54240	1
10649	H	88.73700	44.38180	112.50190	-2510.80954	-1313.94657	1366.60385	1
10650	O	87.05400	43.98480	113.80390	453.46026	474.88097	438.73578	1
10651	H	87.22400	44.78680	114.30390	-843.74822	-2911.98385	-840.63382	1
10652	C	85.56100	45.12680	111.38790	-851.26790	-304.48452	-118.67241	1
10653	O	84.61300	45.60580	112.09190	45.16908	705.48613	-351.96066	1
10654	O	85.32200	44.42480	110.35290	-400.57190	247.81106	633.84467	1
10655	H	79.58954	101.42979	67.58421	-2496.28827	-3262.86163	-2665.72730	2
10656	N	79.69233	100.51405	68.01112	-52.32726	418.35346	-462.87799	2
10657	H	78.70544	100.20935	68.19616	-1273.10898	124.90999	3.04791	2

10658	C	80.56233	100.47808	69.12095	454.87276	-284.58528	-532.26195	2
10659	H	79.96132	100.30827	70.10411	-1245.48904	832.80644	-2158.71392	2
10660	C	81.71383	99.37350	68.92360	588.15512	-238.27061	29.76604	2
10661	H	81.34239	98.37458	68.57855	3839.67046	203.97736	-155.16574	2
10662	H	82.50144	99.50552	68.16530	-303.39311	-3033.71494	890.82898	2
10663	C	82.38890	99.16062	70.26506	752.28396	-410.25994	168.64501	2
10664	H	82.98060	98.24185	70.08739	-823.71335	590.68020	3035.10143	2
10665	C	83.30406	100.34791	70.51796	5.60788	-74.31843	122.28784	2
10666	H	84.03746	100.21114	71.35435	-1992.59065	-350.65737	1532.88338	2
10667	H	83.82912	100.49426	69.57012	599.29607	-434.87408	205.30089	2
10668	H	82.66362	101.24377	70.78005	-2069.08580	2336.22262	2874.53184	2
10669	C	81.49275	99.04405	71.47541	-1062.64556	895.27456	-429.83120	2
10670	H	80.51004	98.64587	71.24759	-1039.04036	2528.11849	-3856.68027	2
10671	H	81.91587	98.23908	72.15882	2224.62914	-271.73813	-1889.99945	2
10672	H	81.23684	99.95808	72.09129	2176.90260	2081.56040	-3120.80292	2
10673	C	81.15883	102.00772	69.04612	253.54715	1088.69676	-370.58867	2
10674	O	81.67510	102.52154	67.96965	667.77442	106.03980	163.51217	2
10675	N	81.16309	102.49616	70.23225	-351.43250	358.98434	148.56166	2
10676	H	80.67627	102.02803	71.00014	-624.79657	1794.67560	-2456.33964	2
10677	C	81.34031	103.92332	70.03394	-941.59473	-128.22282	-917.59403	2
10678	H	80.29709	104.38630	69.91107	-26.96243	-848.86006	962.74728	2
10679	C	82.02863	104.36623	71.44321	357.62842	-316.20201	486.85213	2
10680	H	83.13262	104.07588	71.37153	-3331.91024	-1884.34581	42.95890	2
10681	O	81.52714	103.70365	72.60434	282.50228	206.78430	120.76655	2
10682	H	82.32865	103.21096	72.86125	1324.60997	-34.65537	-1592.71660	2
10683	C	81.88472	105.95335	71.36746	-9.46046	-1110.11653	-10.30381	2
10684	H	82.19634	106.30384	70.36169	639.97045	2347.82096	-1171.31089	2
10685	H	80.87404	106.30597	71.37936	-4507.93131	-804.21909	647.65740	2
10686	H	82.49855	106.43977	72.09257	-1666.64274	1619.47865	-3195.81422	2
10687	C	82.37712	104.18575	68.75854	1106.01473	-438.92102	-315.71700	2
10688	O	83.56424	103.78892	68.80508	213.56340	606.22716	47.88998	2
10689	N	82.02640	105.33786	68.08018	69.30679	-116.34906	-926.61365	2
10690	C	82.99260	105.95955	67.21878	-425.89412	-2.27420	901.10930	2
10691	H	83.59817	105.16094	66.73576	2141.21467	827.54339	-1134.58527	2
10692	C	82.08672	106.85276	66.27693	119.33836	639.17597	297.31301	2
10693	H	82.42846	107.97968	66.30691	2324.81153	4556.79855	-1741.97157	2
10694	H	82.34664	106.64172	65.22217	-93.92332	453.35858	-2372.03657	2
10695	C	80.63746	106.52736	66.77336	237.29199	698.50742	-580.46493	2
10696	H	79.98121	107.48021	66.73181	-27.52302	2483.32866	-1138.49456	2
10697	H	80.24667	105.69764	66.07552	370.92551	2267.57725	2994.10684	2
10698	C	80.79443	106.00644	68.29925	-600.61172	-365.65138	-38.96437	2
10699	H	80.87839	106.82728	69.02844	-2350.55964	-2382.90785	2671.28958	2
10700	H	79.97646	105.31451	68.56812	-978.74851	1168.53283	-1449.66498	2
10701	C	83.99601	106.87747	68.11612	591.91776	-259.22019	291.23345	2
10702	O	83.98289	108.04570	67.75257	648.12929	131.13487	-135.02818	2
10703	N	84.65001	106.28566	69.08831	852.92223	-880.45871	160.39182	2
10704	H	84.56401	105.22590	69.05080	719.82571	1763.50837	-860.84398	2
10705	C	86.06859	106.63744	69.25219	101.95499	-386.17907	-847.65193	2
10706	H	86.16420	107.30869	68.36526	-1448.26558	4290.98257	1803.45728	2
10707	C	86.41750	107.22060	70.68335	-55.22091	508.81522	230.60215	2
10708	H	85.72400	108.07148	70.77033	-404.32648	-1000.19550	3296.53319	2
10709	O	87.77687	107.72589	70.91226	979.11726	277.36434	14.82630	2
10710	H	87.65005	108.74254	70.89711	-5.67523	924.20985	-859.27091	2
10711	C	86.03774	106.06966	71.68885	155.13902	-113.35968	-223.10816	2
10712	H	85.12963	105.49539	71.39878	1841.44240	3366.88484	-2572.45244	2
10713	H	86.97854	105.40637	71.91984	1188.09090	773.25141	-284.63878	2
10714	H	85.69704	106.47929	72.64988	-739.37709	-2077.93891	1074.19111	2
10715	C	87.05328	105.33826	69.01805	799.10243	-255.42652	-299.77926	2
10716	O	87.00203	104.33762	69.68873	-82.50793	164.21234	-68.68794	2
10717	N	87.86025	105.67658	68.05696	398.38915	-28.11871	-699.20258	2
10718	H	87.77559	106.61829	67.57017	-1355.47229	275.09042	568.31956	2
10719	C	88.77715	104.75614	67.45260	-317.06275	788.75231	51.44608	2

10720	H	89.62698	105.37305	67.35200	2755.92518	867.09469	2005.18892	2
10721	C	88.86423	103.45887	68.37204	-784.95946	168.24209	-100.67092	2
10722	H	88.94059	103.73715	69.43351	988.49117	-2584.23998	83.94230	2
10723	H	87.89138	102.89133	68.29448	-2951.28135	162.66371	-856.38972	2
10724	O	89.75018	102.49829	67.78133	80.32295	183.46113	-459.66164	2
10725	H	89.37130	101.68898	68.17962	-1061.78196	-2221.72424	1812.98490	2
10726	C	88.06777	104.35826	66.02174	-241.20155	680.19958	-403.56350	2
10727	O	88.73695	104.65595	65.02796	351.09525	-434.16686	375.23239	2
10728	N	86.82757	103.90235	66.19003	-623.03778	573.19708	-1086.81089	2
10729	H	86.48502	103.72429	67.16177	2005.06146	1424.40409	-2728.50769	2
10730	C	86.10861	103.39844	65.06093	883.79048	539.39113	148.50614	2
10731	H	86.83281	103.29667	64.28173	1482.66768	1738.05117	-1077.94063	2
10732	C	85.51951	101.98647	65.59995	463.29720	310.72414	281.15287	2
10733	H	84.93634	101.55916	64.77754	40.30321	3517.33252	-587.62956	2
10734	C	86.65109	100.99173	65.97296	885.19535	445.08432	-79.28977	2
10735	H	86.31203	99.93495	66.13065	-415.12264	802.19705	1066.65259	2
10736	H	87.35890	100.99761	65.13098	47.44325	-1861.11623	-1494.82979	2
10737	H	87.02344	101.27227	66.97478	-1833.42430	-1474.86425	-1160.65909	2
10738	C	84.55084	102.26781	66.84392	-222.92196	-260.17442	-953.20450	2
10739	H	83.60837	101.65231	66.82883	586.16672	341.63770	-930.17085	2
10740	H	85.11427	102.25300	67.83080	2237.36077	-2956.16963	709.88851	2
10741	H	84.07472	103.18976	66.63019	-2483.40560	934.37387	1422.76781	2
10742	C	84.93586	104.34228	64.58684	403.18200	701.21708	114.58441	2
10743	O	83.85289	103.89482	64.14315	222.94454	357.50458	-382.38165	2
10744	N	85.25346	105.67178	64.75209	504.08732	670.23594	-351.02981	2
10745	H	86.19702	105.83750	65.17958	-967.64766	-2430.42602	-198.15885	2
10746	C	84.82927	106.62874	63.78711	43.77185	-1202.96926	556.99067	2
10747	H	83.97469	106.26464	63.24001	-2014.25422	-2003.16968	-905.15392	2
10748	C	84.73792	108.04915	64.48865	952.67338	168.04692	59.58108	2
10749	H	84.24905	107.85339	65.50943	2398.36156	-2093.60601	878.31520	2
10750	H	85.76025	108.41797	64.72774	192.64787	1421.84279	1251.99622	2
10751	C	83.83300	109.10773	63.66941	-753.53117	161.30559	393.83135	2
10752	H	84.44645	109.71964	62.99696	-3131.18770	1352.92427	1107.43856	2
10753	H	83.16094	108.48748	63.00268	111.70039	2371.65159	-3557.31204	2
10754	C	82.99691	110.00461	64.63366	868.08490	97.01679	85.32002	2
10755	O	82.13888	110.72235	64.14349	421.48925	-481.99928	563.42685	2
10756	N	83.27010	109.86338	65.97312	-501.92731	-32.93925	511.76157	2
10757	H	83.86304	109.36205	66.62320	-2632.99338	-229.33211	970.22956	2
10758	H	82.55747	110.41693	66.42825	952.47130	1045.65846	-235.16989	2
10759	C	86.05003	106.97845	62.77667	324.70284	-905.59524	174.46503	2
10760	O	86.94115	107.79292	63.04272	188.06380	-227.36457	-129.78146	2
10761	N	86.03254	106.07659	61.78223	-417.21037	1155.73585	-270.88890	2
10762	C	86.23818	106.61683	60.46881	840.87414	113.46289	-333.75295	2
10763	H	86.82803	107.56382	60.60440	3946.26537	1538.50372	-2279.39731	2
10764	C	87.05941	105.43767	59.80122	587.85225	-236.90786	-243.76386	2
10765	H	86.79453	105.23530	58.77776	-2521.56474	-1975.66178	-492.08249	2
10766	H	88.19757	105.54851	59.93093	-3040.27069	1144.34145	2118.52260	2
10767	C	86.54310	104.12500	60.43044	742.93346	417.95988	-16.72355	2
10768	H	85.61670	103.77719	59.93800	-789.63466	642.34666	4124.51042	2
10769	H	87.27147	103.22483	60.38578	-2132.58144	-3276.45948	-2234.67842	2
10770	C	86.34715	104.66864	61.94512	-14.47960	-644.58617	-494.80778	2
10771	H	85.44470	104.25443	62.59123	-1998.70033	-1275.11831	1870.99163	2
10772	H	87.26639	104.69042	62.57870	-211.92854	829.19463	-260.88335	2
10773	C	84.81931	106.90015	59.74369	-915.28494	86.83637	-158.41065	2
10774	O	84.66935	107.86166	58.96564	467.57135	-30.70242	-210.88720	2
10775	N	83.82648	106.18334	60.28022	677.84787	220.89574	-236.63463	2
10776	H	84.23880	105.55270	60.99989	3386.53993	814.27333	-518.25369	2
10777	C	82.50324	106.68434	60.10246	-1039.23280	1522.48158	-462.50195	2
10778	H	82.53833	107.28816	59.15681	1017.28889	31.86483	-919.98334	2
10779	C	81.46553	105.44174	60.20605	1004.43928	186.62576	-724.84596	2
10780	H	81.18715	105.18940	61.23806	-1379.78208	-326.46769	455.55576	2
10781	C	80.21216	105.96228	59.43689	30.87619	-100.59611	-149.75588	2

10782	H	79.47824	105.12361	59.26298	-1970.60548	-2787.52719	1264.65637	2
10783	H	79.72099	106.77929	60.00204	510.71797	-1252.12063	-2770.53432	2
10784	H	80.49393	106.28612	58.39799	1535.39109	-1833.62605	791.85698	2
10785	C	82.11973	104.23061	59.40012	-756.35139	324.99703	-968.33747	2
10786	H	81.36360	103.40120	59.69398	4737.67544	2541.34233	-743.05426	2
10787	H	82.18360	104.27590	58.34686	498.83564	-1985.25744	626.71094	2
10788	H	83.15692	103.98949	59.81724	-524.92250	-1549.81983	3253.45122	2
10789	C	82.22864	107.71883	61.34240	-460.13293	-895.24345	293.33585	2
10790	O	81.58669	107.50520	62.36007	374.43925	644.28150	90.59479	2
10791	N	82.81262	108.86034	61.04649	-451.53624	-818.71388	759.84226	2
10792	H	83.40188	108.89088	60.21302	-225.90521	-50.60305	-1589.33061	2
10793	C	81.89609	110.01075	61.02880	459.97703	-197.97207	-971.59717	2
10794	H	81.59140	109.91625	62.07768	2708.32810	1385.51073	-2680.78119	2
10795	C	82.68922	111.34860	60.66249	-1024.35013	-271.84887	-862.38937	2
10796	H	82.02639	112.19312	60.99879	-284.75229	2320.26831	1451.63062	2
10797	H	83.67415	111.42488	61.20560	88.21527	2442.21651	-2716.72515	2
10798	C	83.05449	111.74830	59.18864	204.81734	-26.91273	1065.71251	2
10799	H	82.12465	111.69653	58.49826	-1870.87529	-801.02292	-4880.29888	2
10800	H	83.35913	112.81759	59.09168	-3305.75854	-430.82649	2168.35714	2
10801	C	84.20555	110.86866	58.58146	99.19433	665.96560	389.49757	2
10802	H	85.18511	111.40087	58.61001	-2862.34106	-1735.09558	-1546.65872	2
10803	H	84.43956	109.84152	59.07160	1549.10297	300.49147	-1154.33628	2
10804	C	83.74940	110.43797	57.17787	-788.53896	-358.53723	-290.39857	2
10805	H	83.03654	111.13116	56.65027	-1077.38660	-1925.27639	634.97682	2
10806	H	84.55752	109.99765	56.56878	-388.43611	-1024.65513	299.01179	2
10807	N	83.07562	109.03390	57.25884	1052.22812	918.66922	377.20712	2
10808	H	82.38111	108.99588	58.13585	3013.83136	-1293.00422	-5048.16560	2
10809	H	82.40019	108.72879	56.38560	1222.45926	389.11289	-1478.41655	2
10810	H	83.73441	108.19744	57.41914	-1406.61344	-5016.99386	-3939.81108	2
10811	C	80.76733	109.74764	59.91122	-526.71687	121.28673	-93.67753	2
10812	O	80.95969	108.83199	59.03577	-318.44715	270.35058	340.88596	2
10813	N	80.03662	110.84462	59.83916	-246.54667	516.06620	-355.35773	2
10814	H	80.30830	111.49356	60.59734	-44.90944	-2096.54303	-1041.08456	2
10815	C	78.71171	110.95271	59.35171	69.74307	478.90671	-200.76798	2
10816	H	78.45019	109.95595	59.87527	644.83638	-4506.32062	-1852.54622	2
10817	C	77.69937	112.07976	59.87221	155.00125	-12.35416	93.35071	2
10818	H	78.00557	112.50566	60.90461	-2545.55659	585.69072	-832.78139	2
10819	H	77.74852	113.00532	59.19738	-948.88519	-1663.98451	-505.87371	2
10820	C	76.30150	111.41735	59.90110	519.12576	-397.96880	-442.24346	2
10821	H	76.28053	110.60409	59.15210	2455.16716	-967.64668	-2722.06528	2
10822	H	76.18403	110.85370	60.82843	-232.81993	-48.27987	890.09800	2
10823	C	75.09589	112.46010	59.85900	1360.28532	-469.92695	279.09350	2
10824	H	75.09201	113.00287	58.90693	-1230.91740	-2167.03357	3170.36135	2
10825	H	74.23297	111.73860	59.92725	1383.35014	-3737.14861	530.93089	2
10826	C	74.97993	113.63748	60.89700	-302.18067	-200.03851	286.32551	2
10827	H	75.90104	114.16966	61.08113	1403.34636	208.65345	2077.09092	2
10828	H	74.11730	114.30047	60.66665	-878.67047	-4189.93751	-21.67519	2
10829	N	74.66391	113.14868	62.30860	361.65228	-315.06461	212.73497	2
10830	H	75.43419	112.38860	62.73664	-1298.60371	-629.08150	-3918.03166	2
10831	H	74.54810	113.98817	62.99047	-1000.40360	-2412.71261	-1316.72047	2
10832	H	73.73634	112.69181	62.47908	616.02925	-1298.59838	-1111.26149	2
10833	C	78.47196	110.87183	57.73382	481.10654	-567.64340	370.55881	2
10834	O	77.56469	111.47650	57.18918	458.27799	-127.40671	485.88132	2
10835	N	79.30958	110.00246	57.17720	623.93250	-301.65042	334.73863	2
10836	H	79.86417	109.45712	57.86562	-936.09591	924.85834	-1286.38147	2
10837	C	78.69948	109.23829	56.07053	333.64883	119.41135	745.17911	2
10838	H	78.44448	109.94106	55.29233	-1712.72191	4547.57679	1043.18188	2
10839	C	79.70959	108.20379	55.60964	-401.39665	-696.13142	610.63263	2
10840	H	80.07718	107.73967	56.57926	144.85283	1560.49549	1084.58304	2
10841	O	81.20649	108.80656	55.42836	-594.22340	141.14332	410.20769	2
10842	H	80.97343	109.74024	55.42859	542.75236	949.15645	2204.53463	2
10843	C	79.01232	107.25156	54.54437	157.42321	-31.94533	-716.68284	2

10844	H	79.79861	106.61273	54.07679	-418.01649	-362.24765	-1769.83376	2
10845	H	78.10862	106.70971	54.93641	-1691.45543	-332.07491	-642.97719	2
10846	H	78.66844	107.88187	53.67625	-1585.48923	-24.65045	396.77936	2
10847	C	77.30028	108.48986	56.61180	857.84733	140.66127	113.59050	2
10848	O	76.51787	108.04058	55.80374	-584.37197	81.12620	430.74283	2
10849	N	77.45613	108.07795	57.86553	-873.85359	-322.49386	-32.39729	2
10850	H	78.24931	108.58231	58.24523	2366.49990	-1032.48472	453.61784	2
10851	C	76.29555	107.60166	58.62204	-515.99304	65.80282	100.26119	2
10852	H	75.55076	108.40993	58.44773	-485.51679	-357.39715	-1200.53405	2
10853	C	75.83035	106.25148	57.96872	-599.58085	-58.61843	203.26454	2
10854	H	74.82008	106.03741	58.39572	-2523.01704	-132.80739	2605.37529	2
10855	H	75.60794	106.44406	56.84468	-2686.83382	-61.74908	403.03195	2
10856	C	76.89606	105.12390	58.13402	574.07733	-1524.68724	-812.11113	2
10857	C	76.61900	104.14274	59.10716	-222.20788	-228.07018	-229.22299	2
10858	H	75.67167	104.20741	59.77576	-709.70211	282.26165	1421.79702	2
10859	C	77.97729	105.06181	57.26297	-853.79805	790.81218	334.89628	2
10860	H	78.18485	105.81300	56.41986	265.63289	1283.14081	-2587.84580	2
10861	C	77.46064	103.06766	59.14940	846.30113	395.97138	84.28470	2
10862	H	77.29068	102.30515	59.95447	-2249.19646	956.15650	-2832.34903	2
10863	C	78.86629	104.00866	57.38575	-376.55660	-120.66762	307.38791	2
10864	H	79.76178	103.97912	56.82987	-2135.16909	2051.23717	3569.87235	2
10865	C	78.59832	102.96227	58.31695	-574.87913	445.35567	892.66725	2
10866	O	79.39918	101.75154	58.47343	628.81582	-146.74007	-717.14497	2
10867	H	79.00786	101.43212	59.32107	2193.45459	380.24907	-1108.75141	2
10868	C	76.68938	107.62905	60.13334	375.25194	767.45094	40.15299	2
10869	O	77.50946	108.41463	60.62355	-413.28357	292.21494	-525.30169	2
10870	N	75.78406	106.84757	60.81646	-198.10865	131.20007	-387.67542	2
10871	H	75.13225	106.28962	60.27572	-2289.40196	-2141.15940	-1877.06226	2
10872	C	76.37605	105.93799	61.81672	-592.81439	-258.84353	535.59121	2
10873	H	75.71854	105.05973	61.63991	790.24514	449.00446	399.85247	2
10874	C	77.86600	105.58920	61.42082	1062.66927	-426.83938	384.93024	2
10875	H	77.86057	105.24461	60.34867	-2159.84157	859.71242	-2980.94007	2
10876	H	78.43800	106.54646	61.39438	-608.12565	1225.66092	287.46876	2
10877	C	78.63432	104.56224	62.29280	-56.15533	-379.02494	439.26480	2
10878	H	78.09785	103.65623	62.18740	-1303.13412	-328.68632	-269.08631	2
10879	H	79.65379	104.38737	61.81015	-1261.69630	-921.26353	1291.11624	2
10880	C	78.79567	105.22264	63.74449	-9.77619	-401.67667	-54.94178	2
10881	H	79.40651	106.13970	63.73968	-716.13907	2320.68627	-909.91067	2
10882	H	77.86121	105.48461	64.28366	-1573.25786	-2109.52029	2456.43510	2
10883	N	79.54288	104.24497	64.34160	-373.76937	9.12800	672.01433	2
10884	H	79.07625	103.49267	64.84553	-1775.88509	497.38486	-2476.94488	2
10885	C	80.82161	104.15887	64.28018	-40.20393	179.10722	7.91627	2
10886	N	81.56989	105.04839	63.58788	655.72366	-404.12660	131.95413	2
10887	H	81.17889	105.80413	63.00427	1478.73385	470.26559	-192.73552	2
10888	H	82.60691	104.92116	63.39886	-2045.80144	-1849.38829	655.78014	2
10889	N	81.46226	103.05879	64.98007	-583.94551	312.23903	361.81406	2
10890	H	81.23322	102.80914	65.95426	-120.60626	609.60899	1346.15396	2
10891	H	82.48827	103.08905	64.88772	-1201.87647	2038.48312	-1541.13447	2
10892	C	76.20130	106.66559	63.28419	-770.89880	-1271.69071	289.92910	2
10893	O	75.51430	106.26942	64.21576	-663.40620	-650.96259	-289.97042	2
10894	N	76.93209	107.78327	63.19303	-267.41305	-966.08845	-997.18205	2
10895	H	77.34692	107.99223	62.19171	2384.94080	-1503.43171	-1301.95226	2
10896	C	76.91640	108.90725	64.15039	-1294.87273	83.11625	-301.60080	2
10897	H	76.77323	108.42351	65.12825	-950.66071	-932.68839	-1794.57879	2
10898	C	78.25163	109.63299	63.99937	-8.97036	-439.23588	2.66250	2
10899	H	78.22625	110.04424	62.95957	2411.08041	813.06992	-1102.26435	2
10900	C	78.43184	110.74379	65.01113	-105.26314	-32.36699	-202.64522	2
10901	H	79.23812	111.51710	64.74220	-798.49351	-2227.03905	3000.18782	2
10902	H	77.50932	111.27043	65.08883	1285.16937	-2582.93354	460.30457	2
10903	H	78.71547	110.39469	66.07165	-331.78837	-1788.18710	-1110.37497	2
10904	C	79.51429	108.78505	64.12203	89.12398	-68.61876	583.11055	2
10905	H	80.42869	109.47146	63.86661	892.64338	-103.10350	1401.77051	2

10906	H	79.76744	108.28277	65.08205	1605.90389	-381.01476	913.21594	2
10907	H	79.54506	107.97872	63.42207	-1297.05441	628.55882	2443.37655	2
10908	C	75.78132	109.87798	63.53646	455.06992	-180.03557	-906.90460	2
10909	O	76.05228	110.99204	63.09381	-529.16267	464.36373	-514.11895	2
10910	N	74.61157	109.28827	63.83137	837.09097	661.59368	524.61088	2
10911	H	74.75886	108.39908	64.23382	-1138.37324	288.17119	649.34556	2
10912	C	73.44284	109.77978	63.09934	42.41044	404.67463	-146.52260	2
10913	H	74.02066	110.32717	62.31489	3492.29066	-294.40002	1918.81303	2
10914	C	72.85704	108.41514	62.50142	174.01261	47.38403	317.76066	2
10915	H	73.57481	107.58299	62.31127	2204.39700	-2895.49138	-4032.70138	2
10916	H	72.10620	108.00856	63.24607	-1898.50407	1888.05880	-465.08418	2
10917	C	72.28644	108.64181	61.02840	44.09309	426.44280	860.11377	2
10918	H	71.95372	107.64793	60.68380	-204.89114	-925.40929	2027.88812	2
10919	C	71.05711	109.67338	61.02054	1411.54186	-615.93598	-174.08317	2
10920	H	71.56032	110.65165	60.78253	1605.62344	-93.73957	-323.81072	2
10921	H	70.35286	109.52381	60.18786	-2207.65513	537.20766	-1142.07517	2
10922	H	70.52446	109.71711	61.97396	-1890.94888	-2065.41845	96.96562	2
10923	C	73.39305	109.13565	60.05296	446.18004	-686.60803	95.44946	2
10924	H	74.28749	108.49099	60.06035	-94.40249	2492.46936	849.07351	2
10925	H	73.03350	109.18070	58.98907	-1112.49154	187.31933	2892.11745	2
10926	H	73.78460	110.19219	60.28705	249.87943	561.07887	2240.94895	2
10927	C	72.54555	110.63938	64.08714	770.82701	-146.02497	954.33255	2
10928	O	71.36000	110.52571	64.19777	-379.88746	-663.61775	87.61600	2
10929	O	73.24738	111.72764	64.69585	-613.85959	-50.64132	-253.35743	2
10930	H	74.14436	111.57440	64.48835	2882.55303	-1822.60767	-849.48474	2
10931		5463						
10932		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	100.0000
		0.2500	400.00	0.00	0.00	-25967.2204	0.2251	400.0000
10933	N	58.16043	94.53138	59.17425	-156.39663	-72.22775	-71.80474	1
10934	H	57.95312	95.20225	59.92568	-797.00916	-2728.56626	-1827.92286	1
10935	H	57.74924	95.05926	58.34712	-1892.90999	-109.62552	2072.50020	1
10936	H	63.01319	101.73785	57.12985	-3156.30573	1256.50677	389.41765	1
10937	C	59.49958	94.34519	58.79374	-346.94382	443.68482	284.84162	1
10938	H	60.08457	94.67946	59.67287	3521.71160	3067.24489	-1487.01854	1
10939	C	59.72162	92.75225	58.45927	-171.45862	-233.27461	112.56741	1
10940	H	60.68387	92.58329	57.95797	2470.26020	-2571.23592	2704.12685	1
10941	H	59.05095	92.50518	57.60511	539.66327	1217.65780	517.11301	1
10942	C	59.48950	91.85361	59.70227	-176.92257	353.62024	-744.20013	1
10943	H	58.53080	92.08216	60.21175	-245.73982	-1168.71000	-240.90072	1
10944	H	60.15599	92.18627	60.55457	1826.38436	753.66219	2824.51893	1
10945	S	59.83754	90.21987	59.07100	-451.85990	442.40451	-13.87442	1
10946	C	60.25912	89.45409	60.69386	84.37838	-29.38509	309.19986	1
10947	H	60.92096	90.06490	61.40634	-210.35460	-6.51890	-525.58504	1
10948	H	59.41954	89.43553	61.46632	-790.58890	1390.90566	-14.93259	1
10949	H	60.65255	88.42320	60.68592	-3081.96520	1050.83680	-1676.72995	1
10950	C	59.75184	95.12526	57.36857	-567.71060	593.91430	672.01689	1
10951	O	59.21520	94.86369	56.30226	2.69965	-143.58828	-309.16520	1
10952	N	60.67992	96.08068	57.55617	1352.80810	52.36705	-71.36855	1
10953	H	61.05102	96.42677	58.52144	-1017.24422	-197.67348	-1151.23689	1
10954	C	61.47727	96.35365	56.34318	-289.89867	-446.24647	1044.60613	1
10955	H	60.98707	95.80553	55.51548	-1232.95701	821.13584	130.12214	1
10956	C	61.26351	97.87634	56.10791	475.50521	155.83808	190.05055	1
10957	H	61.08399	98.19100	55.02348	1838.73243	-3756.29542	-1183.84708	1
10958	H	60.38179	98.29397	56.62158	-442.11279	-691.87708	-1946.70058	1
10959	C	62.53727	98.52096	56.76295	662.40337	-237.06835	78.77729	1
10960	H	63.54913	98.19974	56.31459	-357.18865	34.47350	844.63114	1
10961	H	62.53290	98.18478	57.81596	-2663.10972	-1750.95030	-873.15478	1
10962	C	62.37370	100.07448	56.61850	-475.45541	323.24989	-219.95652	1
10963	O	61.55423	100.69342	55.95894	-594.83152	7.77067	537.73660	1
10964	O	63.35378	100.79002	57.38658	-156.07391	-298.95515	422.81224	1
10965	C	63.01484	95.92205	56.54718	-1169.89672	-232.96887	365.94463	1
10966	O	63.97446	96.49602	55.94091	-1035.42237	328.67086	1142.90262	1

10967	N	63.13837	95.06107	57.54224	186.23473	-278.22763	-46.52723	1
10968	H	62.27809	94.69329	57.95342	630.67997	-2083.36788	2300.43816	1
10969	C	64.25224	94.15676	57.43295	-12.31584	163.86153	-309.21754	1
10970	H	64.29198	93.85677	56.34519	-611.45451	2052.12083	-3495.04809	1
10971	H	63.87034	93.20420	57.87857	2748.02657	-805.69292	-1179.30127	1
10972	C	65.75164	94.64245	57.96003	654.42535	-261.73918	252.92292	1
10973	O	66.23858	93.84771	58.72658	-911.87538	-318.29616	228.00144	1
10974	N	66.07397	95.79612	57.42973	419.05104	-547.80496	805.47731	1
10975	H	65.43857	96.27466	56.72471	1387.87194	1716.71901	-853.98759	1
10976	C	66.79601	96.69029	58.31322	314.36854	437.18363	-71.75947	1
10977	H	67.62897	95.98798	58.57776	-1043.43944	1961.15016	-897.92192	1
10978	C	67.26919	98.05746	57.65957	-197.78152	20.37831	263.01072	1
10979	H	67.51257	97.91397	56.63084	-324.13093	-1244.59757	2564.89403	1
10980	C	66.01988	99.01397	57.59478	515.27438	-91.93528	100.79705	1
10981	H	66.07009	100.00747	57.11079	281.93211	21.77721	744.95134	1
10982	H	65.77436	99.29721	58.65101	-2387.13613	-1349.01058	-719.38373	1
10983	H	65.16163	98.35347	57.19284	2672.19666	-801.31379	-345.52991	1
10984	C	68.60562	98.53901	58.41617	-382.08456	-597.51520	-88.14755	1
10985	H	69.32801	97.71412	58.42856	-536.71928	-281.24734	1349.59213	1
10986	H	68.42364	98.72053	59.44598	-437.77383	-401.50131	-786.73556	1
10987	C	69.08727	99.86928	57.74615	405.91255	658.43392	-848.68748	1
10988	H	68.21776	100.57460	57.61691	1951.70162	1369.62460	1257.78539	1
10989	H	69.61257	99.69974	56.76191	1101.60201	-1128.10933	2417.48021	1
10990	H	69.80177	100.35470	58.35155	1900.95282	1739.30517	1134.04575	1
10991	C	66.11269	97.12480	59.68843	-176.25244	182.44215	-95.95372	1
10992	O	66.77388	97.58175	60.63090	-468.24096	379.91793	-690.29471	1
10993	N	64.79372	97.01794	59.70987	-419.14937	345.76278	558.80681	1
10994	H	64.24890	96.72701	58.91317	623.75228	1079.05974	2763.07311	1
10995	C	64.03459	97.57163	60.81630	726.19065	-272.20695	642.11805	1
10996	H	64.77342	98.28940	61.36223	-792.11180	1809.99777	-1901.74733	1
10997	C	62.80948	98.30329	60.24820	460.28213	-102.05800	483.31403	1
10998	H	62.40947	99.15239	60.83872	-1574.11198	1086.81408	-755.98353	1
10999	H	63.14111	98.68011	59.26832	-711.84642	635.49414	-1171.69198	1
11000	O	61.49609	97.41352	59.71803	-141.36330	-404.91390	301.34429	1
11001	H	61.15885	97.19870	60.57552	239.91218	487.87188	-1006.40776	1
11002	C	63.48520	96.34615	61.80070	848.67756	824.41376	-0.89799	1
11003	O	62.93411	96.69945	62.82546	1013.95733	-164.31053	-277.44203	1
11004	N	63.68555	95.17158	61.24116	199.24408	-103.33131	93.63151	1
11005	H	64.19563	95.32509	60.36848	-798.36688	727.84230	-4024.24212	1
11006	C	63.53258	93.86286	61.80589	1021.01121	332.94942	-628.86071	1
11007	H	63.78749	93.19529	60.95840	2169.12266	-118.03273	1796.48722	1
11008	C	64.65410	93.79221	62.99035	-160.28198	-483.92503	122.91378	1
11009	H	64.39834	94.56585	63.76281	-3988.71750	5383.07655	330.86470	1
11010	C	64.71959	92.29292	63.47320	475.35789	1047.33037	-312.81245	1
11011	H	65.40726	92.16803	64.34812	3289.23102	-3324.58332	-237.73729	1
11012	H	63.67690	91.88153	63.66756	-2759.78662	504.91483	-2192.04574	1
11013	H	65.26838	91.64298	62.70001	-94.53429	-1147.86506	-528.83022	1
11014	C	66.09994	94.01275	62.43473	-410.35410	12.51151	257.59936	1
11015	H	66.20534	93.73098	61.36093	-894.64027	-345.69515	1181.80094	1
11016	H	66.76783	93.36558	62.99645	-467.77738	1207.17499	1003.74060	1
11017	C	66.56830	95.51390	62.65662	-908.22021	-249.60988	-606.53789	1
11018	H	67.64908	95.63936	62.38069	578.16447	-1115.75474	574.68683	1
11019	H	65.97646	96.27615	62.09082	-185.62122	776.91407	1361.71517	1
11020	H	66.38284	95.82951	63.74940	-2576.06338	1420.30889	131.25801	1
11021	C	62.05862	93.58051	62.37173	-242.78269	-6.28080	-281.68844	1
11022	O	61.52164	92.53185	61.94332	489.66945	-76.34530	510.90051	1
11023	N	61.51696	94.48627	63.20827	-295.14348	-165.58572	85.43876	1
11024	H	62.02985	95.33206	63.50966	234.93892	1628.24441	1968.30012	1
11025	C	60.05034	94.38349	63.24912	740.87084	397.38608	-303.48704	1
11026	H	59.85008	93.43114	62.72876	-2254.95576	3207.58001	-3152.36758	1
11027	C	59.70098	94.46680	64.77886	265.96245	-107.17317	-345.85454	1
11028	H	59.78050	95.51468	65.12806	-2992.81083	1387.15692	-1386.14991	1

11029	H	60.39520	93.87982	65.45208	773.46291	-2864.08685	-2191.64828	1
11030	C	58.25697	93.91049	64.87388	93.91225	213.75026	252.69791	1
11031	C	58.01697	92.52082	64.89467	307.85125	-381.51808	38.30586	1
11032	H	58.89064	91.81631	64.70514	2177.07880	1050.63759	1766.37330	1
11033	C	56.68054	92.08120	65.10555	325.31073	473.37486	-966.95754	1
11034	H	56.47886	91.08049	65.14152	-5853.99443	1334.15144	1422.25526	1
11035	C	55.61131	93.03075	65.18412	-42.93830	-259.57219	-525.04028	1
11036	O	54.24254	92.58934	65.19868	-8.97560	-363.99506	15.01135	1
11037	H	53.80718	93.45934	65.25008	-37.75048	-1258.39414	6055.49289	1
11038	C	57.20503	94.92393	65.11868	681.12944	-347.41848	636.84165	1
11039	H	57.39155	96.02102	65.09479	-3612.35146	-794.11389	-487.36644	1
11040	C	55.93755	94.42577	65.31080	-214.71130	116.78192	885.93510	1
11041	H	55.10354	95.08805	65.33926	-822.91914	-2188.34689	-279.34936	1
11042	C	59.20714	95.59445	62.61516	-301.27078	-232.36283	591.47100	1
11043	O	57.99354	95.56346	62.49953	884.14248	535.63794	-159.48387	1
11044	N	60.03370	96.63166	62.42705	246.74863	270.18808	-74.01686	1
11045	H	61.01732	96.31920	62.41711	1919.73741	38.00158	-1534.07541	1
11046	C	59.60173	97.99552	62.31106	630.63578	-679.26591	-878.54468	1
11047	H	60.56507	98.53030	61.98903	3653.47627	1244.83822	-1561.18142	1
11048	C	58.37655	98.25356	61.31634	-77.12390	624.34038	912.70820	1
11049	H	58.46092	99.36250	61.27500	95.27370	2481.50067	1235.47830	1
11050	O	57.06368	97.79383	61.48203	150.32224	386.78898	-1.91882	1
11051	H	57.22025	96.84401	61.93178	-139.76533	-533.73871	2489.85035	1
11052	C	59.01444	98.25437	59.85876	-294.33264	176.49738	-676.01205	1
11053	H	60.06569	98.64599	59.85564	-2070.74348	-2556.39960	1532.35949	1
11054	H	59.00735	97.21636	59.53614	623.84751	1671.83231	2021.69577	1
11055	H	58.48455	98.80007	59.10807	702.23365	-6493.63139	-648.56493	1
11056	C	59.15928	98.62790	63.71270	80.23402	-352.36945	-396.49801	1
11057	O	58.64548	97.96416	64.63944	-439.40010	320.79190	-743.96661	1
11058	N	59.31975	99.92186	63.66404	-868.39077	311.37765	456.38930	1
11059	H	59.74527	100.33170	62.82617	925.13336	-390.31174	-1210.97078	1
11060	C	58.99561	100.72919	64.82472	-407.58364	-847.52909	-260.21228	1
11061	H	57.93871	100.43509	65.15246	-1126.88035	527.22360	-1070.00906	1
11062	C	59.98771	100.56367	66.03554	106.70779	-141.62223	-198.69183	1
11063	H	59.65399	101.20294	66.84339	1852.20808	-1211.76849	711.56378	1
11064	H	59.85848	99.46839	66.45839	-726.25611	2023.21172	1829.68880	1
11065	O	61.46372	100.47095	66.05519	-262.70949	-426.16194	391.04369	1
11066	H	61.71813	101.34096	66.37737	-1964.91892	2937.76241	1490.16390	1
11067	C	59.07397	102.29238	64.52414	-141.02831	60.71605	195.55828	1
11068	O	59.68580	102.81051	63.58827	-664.02621	-382.47330	142.40621	1
11069	N	58.58312	102.93519	65.58839	38.62437	490.88921	252.20002	1
11070	H	57.95678	102.38278	66.27601	1525.70027	-1220.07226	27.35274	1
11071	C	58.35764	104.33843	65.46290	-37.48681	-39.26400	-376.82815	1
11072	H	57.83060	104.23668	64.44176	582.62924	2209.50926	700.82479	1
11073	C	57.31118	104.91487	66.45811	-512.85730	-633.41145	-170.54155	1
11074	H	56.35800	105.24601	65.93256	2066.12221	1688.91905	-99.81639	1
11075	H	57.71068	105.83611	66.90430	-86.12253	1100.82793	546.74648	1
11076	C	57.01195	103.97354	67.69776	114.40177	-395.62179	374.14413	1
11077	O	57.04437	102.72931	67.62698	-258.57246	61.30788	-449.06914	1
11078	O	56.55720	104.61043	68.68456	208.28632	401.94260	15.81898	1
11079	C	59.72969	105.28526	65.47728	-4.56373	-260.92987	107.07326	1
11080	O	59.61741	106.38138	65.01887	190.68022	463.24006	426.38984	1
11081	N	60.80900	104.78046	66.07544	923.32918	739.15570	368.69361	1
11082	H	60.62543	103.85164	66.49948	215.52941	968.91746	-3013.98555	1
11083	C	62.04290	105.41845	66.18036	53.08488	583.86293	-1321.51143	1
11084	H	61.77969	106.51061	66.09926	-1562.78633	-982.54085	-750.94095	1
11085	C	62.63031	104.99976	67.62785	753.35890	-528.25821	-395.05766	1
11086	H	61.93899	105.61756	68.26830	-1803.50834	-1328.18188	-1594.59560	1
11087	H	63.68802	105.27289	67.73160	-1055.73521	-3293.52658	-3300.34837	1
11088	C	62.54754	103.46648	67.83976	37.87181	-143.63910	58.99704	1
11089	O	61.47006	102.85763	67.65427	20.15494	252.96067	674.75402	1
11090	N	63.70610	102.93739	68.17832	15.99073	808.19549	776.52983	1

11091	H	63.85078	101.90115	68.42651	-1681.50953	-4070.00030	9.98836	1
11092	H	64.60439	103.45694	68.38335	593.74513	5023.28625	2362.95729	1
11093	C	63.02870	104.92234	64.94154	-1113.08371	-551.69396	-114.53660	1
11094	O	64.19557	105.26538	64.85588	231.18288	283.84603	-302.08764	1
11095	N	62.38217	104.24329	63.97971	-947.16064	-163.18817	-240.28713	1
11096	H	61.42724	103.94021	64.01502	-124.32753	1941.75380	-1824.00279	1
11097	C	63.11755	103.24182	63.28802	-211.33508	812.22395	-318.47940	1
11098	H	64.15879	103.36012	63.44980	-351.23737	44.64401	-1507.00669	1
11099	C	62.65429	101.75579	63.60962	-223.25237	246.37891	-648.05729	1
11100	H	62.39279	101.71956	64.67154	-2285.35201	-16.03896	-1956.23031	1
11101	H	61.78773	101.56505	62.98659	3108.53887	2371.49077	1630.07466	1
11102	C	63.81606	100.76872	63.28128	860.19452	-1029.55108	-1031.78584	1
11103	C	64.75748	100.94499	62.24941	-35.48074	-240.67963	-212.66728	1
11104	H	64.76209	101.79223	61.54518	3135.51994	1663.86651	-3722.34557	1
11105	C	65.87447	100.07335	62.28640	367.91119	699.63192	622.91969	1
11106	H	66.55274	100.44585	61.54299	1381.53458	-2581.49246	770.75236	1
11107	C	66.13252	99.13198	63.24972	-295.46006	58.10350	-570.92727	1
11108	O	67.31466	98.35760	63.24524	155.94314	-487.77632	414.78632	1
11109	H	67.44121	98.06852	62.27149	1477.38790	-1002.85619	3587.70584	1
11110	C	64.01778	99.85910	64.37946	188.38748	-789.08027	955.99833	1
11111	H	63.27486	99.79989	65.17366	1424.95271	1338.62574	1889.81701	1
11112	C	65.15127	99.05143	64.29726	449.55541	3.77414	396.85749	1
11113	H	65.46982	98.34451	65.13137	-2725.52549	-1925.82065	-289.58965	1
11114	C	62.80944	103.53901	61.67296	514.77564	558.04820	445.68621	1
11115	O	63.67492	104.01856	60.96332	428.13545	348.82321	-102.75920	1
11116	N	61.51832	103.32887	61.43574	-51.24309	776.68118	374.31197	1
11117	H	60.83766	102.91422	62.10552	-691.17508	746.99056	292.13966	1
11118	C	61.04354	103.49699	60.11057	267.23162	868.19760	-91.73922	1
11119	H	61.94739	103.18589	59.52076	-2170.96296	1689.80148	-3510.06995	1
11120	C	59.62039	102.76758	59.90675	413.52361	124.48386	-54.49285	1
11121	H	58.93260	103.46420	60.42271	-2951.88448	2097.30721	60.09608	1
11122	O	59.60684	101.54450	60.64423	210.82411	423.54190	-91.62728	1
11123	H	59.42804	101.89278	61.55348	936.04003	-1061.39995	-2545.85953	1
11124	C	59.43044	102.84164	58.34058	-174.68895	157.22758	672.16252	1
11125	H	58.47877	102.52081	57.93813	-1162.28084	3230.74108	2249.34241	1
11126	H	60.08821	102.18789	57.81610	-751.46382	3029.05168	751.68371	1
11127	H	59.57132	103.90916	57.89876	-758.31645	-565.93566	-3005.79959	1
11128	C	60.64193	105.08696	60.15795	204.28305	-325.20123	340.12916	1
11129	O	59.53986	105.46471	59.84136	144.55543	-112.79043	126.88916	1
11130	N	61.73614	105.89431	60.20437	890.30116	-431.21185	357.39776	1
11131	H	62.74937	105.57860	60.29292	-1299.54456	-1521.56650	-1800.50783	1
11132	C	61.55551	107.22336	60.72905	428.36088	-350.02521	-710.77998	1
11133	H	60.81266	107.76589	60.17832	632.29094	2307.64477	3841.34305	1
11134	C	60.88709	106.96321	62.20172	606.23961	-35.24950	-699.84304	1
11135	H	61.07831	105.93236	62.61677	1905.48418	1056.09185	2029.40090	1
11136	H	61.31812	107.58869	63.05323	2451.49126	612.85789	-938.45737	1
11137	C	59.42774	107.36363	62.17581	124.17860	1151.32878	265.75585	1
11138	H	58.91755	106.95431	61.28744	2040.58174	-755.30713	971.26373	1
11139	H	58.94913	107.03719	63.14855	-1054.20832	-428.99845	-2260.28306	1
11140	C	59.02873	108.94312	61.98732	352.55903	-428.69889	300.37233	1
11141	O	57.89530	109.33673	62.32709	397.01454	-589.68386	420.80850	1
11142	O	59.90425	109.65515	61.48713	61.65027	226.85593	381.10453	1
11143	C	62.94939	107.97763	60.73569	502.98499	-54.02938	-77.09174	1
11144	O	64.08413	107.57074	60.48221	-363.56042	323.11782	-497.73454	1
11145	N	62.55209	109.16864	61.31105	678.68854	932.59153	-378.43437	1
11146	H	61.57279	109.13090	61.72444	1334.48772	173.01289	1575.76267	1
11147	C	63.63325	109.80085	62.02465	-827.35378	-73.56550	-467.92244	1
11148	H	64.51336	109.61606	61.40195	491.63715	-2699.44547	-3568.66855	1
11149	C	63.27367	111.31393	62.16935	732.72268	344.01473	-211.78310	1
11150	H	63.96184	111.86744	62.90968	2949.72344	788.65084	-1464.19379	1
11151	H	62.24083	111.40782	62.53153	-810.39613	-1100.72112	1409.25586	1
11152	C	63.64258	112.17985	60.90019	80.92316	-1023.00586	-475.86970	1

11153	H	63.20284	111.79131	59.97962	391.22140	1102.37084	-2619.28236	1
11154	H	63.29633	113.23326	61.03109	-613.71168	840.87620	-3430.85526	1
11155	C	65.28594	112.23295	60.62369	808.84398	303.83824	988.38937	1
11156	O	65.63951	113.16692	59.92292	-581.17834	554.26975	-495.54508	1
11157	O	66.03489	111.31440	60.93844	131.48717	-225.00337	-269.50426	1
11158	C	63.95371	109.08637	63.48557	247.20240	-431.21688	38.59615	1
11159	O	63.09802	108.77629	64.24979	164.17168	-42.07442	-155.88497	1
11160	N	65.28217	109.36218	63.68259	106.91530	75.70519	-592.50668	1
11161	H	65.76602	109.82036	62.87560	2887.13733	-1366.94440	-2667.81325	1
11162	C	66.07973	108.29419	64.34007	-189.82371	23.53692	-453.43481	1
11163	H	65.33549	107.90235	65.04248	427.37409	3784.79439	196.59716	1
11164	C	66.31038	107.28446	63.15976	470.27620	-884.01850	-1147.71114	1
11165	H	65.37174	107.23452	62.63415	-2349.26054	1408.77902	2260.33801	1
11166	H	67.02343	107.88343	62.44661	699.79860	1035.50091	-138.12947	1
11167	C	66.78780	105.86551	63.59701	13.94616	101.28548	-178.73128	1
11168	H	65.96701	105.19452	63.92317	-490.85749	275.73456	398.38031	1
11169	H	67.49548	105.91456	64.44161	2376.03408	1523.87803	692.93109	1
11170	S	67.58522	105.25970	62.00698	-310.92447	353.72983	260.35443	1
11171	C	66.29875	105.78773	60.80891	584.05443	-655.75859	168.31595	1
11172	H	65.24554	105.42126	60.99702	-64.49375	1358.74540	-545.09661	1
11173	H	66.39682	105.30264	59.79649	715.37746	1899.88409	3684.30489	1
11174	H	66.26519	106.93660	60.58952	462.92215	323.01778	-2030.36109	1
11175	C	67.51069	108.83987	64.87765	-50.45770	-148.52743	-496.74390	1
11176	O	68.17743	109.68376	64.33386	-111.78553	-239.63483	-135.45025	1
11177	N	67.83716	107.99639	65.85650	-314.41201	11.87640	223.94481	1
11178	H	67.25303	107.23335	66.17321	2456.45333	-70.93931	-106.97024	1
11179	C	69.06862	108.26654	66.55862	-620.75323	51.30698	90.32566	1
11180	H	69.04411	109.35314	66.44481	118.35733	-2860.11758	-943.61925	1
11181	H	68.92008	107.89839	67.62911	288.06842	-463.89794	71.22159	1
11182	C	70.13040	107.39098	65.73223	134.41312	742.27315	-51.83872	1
11183	O	70.34364	106.24151	66.06017	555.41416	-30.57911	-189.68535	1
11184	N	70.74235	108.13849	64.74768	349.02444	-0.79902	-351.32120	1
11185	H	70.14897	108.99964	64.65151	654.49338	822.76792	1297.44170	1
11186	C	70.76794	107.29642	63.53774	-281.36860	-82.13553	857.97007	1
11187	H	69.91966	106.54143	63.78304	-1253.92820	2224.86621	1904.30450	1
11188	C	70.19145	108.14460	62.35806	182.41299	-152.66610	-899.53346	1
11189	H	69.17303	108.52340	62.64822	-569.78634	1797.42665	-1288.97007	1
11190	H	70.84286	109.02572	62.19314	-1281.85121	108.62635	-4251.36325	1
11191	O	69.85423	107.40081	61.13836	493.41561	19.04452	-604.10443	1
11192	H	69.11721	106.73968	61.51875	-553.61406	1525.50276	2706.93129	1
11193	C	72.22166	106.58528	63.32815	-391.50050	126.41683	-320.03716	1
11194	O	73.01903	106.91541	62.41679	488.00182	828.35011	-156.81582	1
11195	N	72.23459	105.66034	64.22370	882.70265	-235.09174	-757.93151	1
11196	H	71.44086	105.54535	64.83944	-1025.93405	-1043.40405	190.59989	1
11197	C	73.37929	104.75056	64.18004	143.93387	-199.22632	380.41416	1
11198	H	73.23563	104.42112	63.13351	-1712.35828	-356.51973	-1772.23857	1
11199	H	74.28840	105.35372	64.28916	3754.01110	-1394.16163	153.22813	1
11200	C	73.09972	103.60827	65.26525	-201.10451	-152.34894	-527.42847	1
11201	O	72.02840	102.99606	65.21989	-47.06171	26.44443	79.10360	1
11202	N	74.16807	103.30531	65.99753	427.91866	-87.51899	-399.97403	1
11203	H	74.96411	103.94607	66.01817	-432.44016	1113.97898	1145.90603	1
11204	C	73.76727	102.83794	67.33038	-229.79980	-32.77877	445.86577	1
11205	H	72.74978	102.36428	67.10848	2614.22543	1714.33716	-2000.35153	1
11206	C	74.94424	101.89957	67.69541	434.83143	424.05840	564.64060	1
11207	H	74.57644	101.16468	68.47657	268.11154	2116.31864	655.45205	1
11208	H	75.79831	102.43551	68.14942	828.99482	-1508.21808	-411.39966	1
11209	C	75.63544	101.03519	66.40974	350.34096	-95.39365	-239.19871	1
11210	O	76.87638	101.24361	66.43193	638.73423	-541.66347	600.35399	1
11211	O	74.98167	100.35225	65.64339	-450.27898	397.13232	-117.71534	1
11212	C	73.63056	104.00366	68.44834	-268.18714	736.47906	33.87035	1
11213	O	74.17498	103.92513	69.51924	-1371.64737	-350.62952	413.08887	1
11214	N	72.76267	104.88411	67.92287	-282.93065	524.19815	-634.79208	1

11215	H	72.33453	104.71188	67.00539	-897.48876	3514.36989	277.74120	1
11216	C	72.41281	106.02586	68.72693	517.36805	-991.48291	-539.17884	1
11217	H	73.09290	106.04871	69.56047	-1537.74226	-480.32414	3207.13188	1
11218	C	72.70430	107.32393	67.83459	353.64624	-340.71642	-294.04379	1
11219	H	72.13574	108.22231	68.09624	452.70376	-450.69735	3585.50234	1
11220	H	72.46637	107.15850	66.72420	23.22476	951.71328	1392.39576	1
11221	C	74.19723	107.63864	68.02934	613.23938	583.10188	143.74862	1
11222	C	75.27182	106.90277	67.43285	751.95634	-295.07013	307.13935	1
11223	H	75.14895	106.19035	66.66201	1142.85713	2504.04283	2050.14484	1
11224	C	76.52376	106.92914	68.02091	109.49306	-77.39139	305.64294	1
11225	H	77.44803	106.33575	67.65336	1230.29923	-102.24661	1289.03881	1
11226	C	76.76920	107.69322	69.19466	641.52273	319.80942	255.95251	1
11227	O	78.15399	107.78843	69.63017	-24.15643	-479.55967	1000.96270	1
11228	H	78.47595	106.96281	69.31598	927.23231	-974.09399	497.07067	1
11229	C	74.41895	108.40583	69.22701	117.04403	-960.95032	601.80689	1
11230	H	73.62302	108.96338	69.62120	125.52484	-2079.98127	-2891.42308	1
11231	C	75.67404	108.40569	69.80481	848.15901	125.37063	301.85225	1
11232	H	75.84697	108.90832	70.75393	1238.03444	1026.65926	-650.84250	1
11233	C	70.84363	105.83231	69.14363	1246.21488	-324.55033	231.60689	1
11234	O	70.35511	106.77954	69.74485	314.82764	-888.34747	894.84399	1
11235	N	70.32520	104.62703	68.92026	925.25489	-1476.49988	229.10498	1
11236	H	70.86460	103.87856	68.44862	134.55406	1996.93474	1810.17334	1
11237	C	68.91772	104.35292	69.09103	-357.93938	85.55586	-54.96057	1
11238	H	68.46239	104.99885	69.88411	-2074.25025	444.27978	-327.55321	1
11239	C	68.56679	104.74862	67.62645	-613.06506	-862.98718	-766.75482	1
11240	H	69.13612	105.65673	67.27780	4281.62785	2033.90823	-1075.41760	1
11241	H	68.92997	103.91045	66.99055	1692.03310	2684.63519	1773.61381	1
11242	C	66.95477	104.86529	67.50216	-394.81754	-454.91760	-169.98286	1
11243	O	66.51626	105.96492	67.05635	903.37883	135.62580	-516.05756	1
11244	O	66.15551	104.01331	67.94720	124.73162	-599.68039	130.37371	1
11245	C	68.66492	102.74585	69.24550	68.53825	433.61574	70.88525	1
11246	O	69.41347	101.89461	68.72533	1336.51884	239.87426	-164.86074	1
11247	N	67.53202	102.54680	69.88722	-355.88764	50.42948	-188.06551	1
11248	H	67.31110	103.38335	70.40858	2597.87780	3681.47007	-3510.81325	1
11249	C	67.02081	101.24792	70.23352	-289.52377	-714.24095	34.71553	1
11250	H	67.86083	100.60114	70.47117	151.68883	2212.10900	-83.86733	1
11251	C	66.02655	101.65979	71.41761	-9.46592	555.45590	1136.46264	1
11252	H	66.52851	102.26635	72.16628	2690.63739	-2512.72398	-2044.44482	1
11253	H	65.79558	100.69054	71.93172	-108.30834	805.79104	691.98488	1
11254	O	64.77839	102.42420	71.33780	-43.37523	-37.70625	-24.82557	1
11255	H	64.30413	101.87632	70.69978	1184.99759	-729.72001	-60.83379	1
11256	C	66.14553	100.67065	69.03041	92.54136	766.81032	618.15959	1
11257	O	64.91528	100.54362	68.92943	-838.58278	81.22085	516.79002	1
11258	N	67.05129	100.41546	68.12748	-252.38262	-741.61952	277.97045	1
11259	H	68.07923	100.67745	68.34061	3839.67493	1501.27973	-1717.78142	1
11260	C	66.83293	99.54039	67.04729	251.29085	31.74792	-238.50630	1
11261	H	65.73162	99.26425	67.07822	-1580.75676	1787.90157	2357.78623	1
11262	C	67.28141	100.35985	65.70253	393.14486	-135.96802	449.22077	1
11263	H	68.36742	100.45320	65.67047	408.54924	-196.69125	-1241.45080	1
11264	H	67.12310	99.76102	64.76062	-313.87888	-1090.05390	-764.64669	1
11265	C	66.59946	101.75610	65.62345	280.17497	-1401.21201	-77.40187	1
11266	H	65.51149	101.73589	65.81381	-2689.85901	-1469.51149	420.84990	1
11267	H	66.96482	102.15780	66.59509	599.08910	-152.87685	-1144.26058	1
11268	S	67.15497	102.52605	64.05992	-218.62356	-66.06186	-166.58232	1
11269	C	68.92249	102.16217	63.91773	46.70486	-394.45125	-98.84073	1
11270	H	69.20302	101.12467	63.77294	14.53957	1644.09218	30.74574	1
11271	H	69.40781	102.50678	63.00117	-252.53873	-1666.32713	1708.40360	1
11272	H	69.59393	102.45442	64.72459	369.38470	-104.21060	2282.85777	1
11273	C	67.82540	98.26321	66.95846	233.99919	634.35048	-143.72653	1
11274	O	69.03724	98.41170	67.16851	-30.79338	-7.99306	-23.90546	1
11275	N	67.15503	97.21565	66.49559	1048.84349	375.55164	-443.54356	1
11276	H	66.14422	97.26541	66.35083	3106.92371	-1453.11594	-1677.36650	1

11277	C	67.86614	95.98881	66.63024	161.67721	-435.89911	1263.04488	1
11278	H	68.44611	96.00743	67.53331	1239.56547	399.62995	3090.17357	1
11279	C	66.62745	94.97933	66.56833	-22.80054	92.70211	451.64518	1
11280	H	65.71999	95.29891	66.04500	468.05641	963.00803	-595.11784	1
11281	H	66.91235	94.11534	65.89597	-790.23620	51.39172	253.32676	1
11282	C	66.32728	94.58814	68.05974	-921.58687	32.72127	-152.90848	1
11283	H	65.30003	94.14983	68.19590	-1830.07493	3299.40627	2001.80795	1
11284	H	66.31594	95.48493	68.72842	-1703.99975	-2188.74565	58.45502	1
11285	C	67.27256	93.39899	68.50984	415.87422	394.48054	451.61632	1
11286	H	68.29487	93.57836	68.21212	-517.94278	2843.59263	1620.38701	1
11287	H	66.98738	92.43749	68.05680	-1926.41545	-734.41503	242.85655	1
11288	C	67.26154	93.27874	70.07948	-315.76774	-344.83956	-410.33961	1
11289	H	67.66023	92.26693	70.40717	2146.14349	2648.62169	475.40115	1
11290	H	66.25078	93.42775	70.57397	43.84899	1406.69041	-560.66045	1
11291	N	68.12615	94.34746	70.64732	-357.45933	736.85635	-26.25432	1
11292	H	68.15130	94.34349	71.70228	-959.42785	-1312.74203	3890.04788	1
11293	H	69.32194	94.17276	70.41352	64.08081	-1238.44023	177.82887	1
11294	H	67.88021	95.39016	70.41054	2026.92808	653.96691	819.40095	1
11295	C	68.77974	95.80567	65.30545	-68.43240	-282.12631	29.69206	1
11296	O	68.43682	94.91988	64.54145	-661.50531	-44.12424	380.17086	1
11297	N	69.69114	96.77802	65.25534	-139.75103	-14.30604	362.34367	1
11298	H	69.92088	97.42801	65.96206	-884.17647	1730.95089	-2079.61381	1
11299	C	70.74081	96.57353	64.28069	230.66091	-508.47265	-62.68953	1
11300	H	70.80931	95.49264	64.11806	1779.40337	275.37781	1862.28894	1
11301	C	70.10298	97.23460	62.98608	-84.60383	-646.29580	219.44332	1
11302	H	69.03825	96.89064	62.89464	-4305.66583	1213.04793	-280.54886	1
11303	H	70.16914	98.32631	63.19315	423.16561	-1781.98860	-234.46853	1
11304	C	70.92904	96.75308	61.75900	-263.73439	404.16497	544.05469	1
11305	H	70.28460	95.95446	61.33359	1010.79569	-4087.27651	-2617.12887	1
11306	H	71.89886	96.35153	61.96373	2139.91577	-1138.32203	812.55705	1
11307	C	70.88284	98.14992	60.91580	83.25741	-130.43483	-62.86435	1
11308	O	71.22611	97.98068	59.71860	229.99123	152.63466	263.04383	1
11309	O	70.46836	99.20481	61.41362	-250.11485	-103.93697	689.77311	1
11310	C	72.04007	97.41959	64.82450	502.82035	-402.58522	194.94022	1
11311	O	73.09675	97.05417	64.31491	-958.76038	-162.61653	-595.52374	1
11312	N	71.78383	98.45540	65.60489	372.01245	14.11304	-334.79264	1
11313	C	70.90442	99.58339	65.23804	257.65951	184.13489	-202.85616	1
11314	H	69.84263	99.23321	65.03439	-739.18443	3741.28380	-432.68576	1
11315	H	71.16419	99.97566	64.22983	626.97979	-2982.76850	4033.10978	1
11316	C	72.71304	98.74872	66.67588	-353.53637	405.52377	-404.97551	1
11317	H	73.63063	98.53413	66.12374	352.29602	161.68376	-2480.28466	1
11318	C	72.45631	100.28478	67.05442	-224.32335	-502.44172	-567.76142	1
11319	H	73.13823	101.01363	66.50255	2811.50815	-925.63415	446.99879	1
11320	H	72.42195	100.37083	68.14386	-3155.22934	-1754.36859	-156.66152	1
11321	C	71.00278	100.53088	66.49564	199.39940	-822.80520	-4.85614	1
11322	H	70.74465	101.60972	66.26808	2159.86850	-1173.27392	1502.99619	1
11323	H	70.35177	100.12555	67.32751	-3457.70599	-1682.23505	41.94081	1
11324	C	72.84686	97.59318	67.85654	677.73157	712.68530	38.46164	1
11325	O	72.37887	97.89508	68.90687	169.86118	421.82225	835.67013	1
11326	N	73.74846	96.67941	67.53024	101.43347	-290.29677	-623.65850	1
11327	H	74.10369	96.66328	66.50598	1363.39340	-2165.54807	-1840.48451	1
11328	C	73.52464	95.35712	68.12944	-295.72298	898.08525	-298.68095	1
11329	H	73.23876	95.62027	69.21155	1378.28976	3012.40034	-1202.48673	1
11330	C	72.63584	94.41979	67.30026	-230.24819	-225.95993	918.20035	1
11331	H	72.63344	94.72466	66.17112	-1442.28104	-2695.04920	487.90383	1
11332	H	73.07467	93.34841	67.28221	2071.90603	1520.76862	-1950.99572	1
11333	S	71.01080	94.62013	68.07644	-328.27363	177.70906	-86.57197	1
11334	C	75.02284	94.58822	68.21039	534.94857	-446.13637	34.97189	1
11335	O	75.15297	93.52080	67.65379	99.60239	-268.08605	-360.24208	1
11336	N	76.04303	95.30371	68.71406	53.04421	-160.74423	910.97413	1
11337	H	75.68649	96.23074	68.99587	3352.50010	45.34741	-2702.06897	1
11338	C	77.26189	94.69038	69.10898	436.83570	-296.42516	-796.34515	1

11339	H	77.23403	93.61961	68.82971	1000.42378	-1639.82358	-1897.64634	1
11340	C	78.49906	95.45921	68.45472	-320.67938	420.00699	570.22313	1
11341	H	79.44574	94.95672	68.51681	1143.12573	608.20009	-1391.44073	1
11342	H	78.54609	96.31958	69.17440	2333.81558	-1839.33523	-1065.51832	1
11343	C	78.17579	95.84504	67.00851	-83.39429	-133.51862	493.90657	1
11344	C	79.10889	95.36106	66.00767	-868.18030	550.61057	424.39634	1
11345	H	79.97637	94.73310	66.38056	-1771.68444	2598.98699	1387.99276	1
11346	C	79.02932	96.03083	64.78161	362.00835	-972.49609	822.55677	1
11347	H	79.83499	95.70499	64.09403	2303.87754	1843.38201	1133.80563	1
11348	C	78.07012	97.02229	64.45891	76.29605	-832.94021	646.71875	1
11349	H	77.99201	97.35335	63.41028	-3861.54253	1767.07693	751.63010	1
11350	C	77.31420	96.99232	66.78515	685.81525	539.33723	-91.87864	1
11351	H	76.70479	97.40657	67.55700	1320.53512	-910.57421	-665.32631	1
11352	C	77.22953	97.57242	65.47036	-273.29685	-466.38828	564.89622	1
11353	H	76.50788	98.31646	65.22122	-888.67334	2707.24612	2044.03437	1
11354	C	77.29327	94.84498	70.70580	-10.84967	834.19885	-239.60633	1
11355	O	77.65111	95.92240	71.20957	356.94753	70.76114	-138.78146	1
11356	N	77.13245	93.68021	71.34718	-388.84723	-870.35964	-41.07583	1
11357	H	76.91396	93.01979	70.60891	1331.86455	1219.35968	2583.12181	1
11358	C	76.42655	93.65284	72.60333	481.51325	68.76401	88.85280	1
11359	H	75.52338	94.34970	72.40318	1508.65913	943.86221	2640.27256	1
11360	C	76.06786	92.10470	72.82220	275.73804	-392.60452	432.86011	1
11361	H	76.54351	91.83017	73.81599	599.10260	-1646.82527	-2478.77429	1
11362	H	76.65660	91.52418	72.04400	-2492.41754	-621.35266	-1041.32385	1
11363	C	74.56110	91.78880	72.79106	393.98922	-710.13741	-219.79879	1
11364	H	73.99570	92.51368	72.20639	662.96904	-3619.65712	-1604.36106	1
11365	H	74.43564	90.71188	72.42748	-676.42934	-476.96797	1751.73158	1
11366	C	74.13549	92.12913	74.32510	-273.50151	351.56797	765.69232	1
11367	H	74.54607	93.11611	74.66390	216.69680	316.45294	-2057.09060	1
11368	H	74.23014	91.25377	75.04143	2673.50917	-809.49044	-1860.03011	1
11369	N	72.79061	92.29889	74.05164	578.76202	-141.84791	873.34805	1
11370	H	72.58989	93.31629	73.93334	-1563.28473	-32.77979	756.19429	1
11371	C	71.79685	91.47911	73.93251	365.42825	-563.34365	-315.46510	1
11372	N	72.09286	90.16789	74.03933	299.47555	-499.05273	95.60688	1
11373	H	73.08322	89.82147	74.14030	4536.90019	-1644.92287	-2091.14595	1
11374	H	71.42044	89.32770	73.91754	-408.98225	-1305.96704	-296.01883	1
11375	N	70.56546	92.14338	73.69237	-908.19951	-54.02008	-628.54682	1
11376	H	70.30127	93.14818	73.85028	-308.46517	1458.06751	-287.14190	1
11377	H	69.74097	91.57950	73.39945	1726.89836	250.08968	956.28171	1
11378	C	77.24245	94.29572	73.79936	468.48499	114.14667	-432.57972	1
11379	O	76.93592	94.11984	74.99707	-597.47414	-8.33621	358.31735	1
11380	N	78.33717	94.86267	73.36601	494.09257	-240.61375	705.83507	1
11381	H	78.59841	94.92796	72.33805	1085.70782	1513.90196	-446.32169	1
11382	C	79.09552	95.65578	74.25406	274.65487	600.21377	941.94363	1
11383	H	79.79482	96.09394	73.60659	-2962.69170	-1015.73164	-2221.57572	1
11384	C	78.05908	96.72921	74.88136	-513.98327	82.86138	-225.51852	1
11385	H	77.01687	96.30629	74.91963	2277.77546	-1752.62787	569.20428	1
11386	H	78.29863	97.08584	75.87556	-2195.98452	-1578.69190	1658.79225	1
11387	C	78.23229	97.93276	73.90111	970.08894	-480.64912	752.38164	1
11388	H	77.49603	98.73525	74.05717	254.07479	108.78987	-853.56107	1
11389	H	78.02191	97.68394	72.82268	969.10678	37.65380	1.18004	1
11390	C	79.77194	98.45722	74.25103	-74.43353	-447.99158	-189.55178	1
11391	O	80.41880	97.84684	75.12125	288.66704	421.00229	-201.64734	1
11392	O	80.06800	99.39882	73.52676	-456.46626	-1146.49405	-152.42248	1
11393	C	79.74226	94.60515	75.29595	288.20682	-29.03680	-519.58203	1
11394	O	79.77528	93.41151	75.20986	890.68934	-879.89428	-137.05639	1
11395	N	80.41559	95.36526	76.17821	-393.51440	241.48654	-1282.77550	1
11396	H	80.18919	96.41357	76.17162	-2243.37318	795.58576	-1458.04252	1
11397	C	80.71059	94.71703	77.42307	844.93414	-33.88872	-817.00611	1
11398	H	80.27895	93.67328	77.55180	-1209.81864	-11.89462	1381.02741	1
11399	C	82.33699	94.84849	77.51916	297.75473	1192.88296	500.07913	1
11400	H	82.71053	95.01951	78.49902	619.56678	3109.70055	229.52586	1

11401	H	82.75533	95.71274	76.90872	64.44594	961.99456	-3241.13612	1
11402	C	82.67408	93.43985	76.93440	-673.92328	772.25234	423.17725	1
11403	H	83.74576	93.36391	76.56226	-213.74939	-634.98583	1384.03033	1
11404	H	81.98536	93.20657	76.05656	-144.38205	-303.78358	-921.25032	1
11405	C	82.41254	92.35248	78.14345	830.78303	394.75272	-22.42168	1
11406	O	83.35955	91.78444	78.66391	-197.25227	-508.00322	-272.75463	1
11407	O	81.21649	92.09634	78.55454	208.20973	-497.81389	713.58826	1
11408	C	80.21698	95.68750	78.60109	303.10548	17.84436	-743.03084	1
11409	O	80.42598	96.86050	78.57732	59.27966	66.00758	-409.10113	1
11410	N	79.85514	94.92939	79.69217	-670.55085	-846.99243	291.41002	1
11411	H	79.93079	93.93675	79.56463	-3436.54819	806.11043	2954.16571	1
11412	C	79.53670	95.59449	80.88683	-614.02787	612.90552	441.72139	1
11413	H	79.22368	96.63102	80.59859	1184.89186	-3115.39747	1552.85648	1
11414	C	78.46623	94.61226	81.48924	232.44503	-286.03837	466.25942	1
11415	H	78.92357	93.57927	81.34688	-848.24764	-454.05197	-2245.88323	1
11416	H	77.49694	94.63965	80.90213	294.87859	-685.80184	82.10260	1
11417	C	78.03874	94.78117	83.00671	736.09837	-372.89636	251.89513	1
11418	O	78.00270	95.95865	83.37221	918.79314	567.47417	194.32690	1
11419	N	77.83682	93.63774	83.60683	-525.80527	259.15303	75.14851	1
11420	H	77.98011	92.71117	83.17349	-1757.52290	-2527.87859	832.01751	1
11421	H	77.79821	93.57329	84.63501	431.62780	1547.68321	-2232.98641	1
11422	C	80.85251	95.44245	81.88383	307.13946	459.76288	1212.31759	1
11423	O	81.30990	94.35107	82.27328	-486.45472	327.39260	837.58809	1
11424	N	81.36480	96.62149	82.09259	557.14458	15.96389	519.64719	1
11425	H	80.88634	97.43063	81.70130	-770.27641	863.93471	-2246.74092	1
11426	C	82.64851	96.67114	82.76415	-1190.70117	389.60163	157.78664	1
11427	H	83.11140	95.67521	82.47865	-2444.13731	-249.25234	-723.13339	1
11428	C	83.37546	98.01988	82.46011	-46.25847	-328.47089	-28.90800	1
11429	H	83.45512	98.06683	81.35225	-553.61455	545.14948	1672.53127	1
11430	H	82.83506	98.89740	82.90733	1405.98320	455.28287	1315.49029	1
11431	H	84.40937	98.07867	82.78246	83.27796	-2573.33601	5126.59496	1
11432	C	82.42284	96.65625	84.37860	-573.72812	1523.82412	-29.61310	1
11433	O	82.58524	97.56734	85.17034	70.66431	-262.52996	337.12420	1
11434	N	82.11326	95.41220	84.72066	535.43481	-292.96572	-706.53520	1
11435	H	81.96991	94.68081	83.99833	2095.27727	280.55157	414.99762	1
11436	C	81.31326	95.36593	85.93960	819.45862	184.17419	-67.87842	1
11437	H	81.95424	96.08358	86.47464	1139.44780	-542.49873	2716.23890	1
11438	C	79.90518	95.93529	85.45179	1541.76247	-1114.84779	263.09155	1
11439	H	79.41238	95.17328	84.69315	-1769.30675	660.00079	2700.10018	1
11440	H	80.16191	96.81967	84.80175	87.26739	-1245.81385	-375.66445	1
11441	C	79.02647	96.24642	86.69185	543.23257	1133.51821	-1374.50448	1
11442	O	79.26443	96.17264	87.86898	794.97601	-47.76832	229.19705	1
11443	N	77.82197	96.50472	86.10983	366.42941	-304.03278	1051.43166	1
11444	H	77.67628	96.44916	85.06150	1672.77739	2169.37344	2509.43802	1
11445	H	76.99669	96.94537	86.49000	1091.04405	696.18253	996.36093	1
11446	C	81.37512	93.82256	86.46255	50.74411	-720.58329	40.35588	1
11447	O	82.01148	93.40347	87.38380	-317.51175	-500.24867	-31.13496	1
11448	N	80.52868	93.07061	85.67567	296.27155	529.80057	318.07118	1
11449	H	79.91851	93.46344	84.92181	-344.75220	-1874.06393	-2056.24145	1
11450	C	80.48620	91.71550	86.08841	-304.82927	688.56816	993.09886	1
11451	H	80.77324	91.53789	87.11840	2164.08262	5574.24335	78.75699	1
11452	C	79.11593	91.03322	85.65839	634.76314	246.06392	1067.36430	1
11453	H	79.25605	89.94521	85.71328	-536.85069	-40.65094	-2150.91411	1
11454	H	78.95628	91.19233	84.59339	1224.01963	-1954.96470	-3145.00098	1
11455	C	77.82072	91.54644	86.41048	695.37517	393.69065	-311.61478	1
11456	C	76.57207	91.31724	85.70441	541.00234	-271.92095	42.27348	1
11457	H	76.59075	90.75875	84.72240	-5003.01819	1913.01303	-3565.51650	1
11458	C	75.42721	91.76552	86.32107	102.27512	327.17349	-393.90421	1
11459	H	74.48701	91.42158	85.90779	553.23530	-1477.46684	-665.91928	1
11460	C	75.51560	92.50256	87.55649	432.96990	848.60269	-416.31617	1
11461	H	74.58202	92.92256	88.00801	-3392.08628	2971.84169	2185.76719	1
11462	C	77.94612	92.25476	87.61706	515.29408	-455.65852	-333.67203	1

11463	H	78.93278	92.49136	87.90969	1587.82556	806.62594	-622.21915	1
11464	C	76.72443	92.77268	88.19256	1474.26888	-1118.31851	541.13537	1
11465	H	76.67939	93.30798	89.17986	593.66685	-1375.44247	954.86653	1
11466	C	81.44235	90.73996	85.13067	164.23022	-565.82092	-403.02775	1
11467	O	81.81828	89.60468	85.40251	-419.45843	-103.60391	-436.16583	1
11468	N	81.56585	91.40209	84.01124	-352.36359	220.65365	632.85928	1
11469	H	81.10019	92.29300	83.96610	3478.39316	770.37576	829.22093	1
11470	C	81.81026	90.70659	82.77971	-609.31726	-120.33158	-243.50671	1
11471	H	81.37410	89.74252	83.12468	-2294.20912	2117.07118	-710.07520	1
11472	C	81.17882	91.45579	81.51895	221.94831	-230.95294	-338.97845	1
11473	H	81.54716	91.01722	80.56320	330.93681	2825.56823	-3472.16174	1
11474	H	81.60495	92.49981	81.65592	-321.48524	1595.97642	-2905.60177	1
11475	C	79.62744	91.33323	81.50901	-199.75125	845.20715	-70.29301	1
11476	O	78.81381	91.46075	82.44563	-131.24983	-243.87615	231.77711	1
11477	N	79.16142	91.23619	80.22541	-292.53363	-214.84751	-91.84691	1
11478	H	79.85582	91.51892	79.50121	2365.79957	-1078.63719	-1808.33385	1
11479	H	78.26068	91.71462	79.98303	767.53665	-335.33227	-775.30272	1
11480	C	83.42360	90.55036	82.62484	-245.32590	213.11428	336.09328	1
11481	O	83.82206	89.81004	81.74894	219.53648	537.45653	164.89408	1
11482	N	84.06511	91.41981	83.39191	523.78021	-72.56380	-314.89073	1
11483	H	83.45657	91.97448	84.01527	915.23011	-3003.29133	-152.41858	1
11484	C	85.47987	91.40157	83.41841	514.57968	353.26018	-382.13814	1
11485	H	85.69835	90.41124	82.87607	-3221.82827	-1149.33658	311.86338	1
11486	C	86.08262	92.71603	82.78334	-169.17693	-51.15067	422.72072	1
11487	H	87.20801	92.68992	82.62164	2227.31746	5049.70118	886.53879	1
11488	H	85.76935	93.65377	83.34811	2254.51980	2371.27650	-225.21125	1
11489	C	85.56141	92.84518	81.33311	-427.03376	561.99834	-244.26773	1
11490	H	84.47330	92.69958	81.27427	-2477.72595	495.34039	2196.13846	1
11491	H	85.91792	91.94058	80.85249	1522.44215	1319.51912	-280.79977	1
11492	C	85.75983	94.13169	80.58304	234.57821	-340.23329	525.37574	1
11493	H	86.70746	94.70413	81.00787	2058.14685	-1230.19905	-1630.84457	1
11494	H	84.85565	94.76322	80.77732	-1322.84966	432.93313	-2681.38487	1
11495	C	85.78762	93.66259	79.07108	-502.41544	61.13171	22.72944	1
11496	H	86.71050	93.06289	78.84900	538.21076	-506.19232	-1076.68167	1
11497	H	84.87628	93.10857	78.66411	-1387.39874	-2294.76672	2499.73969	1
11498	N	85.85856	94.92234	78.31017	-400.59203	-243.89856	-631.84479	1
11499	H	85.15746	95.61010	78.57185	-1225.31757	1011.38627	223.96607	1
11500	H	85.83336	94.80048	77.34178	-26.79458	3429.39720	-3462.54216	1
11501	H	82.52832	98.60599	79.44460	1957.35547	-1696.37778	-1580.80164	1
11502	C	85.87667	91.29917	85.00630	-656.68327	-48.69138	131.04006	1
11503	O	86.99952	91.64269	85.34082	-642.20030	-113.48988	912.98838	1
11504	N	84.95950	90.63355	85.70741	-184.66276	-434.99060	-8.78085	1
11505	H	84.02987	90.39349	85.34613	812.62458	-1875.22501	242.32648	1
11506	C	85.26202	90.53420	87.12363	46.96894	724.27998	-526.86571	1
11507	H	86.32679	90.84437	86.97658	-1430.14349	-593.86160	-5083.72372	1
11508	C	84.56963	91.79369	87.80059	740.23894	-151.02669	-326.15397	1
11509	H	83.57611	92.09905	87.25581	-1370.69885	-2226.76296	-1885.89679	1
11510	C	84.22835	91.45222	89.28757	-319.46729	77.27926	112.53531	1
11511	H	83.88787	92.39998	89.88720	385.97517	860.08743	-83.23172	1
11512	H	85.07438	90.93345	89.79410	-296.00780	-643.01675	-469.96926	1
11513	H	83.36760	90.73779	89.36864	-1667.57712	1976.64421	-353.60463	1
11514	C	85.53997	93.02897	87.79376	560.64661	-225.04601	-335.55743	1
11515	H	85.56293	93.58543	86.86012	-322.95342	2807.53814	-1195.51979	1
11516	H	85.03118	93.74704	88.45226	-241.63079	-2366.06491	-3499.93880	1
11517	C	86.99509	92.62230	88.21889	875.54247	-723.98438	-157.82176	1
11518	H	87.64584	93.48823	88.57830	-235.86492	1762.40204	-3648.97080	1
11519	H	87.06131	91.86842	89.01157	-325.72652	-1252.04540	-419.95834	1
11520	H	87.47249	92.25320	87.29700	-183.13591	-2275.02910	-304.62135	1
11521	C	84.94275	89.00052	87.53926	-349.15418	113.14135	879.21519	1
11522	O	85.81082	88.30177	88.03899	142.56165	-310.17138	58.25017	1
11523	N	83.61761	88.79366	87.36803	477.96514	-495.26630	-283.28837	1
11524	H	83.07515	89.46669	86.82290	347.27302	2052.50466	-1008.18793	1

11525	C	83.25766	87.45041	87.77656	-272.16292	157.92721	346.74175	1
11526	H	83.85433	87.28529	88.70338	560.80942	2994.74999	-1586.58857	1
11527	C	81.69224	87.48938	88.04553	76.54641	613.82393	838.77748	1
11528	H	81.24740	87.84680	87.05602	-334.21064	-2651.98282	-1881.97423	1
11529	H	81.56540	88.25446	88.81850	-416.92601	646.55158	1204.96891	1
11530	C	80.91902	86.19862	88.51144	82.38758	-1347.30315	-805.11703	1
11531	C	80.17175	85.46432	87.54707	-113.83590	49.33001	153.63423	1
11532	H	80.19341	85.71766	86.44265	939.31247	-547.10901	2976.22042	1
11533	C	79.40000	84.34180	88.00890	148.59986	-886.08935	-155.61086	1
11534	H	78.84100	83.76780	87.28590	-323.95670	-2958.00140	1021.52142	1
11535	C	79.47800	83.93480	89.35490	-638.99266	453.47035	-466.37326	1
11536	H	78.96900	83.02580	89.64090	-632.11128	-440.06841	3050.41003	1
11537	C	80.97371	85.85117	89.88926	-173.47880	345.64588	-682.26845	1
11538	H	81.55404	86.41607	90.58274	267.47433	1683.48618	-338.60285	1
11539	C	80.30600	84.65280	90.26790	24.69251	-623.90608	-664.51674	1
11540	H	80.48200	84.28180	91.26690	-2373.94869	-1191.52542	-1686.07859	1
11541	C	83.56912	86.43630	86.54827	19.36746	100.17810	307.82461	1
11542	O	83.88045	85.26363	86.74237	-348.09155	384.44185	312.08642	1
11543	N	83.43273	87.00649	85.34615	-408.16943	291.97699	-998.55355	1
11544	H	82.97337	87.92924	85.35862	-1332.49050	-260.88052	-317.83713	1
11545	C	83.56022	86.27484	84.14466	-52.85214	-129.96311	93.85344	1
11546	H	82.75486	85.53600	84.33125	-1818.03325	-259.64653	1163.27761	1
11547	C	83.25325	87.23799	82.87141	599.31846	-124.21472	54.72017	1
11548	H	83.78308	86.86058	81.99439	4674.33787	794.17026	-1864.50793	1
11549	H	83.54699	88.29774	82.94201	-1434.66954	-34.61166	62.95397	1
11550	C	81.72290	87.20036	82.69007	-276.39415	-68.94024	464.91942	1
11551	H	81.39023	87.77140	83.60534	-1175.96624	250.08768	1079.20566	1
11552	C	81.57286	87.82507	81.24730	23.54488	-795.09570	126.64712	1
11553	H	82.15525	88.71242	80.97738	13.53142	-2785.62643	1889.97494	1
11554	H	80.54511	88.11782	81.09534	-1282.73676	-581.17038	1779.09678	1
11555	H	81.75408	87.05863	80.52671	-3273.40711	-1099.98688	2822.25289	1
11556	C	80.99207	85.81358	82.80247	-189.45726	668.54278	-62.46674	1
11557	H	80.96473	85.45148	83.82326	-2704.52722	2012.00317	3145.66827	1
11558	H	81.43856	85.04401	82.09515	2067.04558	-1799.38696	-1735.58538	1
11559	H	79.90353	85.98227	82.60372	-1639.25749	-3159.47536	89.09852	1
11560	C	84.92835	85.42613	84.07887	-40.76890	41.52512	82.86406	1
11561	O	84.87300	84.21580	83.92590	489.99464	-232.86132	573.85372	1
11562	N	86.09207	86.11645	84.20324	-132.65740	207.63224	837.82017	1
11563	C	86.06566	87.56451	84.16637	-156.54843	1354.77790	-457.40520	1
11564	H	86.14646	87.97179	85.17901	-296.54852	1272.20169	3933.27423	1
11565	H	85.21197	87.88444	83.55031	-1809.75797	-2306.79602	-3504.86744	1
11566	C	87.37242	85.51127	84.20600	-462.93494	-69.57352	97.50193	1
11567	H	87.36000	84.75980	83.39390	-1951.11782	-1726.41590	-1763.76122	1
11568	C	88.32645	86.78670	84.28881	151.98228	-69.36847	154.99286	1
11569	H	89.26953	86.53875	83.74327	-227.96448	-1480.07404	-2379.92353	1
11570	H	88.62532	87.10834	85.26540	3235.93536	365.23257	1639.91630	1
11571	C	87.48501	87.84048	83.50907	-398.36289	-1333.53834	123.11891	1
11572	H	87.77977	88.94664	83.56465	1702.08954	-1131.35377	235.73713	1
11573	H	87.50351	87.73811	82.41152	1121.44379	-3901.50156	-65.63749	1
11574	C	87.49300	84.44880	85.47990	485.99674	-771.15644	-23.99827	1
11575	O	88.17500	83.43780	85.31690	667.02038	338.23839	-253.58595	1
11576	N	86.94800	84.79480	86.61690	-351.21097	360.46375	-677.78243	1
11577	H	86.39371	85.66439	86.57860	-451.18448	1965.92666	-1546.28294	1
11578	C	86.99100	84.05980	87.81290	752.58343	418.51104	-299.86278	1
11579	H	88.04200	83.90580	88.00490	-1282.28310	1354.76212	-2533.49480	1
11580	C	86.54200	84.90880	89.03390	422.30738	559.35235	-583.29447	1
11581	H	85.43503	85.11032	88.93690	1269.65617	439.94997	2564.40618	1
11582	O	87.33741	86.12270	89.01471	343.51056	248.19543	-74.92673	1
11583	H	86.77832	86.88118	88.75541	273.23515	-394.72913	38.29735	1
11584	C	86.58800	84.13880	90.31390	-280.22500	861.65118	102.38256	1
11585	H	86.42200	84.88380	91.12190	-1792.57882	1437.36362	2149.15640	1
11586	H	87.58000	83.65880	90.45790	-432.47922	1218.71390	2868.08723	1

11587	H	85.87300	83.28880	90.33790	850.54544	-2923.52327	792.34485	1
11588	C	86.28000	82.71080	87.71290	352.70556	-609.86529	-578.89043	1
11589	O	86.82200	81.66680	88.07090	491.28648	-367.68551	-497.06357	1
11590	N	85.01900	82.70380	87.12790	152.03866	116.75225	-822.14685	1
11591	H	84.59100	83.60380	87.13890	-2670.47446	1533.40975	-644.55172	1
11592	C	84.34600	81.49680	86.73990	-169.54950	895.80157	-15.60477	1
11593	H	84.30700	80.75780	87.52590	2630.13013	725.45100	-1566.64054	1
11594	C	82.88500	81.78680	86.44690	476.61807	489.67358	603.74332	1
11595	H	82.91900	82.67580	85.78090	-1563.19923	-1396.76035	2345.99551	1
11596	C	82.17700	80.62380	85.67890	-681.83180	-555.91392	-239.82518	1
11597	H	81.07800	80.71880	85.54690	602.73017	-2089.52721	-2273.50360	1
11598	H	82.70400	80.35880	84.73790	465.57596	2498.61775	-1854.28546	1
11599	H	82.32100	79.72080	86.31090	1408.56024	-2171.16793	1788.91422	1
11600	C	82.07000	82.12980	87.72690	833.83245	-259.28105	262.57912	1
11601	H	81.10200	82.37580	87.23990	2009.33983	-1845.03907	-1567.35782	1
11602	H	82.53400	83.06080	88.11890	2001.44440	-772.01096	2301.40079	1
11603	C	81.94500	81.05480	88.81990	-711.29367	296.77117	-487.27733	1
11604	H	82.88100	80.59980	89.20790	-587.70429	3052.00527	-487.94852	1
11605	H	81.31400	80.20680	88.47790	2819.11105	-507.83191	1301.13253	1
11606	H	81.40000	81.55980	89.64590	-694.54622	-1642.16649	2592.12673	1
11607	C	85.05200	80.71580	85.59890	-4.22895	117.73405	-904.19678	1
11608	O	85.24900	79.52680	85.71490	33.01373	785.75877	71.55753	1
11609	N	85.49400	81.43280	84.53190	-389.96503	-638.06614	-391.75397	1
11610	H	85.40200	82.42480	84.48490	-912.91230	-3006.00745	-169.51857	1
11611	C	86.03100	80.79380	83.32290	-680.12736	-510.63371	328.83277	1
11612	H	85.31500	80.12480	82.86790	2092.89870	-1750.34149	1566.62246	1
11613	C	86.55300	81.83280	82.24690	-280.07891	679.12645	-540.17967	1
11614	H	87.16500	81.34780	81.45690	-401.43550	1247.37788	2860.26646	1
11615	H	87.19100	82.46680	82.89890	-1414.90619	-2747.45996	589.68677	1
11616	C	85.50700	82.73980	81.58390	-381.73017	-518.08598	-646.00309	1
11617	C	84.15500	82.39380	81.53690	13.98738	736.61994	537.25824	1
11618	H	83.79200	81.55280	82.10890	-1971.37046	-504.49935	-2399.45934	1
11619	C	83.21100	83.32080	80.93390	-807.86256	349.76018	-237.64869	1
11620	H	82.15600	83.09880	80.98090	2041.51106	1767.43141	-1614.51077	1
11621	C	83.64600	84.52480	80.37890	778.54054	-29.86410	473.74442	1
11622	O	82.57912	85.38324	79.71476	235.28962	-26.04621	310.29669	1
11623	H	81.83700	84.81180	79.82390	-1073.70180	-2324.00967	1828.76181	1
11624	C	85.92600	83.94280	80.96390	12.02304	-905.25558	-108.71426	1
11625	H	86.96400	84.21780	81.07890	2835.24504	-600.94536	-1224.12273	1
11626	C	84.98800	84.82180	80.36790	-671.76561	494.51852	-368.28440	1
11627	H	85.17180	85.83155	79.96900	414.17976	-554.22592	-3026.33487	1
11628	C	87.28100	79.90080	83.70090	-597.77310	657.57265	-204.24626	1
11629	O	87.52500	78.85780	83.08590	-544.70164	560.35624	113.70242	1
11630	N	88.11400	80.46780	84.61090	647.50288	512.31416	-175.91620	1
11631	H	87.81200	81.38580	84.85490	559.06666	2850.33201	1208.83337	1
11632	C	89.22100	79.75680	85.24590	-797.62956	436.77539	66.82327	1
11633	H	89.95300	79.50280	84.49390	-1460.06880	-2547.55562	1129.77241	1
11634	C	89.96200	80.65580	86.28690	-454.18283	-344.00928	711.91753	1
11635	H	90.83200	80.05380	86.62590	2287.01729	-336.87369	-2134.07926	1
11636	H	89.32800	80.96580	87.14490	935.25630	2256.94615	-1982.35111	1
11637	O	90.43900	81.84080	85.66990	614.75734	91.34602	487.19252	1
11638	H	89.67500	82.42080	85.62090	2373.53990	-1179.91475	1694.79668	1
11639	C	88.73400	78.47380	85.93690	-905.12227	101.27148	44.14489	1
11640	O	89.25800	77.41880	85.68690	455.97762	479.88502	430.60655	1
11641	N	87.62200	78.53080	86.72490	-698.23013	282.60942	-381.15468	1
11642	H	87.11900	79.38180	86.85290	1749.77418	2397.46164	-1043.40512	1
11643	C	87.01300	77.34680	87.36090	-109.87209	694.32003	580.77433	1
11644	H	87.78600	76.78980	87.87090	2154.73553	2267.17444	339.50120	1
11645	C	85.83700	77.64780	88.31690	-570.15198	-362.84637	-612.14396	1
11646	H	85.15200	78.26580	87.69790	2173.88273	954.33054	2064.39176	1
11647	C	85.23200	76.35180	88.91690	-581.57871	629.52021	-311.32219	1
11648	H	84.85900	75.70780	88.09290	1916.25287	867.57994	-2339.55257	1

11649	H	85.99500	75.79680	89.50290	-1845.52259	-1492.04024	2065.45117	1
11650	H	84.35600	76.61180	89.54990	-672.14676	3070.81391	128.63473	1
11651	C	86.39100	78.49780	89.48490	356.99775	773.14505	-325.96063	1
11652	H	87.06500	79.27980	89.07290	1431.02713	-2197.52367	-1738.18218	1
11653	H	87.08200	77.89680	90.11390	-988.36040	-1147.52745	2757.63498	1
11654	C	85.32100	79.24980	90.26490	550.97854	-644.36010	-335.66904	1
11655	H	85.66100	79.80480	91.16590	-1836.89018	-1093.54418	2308.29413	1
11656	H	84.50800	78.55480	90.56390	2591.63684	369.16478	-1745.09658	1
11657	H	84.81600	79.99880	89.61990	946.08171	-1654.16507	-2503.37643	1
11658	C	86.59100	76.33380	86.29590	40.75260	705.04492	-576.80317	1
11659	O	86.87600	75.13580	86.32990	266.79178	-247.24634	-700.94124	1
11660	N	85.94400	76.86980	85.20790	-711.83126	-4.55967	453.81467	1
11661	H	85.63800	77.81680	85.14890	842.37471	1784.07581	-2450.65391	1
11662	C	85.54400	75.97380	84.09090	-585.75515	55.87593	-696.57719	1
11663	H	84.97100	75.16780	84.52390	-586.97010	-2292.83159	-2072.82793	1
11664	C	84.70500	76.68680	83.02590	816.47427	-154.59043	-375.39655	1
11665	H	85.34800	77.43880	82.51990	-2027.81144	-1170.43123	-2101.49893	1
11666	C	84.27500	75.71480	81.91990	390.62822	-9.12547	823.87943	1
11667	H	85.09700	75.06980	81.54390	-1043.18891	1845.65843	-2324.54901	1
11668	H	83.47900	75.04880	82.31590	-1130.74826	2166.20224	1981.71705	1
11669	H	83.83700	76.40380	81.16690	-1216.70776	-1778.85079	-2292.05984	1
11670	C	83.45000	77.48980	83.55590	419.46463	384.39946	712.55700	1
11671	H	82.97200	77.88180	82.63290	2756.57425	499.32282	1431.85241	1
11672	H	83.89400	78.25780	84.22490	-2550.79173	-1013.73960	-1537.53692	1
11673	C	82.33100	76.72480	84.30590	-569.19555	-645.58374	-301.14624	1
11674	H	81.47300	77.36780	84.59690	625.84537	408.42952	3056.09704	1
11675	H	82.01000	75.87880	83.66190	-2554.73294	-333.43172	1805.65477	1
11676	H	82.78500	76.35380	85.24990	1986.33564	2424.54117	-272.57487	1
11677	C	86.82000	75.33080	83.39190	637.84342	6.19652	651.58912	1
11678	O	86.93000	74.10180	83.14490	-599.14387	513.65301	28.53841	1
11679	N	87.87300	76.12580	83.05390	-663.86913	290.65683	-432.97653	1
11680	H	87.78700	77.10580	83.21590	969.26659	2388.87271	1803.34014	1
11681	C	89.14600	75.69580	82.51290	630.94474	149.00597	-641.21522	1
11682	H	88.77200	75.17380	81.64490	1623.04462	-2062.26052	-1735.23311	1
11683	C	89.90200	76.92480	82.03590	429.36837	562.65273	-574.90495	1
11684	H	89.27500	77.50780	81.32890	-1806.21469	1033.38445	2359.64643	1
11685	H	90.24800	77.70980	82.74190	968.87177	-2107.61869	2125.43106	1
11686	C	91.23100	76.59480	81.38190	335.66772	-777.81997	337.30443	1
11687	C	91.21500	76.27080	80.01490	-23.36967	907.47043	86.03647	1
11688	H	90.34000	76.17680	79.38890	-467.53920	-1960.65393	-2415.67164	1
11689	C	92.38300	75.83580	79.33690	124.29451	103.54849	897.37372	1
11690	H	92.23500	75.47680	78.32890	1781.61946	-2563.46973	-390.74451	1
11691	C	93.59700	75.74780	79.99190	629.41964	-214.97680	-623.75227	1
11692	H	94.46100	75.44580	79.41890	-281.46604	2946.36560	1066.73935	1
11693	C	92.48600	76.63880	82.03490	851.84921	315.37290	-79.64839	1
11694	H	92.45700	76.91580	83.07890	1218.97345	-2335.50035	1719.81629	1
11695	C	93.65300	76.24480	81.37190	120.85959	619.33722	658.22896	1
11696	H	94.58100	76.33180	81.91690	2968.31632	-683.86815	787.17776	1
11697	C	89.91100	74.63880	83.25790	-899.20530	-97.73742	115.44797	1
11698	O	90.31700	73.58680	82.77890	113.37404	592.87936	-509.18329	1
11699	N	90.07200	74.84380	84.60690	-64.86282	763.94033	-353.35574	1
11700	H	89.75100	75.72580	84.94490	-1902.98710	2503.37145	99.98835	1
11701	C	90.99200	74.14780	85.47890	176.20601	833.55186	324.95190	1
11702	H	91.87600	73.95580	84.88990	-1938.84985	1230.85296	2150.36938	1
11703	C	91.44100	74.96580	86.68890	173.02299	894.91988	-25.14875	1
11704	H	90.54900	75.39680	87.18990	1719.42224	-1244.72462	-2322.17011	1
11705	H	91.98500	74.47680	87.52490	-140.95733	3113.86396	-426.85887	1
11706	C	92.29500	76.20180	86.29890	-749.23088	-254.34103	453.22702	1
11707	H	91.81200	76.81980	85.51190	2493.22330	789.70012	-1748.83891	1
11708	C	92.49600	77.08680	87.49090	615.93485	-41.19508	671.10225	1
11709	H	93.34000	76.67480	88.08490	-644.39557	2184.95975	-2170.00725	1
11710	H	92.75900	78.11980	87.17690	-2280.25586	-592.01586	-2085.22821	1

11711	H	91.62000	77.10680	88.17290	-2013.59702	1687.69269	1730.70698	1
11712	C	93.63900	75.80880	85.71290	-662.53911	-597.98125	186.84578	1
11713	H	94.39500	76.62280	85.73390	2425.53471	-1273.93938	-1546.63701	1
11714	H	94.08800	74.94380	86.24590	218.14437	-1964.51532	2447.71706	1
11715	H	93.51200	75.52980	84.64590	2280.59240	1358.96732	-1688.29274	1
11716	C	90.49500	72.83780	85.92890	-810.95123	-84.95218	408.15712	1
11717	O	91.27500	71.96380	86.38890	-129.50298	-269.20414	731.01665	1
11718	N	89.19100	72.60280	85.69690	-251.93515	121.47951	796.51974	1
11719	H	88.59100	73.30280	85.31790	43.31501	-3145.28314	-59.53133	1
11720	C	88.45900	71.35680	85.94490	726.48390	-372.36520	406.22199	1
11721	H	89.12800	70.64180	86.40090	2333.32560	-2080.92148	351.54472	1
11722	C	87.22600	71.64880	86.78490	631.74897	106.00902	648.92706	1
11723	H	86.71000	70.67580	86.92890	-1829.54859	1647.60973	1958.66290	1
11724	O	86.29500	72.52080	86.19690	722.07675	-294.97409	123.38023	1
11725	H	86.60700	73.42780	86.23990	272.75475	493.84464	-3095.14920	1
11726	C	87.61600	72.22880	88.17090	-735.97154	-495.50351	-210.41188	1
11727	H	86.73200	72.42180	88.81590	-1085.15946	2935.96839	317.40318	1
11728	H	88.12700	73.21380	88.10690	-35.06783	-1908.79420	2500.70014	1
11729	H	88.25200	71.51380	88.73390	1027.51984	2137.29586	-2067.46115	1
11730	C	88.17800	70.69480	84.65590	-47.19641	571.30404	-709.10874	1
11731	O	88.41700	69.53780	84.41390	235.50712	-361.22663	-661.57309	1
11732	N	87.69700	71.45480	83.66790	-641.78769	345.94488	-425.56196	1
11733	H	87.49600	72.42580	83.77290	2623.53799	492.24444	1665.22373	1
11734	C	87.33000	70.99180	82.32790	-514.93006	-529.73946	-534.48494	1
11735	H	86.87200	71.79880	81.77690	-1048.08217	-1588.60383	2505.21214	1
11736	H	86.53900	70.25880	82.39390	3137.72187	-193.95131	123.73591	1
11737	C	88.38800	70.38780	81.46990	-130.35224	-889.90919	-150.06972	1
11738	O	88.07800	69.34780	80.89690	-369.07184	-568.54953	405.17236	1
11739	N	89.50700	71.10180	81.21690	-378.33265	-574.17396	489.75602	1
11740	H	89.71200	71.85980	81.82990	-620.69684	-1577.17562	2650.56197	1
11741	C	90.54000	70.62380	80.30890	-321.64006	682.06396	512.62797	1
11742	H	90.04700	70.37080	79.38190	2550.62627	-1531.66824	1022.99769	1
11743	C	91.49700	71.77680	80.00190	-684.88866	-170.05872	577.45871	1
11744	H	90.87200	72.69580	80.01990	-275.26504	2904.80995	-1176.66246	1
11745	C	92.63800	71.97780	81.09890	362.06379	824.28792	144.60375	1
11746	H	93.11400	72.96780	80.93290	-1446.05167	-651.16070	2717.19534	1
11747	H	93.41500	71.18380	81.09390	-1775.22326	-144.94800	-2593.41448	1
11748	H	92.18000	72.00080	82.11090	2936.47914	-377.82875	1064.21893	1
11749	C	92.06200	71.74980	78.55590	282.82799	-290.71302	816.66717	1
11750	H	91.23500	71.68480	77.81690	-1767.79188	2090.98319	1549.49263	1
11751	H	92.43600	72.79180	78.45790	-1695.32947	2126.98507	1581.14475	1
11752	C	93.19900	70.75380	78.20890	626.50407	-561.61670	-351.46882	1
11753	H	94.09500	70.93880	78.83990	-2524.82516	385.19354	-1837.14727	1
11754	H	93.64100	70.73480	77.18990	902.56296	-2279.38943	1971.79871	1
11755	H	92.87200	69.72480	78.47090	-2537.52079	633.89517	1748.53978	1
11756	C	91.19200	69.33780	80.85890	-845.85400	40.75214	338.11430	1
11757	O	91.46200	68.34780	80.13890	-212.93731	675.59238	-349.08432	1
11758	N	91.48600	69.32480	82.18790	-413.14054	594.69609	-433.96284	1
11759	H	91.23100	70.17480	82.64090	2768.65843	-1191.23536	902.06154	1
11760	C	91.91500	68.12480	82.90290	674.76662	-4.89852	-613.28380	1
11761	H	92.79300	67.74880	82.39990	1137.05328	2474.96393	1574.76652	1
11762	C	92.25100	68.54980	84.34890	-623.70194	-217.42377	628.62850	1
11763	H	91.36300	68.83680	84.95190	2031.03728	-2134.16384	-1103.83808	1
11764	C	92.93000	67.35280	85.13090	-38.21424	545.58213	729.61004	1
11765	H	93.39500	67.66780	86.08990	2816.88312	785.42742	-1160.38765	1
11766	H	93.59900	66.86780	84.38790	683.50592	2165.82641	2177.20965	1
11767	H	92.08600	66.72380	85.48590	-1297.42712	-2085.69786	-1965.90273	1
11768	C	93.12200	69.81780	84.36490	-82.64499	-713.48418	-561.74829	1
11769	H	92.59100	70.79080	84.28690	418.05189	-1824.98671	-2528.41499	1
11770	H	93.47800	69.79780	85.41690	-1799.71518	611.07834	-2507.15671	1
11771	H	93.92400	69.74080	83.59990	-2110.06411	-1558.22569	-1737.17828	1
11772	C	90.88500	67.01480	82.85490	-556.90750	641.70428	-330.93904	1

11773	O	91.19100	65.97680	82.31990	578.50465	275.09237	-461.82658	1
11774	N	89.59800	67.27880	83.21290	527.47058	507.40287	420.70109	1
11775	H	89.33800	68.17280	83.56890	-3101.06471	-449.88638	281.47141	1
11776	C	88.50800	66.28280	83.31090	-543.31176	554.50542	478.31693	1
11777	H	87.63400	66.81180	83.66190	-1058.56279	-2935.79372	398.47993	1
11778	H	88.77800	65.52880	84.03490	13.31072	2345.67527	2096.62981	1
11779	C	88.13700	65.55880	82.06790	314.14467	-561.63813	-646.00831	1
11780	O	88.04400	64.34280	82.03790	301.13903	-577.45636	446.63929	1
11781	N	87.94300	66.29480	80.94490	-133.31966	640.18901	-533.90653	1
11782	H	88.08700	67.28080	80.99990	-2812.65001	978.91141	-1014.37598	1
11783	C	87.72000	65.63780	79.67190	413.69976	-526.35060	-619.07879	1
11784	H	87.02600	64.82080	79.79990	1059.06714	206.50054	2955.32748	1
11785	C	86.96700	66.60780	78.71390	-92.17659	171.75748	-890.76026	1
11786	H	87.46400	67.58080	78.50890	3104.91925	80.66297	501.19475	1
11787	H	86.78100	66.01880	77.79090	2249.29314	359.21715	-2170.22340	1
11788	C	85.61000	66.79680	79.39290	257.20112	777.19145	-401.58690	1
11789	O	84.83300	65.81480	79.48890	41.48806	742.67780	265.20870	1
11790	N	85.34400	67.99780	79.87490	293.16062	776.53241	154.03428	1
11791	H	86.08300	68.66580	79.96190	-2086.18902	-1479.44611	1832.28840	1
11792	H	84.39500	68.15680	80.14790	-3074.19845	130.00965	656.22221	1
11793	C	88.89800	64.98780	79.03490	729.59863	376.10731	-397.08957	1
11794	O	88.72200	64.04280	78.34190	-693.58536	354.52459	-129.91881	1
11795	N	90.14400	65.40080	79.46790	210.13862	-791.79120	-203.91357	1
11796	H	90.25700	66.25580	79.96790	-1062.04363	2020.92879	-2164.74858	1
11797	C	91.31700	64.73480	79.05890	97.70485	515.88956	745.49495	1
11798	H	91.30700	64.62180	77.98490	-2927.03199	1151.10278	-75.31504	1
11799	H	92.21500	65.29480	79.27790	1062.09970	-1925.40192	2250.11064	1
11800	C	91.40100	63.43180	79.75790	310.82975	-796.83060	-316.06465	1
11801	O	91.82500	62.42080	79.26990	-577.07887	332.13922	424.60658	1
11802	N	91.02800	63.38680	81.05790	661.05041	154.45958	-501.82356	1
11803	H	90.80500	64.21680	81.56290	-2517.52490	1601.70543	-997.41382	1
11804	C	90.91800	62.15580	81.79590	275.37986	-734.86526	-464.31669	1
11805	H	91.86200	61.64080	81.70190	-1066.15996	2389.99152	1746.27308	1
11806	C	90.82800	62.40680	83.27890	331.56885	-794.75202	299.80382	1
11807	H	90.54300	61.55180	83.92790	1677.69666	2644.70176	298.51762	1
11808	H	89.92600	63.04680	83.38890	-2285.97755	-1673.79653	1367.82238	1
11809	C	92.01900	63.17780	83.96190	-507.29365	-341.32403	-676.46291	1
11810	H	92.39400	64.07880	83.43090	2371.87763	457.82649	2015.64324	1
11811	C	91.67700	63.61180	85.38990	-427.74577	655.48410	467.78751	1
11812	H	91.21000	62.80180	85.98990	-2952.71904	-361.96864	-1024.03866	1
11813	H	92.58900	63.86880	85.96890	1883.89389	-747.97171	-2406.18128	1
11814	H	90.99500	64.48680	85.45990	-1863.27798	1324.56257	-2161.47065	1
11815	C	93.24800	62.26580	83.90690	395.64209	142.65578	809.05356	1
11816	H	93.04800	61.32980	84.47190	2319.96381	-1501.10801	1504.21703	1
11817	H	94.12500	62.84280	84.26990	-1438.91126	1875.01864	-2076.55140	1
11818	H	93.55700	61.98580	82.87690	1529.33518	1892.55504	1994.39103	1
11819	C	89.83700	61.22880	81.39190	-670.64914	389.97123	-479.16926	1
11820	O	90.05200	60.01880	81.38790	781.35197	-104.16432	47.60376	1
11821	N	88.67800	61.73480	81.04490	330.59139	-215.15975	746.38322	1
11822	H	88.46700	62.70780	81.09490	-1221.30094	-2124.56655	1973.03503	1
11823	C	87.67100	60.85880	80.39390	540.49009	460.58516	571.99894	1
11824	H	87.32000	60.08580	81.06090	-2109.82119	420.31282	-2295.69552	1
11825	C	86.36900	61.62080	80.15290	437.16704	378.29483	705.14467	1
11826	H	86.66700	62.53680	79.59990	-931.64399	-1905.93439	2323.29073	1
11827	C	85.41000	60.79180	79.24990	-40.18690	139.68571	-900.17994	1
11828	H	85.78800	60.71980	78.20790	-337.71721	2233.51169	2189.88558	1
11829	H	84.42100	61.27980	79.11590	-2232.42026	1456.66377	1671.12438	1
11830	H	85.21300	59.82180	79.75490	-1555.71342	-964.44593	-2558.87202	1
11831	C	85.66900	62.05280	81.46790	59.94967	164.68914	894.83771	1
11832	H	84.86800	62.78280	81.22090	2288.98316	-975.36532	-1925.47262	1
11833	H	85.26400	61.20280	82.05790	1418.49257	-211.68327	-2800.23128	1
11834	H	86.41700	62.61580	82.06690	1686.79616	1795.69322	-1956.63763	1

11835	C	88.14800	60.21080	79.10090	-460.61643	407.85428	673.00698	1
11836	O	87.98300	59.02080	78.84890	-678.66037	361.86766	-179.16229	1
11837	N	88.93200	60.97080	78.26790	603.21865	-484.47884	-337.75701	1
11838	H	88.88200	61.95180	78.43890	950.00296	-2010.56634	-2225.61084	1
11839	C	89.63900	60.42180	77.09990	725.26411	366.18609	413.94532	1
11840	H	88.99200	59.82980	76.46890	-2637.04200	-778.25505	-1529.23341	1
11841	C	90.13200	61.55680	76.21090	-245.39354	328.56694	-814.41806	1
11842	H	90.77500	62.20780	76.84090	2388.04920	1975.44820	-541.34249	1
11843	C	91.04800	61.07380	75.04890	-454.31315	-405.65078	-678.60004	1
11844	H	91.94600	60.50580	75.37390	-1639.17125	-2672.23587	265.51703	1
11845	H	91.50200	61.91580	74.48490	2378.32481	2035.61491	313.16012	1
11846	H	90.55600	60.35680	74.35590	-884.49316	-328.70926	-3001.30776	1
11847	C	89.00800	62.48180	75.66090	7.02713	567.02539	714.06151	1
11848	H	88.47400	61.93980	74.85190	2612.78447	-1684.72838	-482.98432	1
11849	H	88.14100	62.60780	76.34490	-2631.13738	-1490.45271	-868.27012	1
11850	C	89.53000	63.78780	75.11390	-553.20240	-415.10246	594.22895	1
11851	H	90.19400	63.52080	74.26490	942.90686	-3000.78915	66.46305	1
11852	H	88.68400	64.35180	74.66590	-2106.33165	2266.34950	-570.30969	1
11853	H	89.97900	64.42080	75.90890	-2572.36207	1655.35637	-735.50996	1
11854	C	90.77300	59.45680	77.46190	332.79423	-609.46388	-590.97613	1
11855	O	90.96700	58.38780	76.89490	-33.13991	738.45028	277.88517	1
11856	N	91.47500	59.73380	78.58890	-205.99053	-461.63039	676.11949	1
11857	H	91.42900	60.64380	78.99590	1676.62045	1711.55738	2039.05405	1
11858	C	92.46700	58.82380	79.17890	-724.88543	-475.55518	-282.55864	1
11859	H	93.13400	58.59180	78.36190	-2154.49200	2198.57070	-650.13636	1
11860	C	93.39400	59.54580	80.25190	-727.45292	-66.62977	545.73229	1
11861	H	93.67500	58.93680	81.13790	-477.43093	1900.27554	2461.55211	1
11862	H	92.68800	60.32980	80.60090	-1885.56164	2439.64756	-625.30258	1
11863	C	94.60100	60.20980	79.64990	0.07779	136.16699	-901.61497	1
11864	H	94.23900	60.46180	78.62990	-1494.27344	2209.19348	-1668.78317	1
11865	C	95.06300	61.43480	80.47190	181.28753	817.11273	-361.81848	1
11866	H	95.28300	61.04180	81.48790	-1711.81780	-2403.28153	1091.85344	1
11867	H	94.26400	62.20680	80.47790	-1638.91079	-1988.92275	-1804.54535	1
11868	H	96.00300	61.82780	80.02690	789.63194	-1754.67722	2489.13951	1
11869	C	95.76500	59.20580	79.52190	-723.88704	514.99269	205.47768	1
11870	H	96.08900	58.91780	80.54590	-2579.66576	1679.81506	649.43986	1
11871	H	95.53700	58.21280	79.07790	1397.94009	-2453.65391	1386.92906	1
11872	H	96.53300	59.68580	78.87890	591.89494	-2907.09292	1047.23319	1
11873	C	91.86500	57.57880	79.69390	-582.56779	-303.19306	-632.56600	1
11874	O	92.42900	56.49880	79.48290	535.77260	-24.90168	-579.61613	1
11875	N	90.65400	57.56080	80.28190	-381.42184	-696.43704	286.64460	1
11876	H	90.21300	58.42780	80.50190	-2074.13190	2027.32988	-1219.07205	1
11877	C	89.92200	56.39580	80.60690	-269.30077	-32.73197	-870.54966	1
11878	H	90.56100	55.73180	81.16890	2609.90647	-683.93234	-1618.28644	1
11879	C	88.72200	56.64380	81.52490	-255.95642	818.20196	-310.61692	1
11880	H	88.11700	57.51680	81.19890	-2200.53987	-872.08249	2072.51602	1
11881	C	87.81900	55.37180	81.65790	-270.06871	308.71118	-814.37786	1
11882	H	87.24900	55.30580	80.70590	-1679.32935	2605.55697	537.72862	1
11883	H	88.39100	54.44580	81.87890	2325.06348	1309.71624	-1666.41814	1
11884	H	87.10100	55.43280	82.50390	1541.58712	-1896.34312	-1981.31727	1
11885	C	89.30500	57.08480	82.90890	-335.17659	787.08053	-315.61352	1
11886	H	89.91800	58.00280	82.78290	2332.24242	609.63530	-2021.68651	1
11887	H	89.92900	56.23680	83.26390	-1968.73005	1708.57905	1761.55779	1
11888	H	88.39800	57.27180	83.52290	-1980.23295	-1726.76671	-1730.65895	1
11889	C	89.44700	55.63980	79.32990	-359.27848	576.33568	608.44652	1
11890	O	89.89800	54.49180	79.18290	-449.67866	648.30608	33.39991	1
11891	N	88.71500	56.24380	78.37590	-687.55598	361.92186	-330.07821	1
11892	H	88.39800	57.18380	78.48190	-1682.32476	-210.17816	-2650.25183	1
11893	C	88.13600	55.43780	77.35890	481.60797	-515.20904	-577.98305	1
11894	H	87.98700	54.42380	77.69790	2167.44450	1544.81508	-1677.48530	1
11895	C	86.80000	55.99480	76.89190	518.43415	-69.51995	746.88955	1
11896	H	86.79700	57.04880	76.53890	-1143.95498	2795.22945	-881.07069	1

11897	H	86.30400	55.48680	76.03690	1254.94298	2533.45344	-1380.20217	1
11898	C	85.67600	55.90280	77.97190	-484.48634	-150.54762	757.66708	1
11899	H	86.01400	56.61080	78.75890	1871.95387	1227.76250	2210.56875	1
11900	H	85.62800	54.90080	78.44890	-2218.83620	1002.44526	1992.50988	1
11901	S	83.95900	56.24880	77.57990	-404.97605	-144.73323	355.32703	1
11902	C	84.12800	58.00880	77.20090	-197.22130	-509.73989	-729.87671	1
11903	H	83.24300	58.67880	77.24590	-414.07682	-2980.23816	919.21005	1
11904	H	84.54900	58.20380	76.19090	411.47298	2082.84638	-2321.78103	1
11905	H	84.85200	58.45580	77.91490	2087.45348	1033.17280	-2115.02202	1
11906	C	89.02800	55.25480	76.12090	452.00509	-403.62784	-681.34204	1
11907	O	88.67300	54.33880	75.34490	-482.40885	216.79530	-586.43732	1
11908	N	90.17100	55.99680	75.92590	-667.46038	-222.59038	466.50022	1
11909	H	90.45000	56.78180	76.47390	1347.87838	2726.98930	-803.10612	1
11910	C	91.03600	55.84080	74.74190	-889.83329	191.54029	-54.40627	1
11911	H	91.33000	56.77180	74.28090	-1586.87762	296.94965	-2700.34564	1
11912	H	90.59400	55.18780	74.00390	-572.29216	2941.77648	957.42313	1
11913	C	92.32500	55.26980	75.05690	636.94938	-640.72478	123.36225	1
11914	O	92.92800	54.78180	74.07790	-199.28590	-698.80068	309.17628	1
11915	N	92.85900	55.28180	76.31390	-420.26493	-726.64527	89.64558	1
11916	H	92.39700	55.80080	77.02990	-2179.54868	-321.32446	2246.00632	1
11917	C	94.18600	54.76780	76.54990	-516.28029	736.80378	-148.41107	1
11918	H	94.42000	54.19980	75.66190	2046.46465	2181.63635	-975.02384	1
11919	C	95.24000	55.87480	76.84190	-403.38982	768.94288	-278.30649	1
11920	H	96.23400	55.39980	76.97990	1643.87484	994.04106	-2491.54252	1
11921	H	94.96800	56.43880	77.75990	1807.35693	-538.28990	-2518.31911	1
11922	C	95.32500	56.83880	75.67490	658.83343	599.46334	-195.02109	1
11923	C	94.57400	58.04680	75.56990	735.77653	-405.26549	354.74468	1
11924	H	93.81100	58.35680	76.26890	1625.72964	-2631.85930	573.18932	1
11925	C	94.76300	58.89280	74.47790	-420.74497	-268.55247	-763.08862	1
11926	H	94.19800	59.78980	74.27190	-2210.21796	872.57426	2061.98374	1
11927	C	95.64700	58.60780	73.44990	417.26536	581.36110	565.11937	1
11928	O	95.87200	59.44180	72.41690	-555.02119	-364.40461	427.53712	1
11929	H	96.32200	59.00280	71.69190	1960.54608	-1695.32460	1783.35632	1
11930	C	96.26800	56.58880	74.66090	-707.17336	-527.74710	-229.86917	1
11931	H	96.92000	55.72780	74.64290	-1392.07536	228.65270	-2812.12915	1
11932	C	96.40200	57.42980	73.55890	243.88306	-863.32614	-163.21773	1
11933	H	97.07000	57.15380	72.75690	1815.36562	1085.64151	-2328.96037	1
11934	C	94.25100	53.70880	77.63690	517.31090	682.10256	-313.96900	1
11935	O	94.75800	52.60880	77.40090	-416.13956	-623.25887	-249.00497	1
11936	N	93.66100	53.96080	78.80590	256.79754	-672.06997	441.64383	1
11937	H	93.27600	54.86780	78.95390	-1234.01676	-2604.29812	1262.16487	1
11938	C	93.44100	53.00680	79.89090	-599.56266	600.82935	-333.13618	1
11939	H	94.35700	52.47780	80.10790	1827.87857	1575.23439	2018.84194	1
11940	C	92.94400	53.62880	81.25290	445.77242	-396.55549	-689.55181	1
11941	H	92.05600	54.20480	80.91490	1528.57417	1902.28294	1985.70059	1
11942	H	92.64800	52.84180	81.97990	1217.80572	896.89466	2758.75976	1
11943	C	93.94700	54.46080	82.04690	-393.38206	815.68796	106.55845	1
11944	H	94.47900	55.07880	81.29190	-1516.57166	-2750.17328	186.50351	1
11945	H	94.64500	53.84780	82.65590	2442.85213	-1927.82729	462.79762	1
11946	C	93.27700	55.39580	83.02990	-567.21803	42.86215	712.65528	1
11947	O	92.47900	54.97380	83.85390	278.53089	-654.64459	342.76557	1
11948	N	93.52300	56.72180	82.88790	-587.28231	-86.24744	600.27756	1
11949	H	94.41900	57.02380	82.56290	-2097.16996	45.48301	-2344.78905	1
11950	H	92.86000	57.35880	83.28190	1729.79074	364.51200	-2602.53362	1
11951	C	92.57700	51.86780	79.50590	309.23997	595.98626	616.94572	1
11952	O	92.78500	50.65780	79.79990	-586.64018	395.11844	-351.22919	1
11953	N	91.47300	52.18080	78.75590	361.09023	362.27129	671.59932	1
11954	H	91.20800	53.14080	78.70990	2028.97080	263.32461	2390.01337	1
11955	C	90.61600	51.17280	78.07990	625.30084	-488.83724	448.87417	1
11956	H	90.80800	50.23680	78.58390	-2144.40996	-1361.23221	-1856.55030	1
11957	C	89.08300	51.53180	78.20090	477.40451	-650.07167	425.37367	1
11958	H	88.90900	52.51580	77.71390	-2984.13350	-814.07351	574.85456	1

11959	H	88.49600	50.75480	77.66490	387.63192	2809.97985	1360.87507	1
11960	C	88.66600	51.54680	79.65090	-16.46731	727.72636	549.17591	1
11961	H	89.15400	52.39480	80.17690	1412.95289	2456.78161	-1366.02141	1
11962	H	89.07300	50.61780	80.10390	2470.71274	-1055.01199	-1637.30098	1
11963	C	87.13900	51.48180	79.68990	-432.57797	-796.00644	-103.44587	1
11964	H	86.76700	52.34880	79.10290	822.00885	-1659.18601	2543.54663	1
11965	H	86.88900	50.48680	79.26190	-2959.95700	805.02226	699.15660	1
11966	C	86.57500	51.74980	81.08890	626.28866	582.54457	-315.99896	1
11967	H	86.92000	52.73180	81.47690	-1470.60068	2538.39473	-1136.71109	1
11968	H	86.98500	50.92780	81.71390	428.27849	-2564.59065	-1771.34937	1
11969	N	85.12500	51.68880	81.07790	-325.89062	634.10551	-452.08162	1
11970	H	84.77400	50.75480	80.78390	2061.34753	2252.62626	-758.12104	1
11971	H	84.69900	52.02580	81.96490	-2254.09242	-2171.37274	-320.05317	1
11972	H	84.83800	52.34680	80.32490	2702.72499	846.95956	-1369.73113	1
11973	C	90.95300	50.94980	76.60790	-791.95575	415.04482	178.87113	1
11974	O	90.98900	51.89480	75.82090	-477.04654	-343.75641	-527.14833	1
11975	N	91.05100	49.72080	76.17790	-649.59839	398.10287	363.60462	1
11976	H	90.96200	48.97080	76.82890	1458.14370	2348.37727	-1502.38722	1
11977	C	91.29900	49.34780	74.85290	-196.54250	852.49423	257.05181	1
11978	H	91.82800	50.10280	74.28990	810.25378	-484.59869	-3001.14631	1
11979	C	92.38200	48.18380	74.82990	-232.57955	668.07899	-575.35052	1
11980	H	92.07000	47.34480	75.48790	1997.64510	893.54082	2260.35950	1
11981	H	92.30400	47.74580	73.81190	-1462.04695	-2629.60319	919.69126	1
11982	C	93.85500	48.62380	74.83190	-424.38912	617.07221	520.16032	1
11983	H	94.07900	49.05780	73.83490	-1533.42661	-1555.59845	-2264.27527	1
11984	H	94.46100	47.69280	74.87390	-1012.94100	-909.17038	-2836.47422	1
11985	C	94.33100	49.57380	75.99790	-123.48169	749.27765	504.76358	1
11986	H	93.81300	50.55380	75.93290	2516.78984	1864.77128	294.31821	1
11987	H	94.18600	49.06480	76.97490	-1086.76355	2939.52485	-276.34191	1
11988	C	95.82100	49.84980	75.84490	662.05657	334.81084	530.12621	1
11989	H	96.00100	50.55280	75.00390	1609.52510	-840.60521	2569.24854	1
11990	H	96.33200	48.90480	75.56290	-1866.05211	2255.16258	1153.39391	1
11991	N	96.36400	50.35680	77.12790	83.85254	-840.00723	-5.37561	1
11992	H	95.93900	49.92380	77.97290	366.75803	-1847.68540	-2519.87568	1
11993	H	96.24700	51.38080	77.26290	-212.69305	-2418.09462	-2001.45105	1
11994	H	97.39300	50.20580	77.11590	2220.86465	1037.98853	1971.94479	1
11995	C	90.00100	49.00580	74.10290	-646.14395	-433.52289	475.40183	1
11996	O	90.08300	48.49180	72.98190	-109.13754	630.33862	463.02208	1
11997	N	88.81000	49.29580	74.67490	645.30425	-291.62975	459.57241	1
11998	H	88.70200	49.78880	75.53390	-1336.66204	-690.57977	2763.08892	1
11999	C	87.55400	48.97680	74.08890	810.69662	332.42387	252.42102	1
12000	H	87.68600	49.00780	73.01690	1261.16373	-2809.95431	641.75465	1
12001	C	87.15200	47.53380	74.50490	195.68149	-372.14895	-809.11366	1
12002	H	87.00100	47.55280	75.60590	627.64980	-2730.86972	1430.60566	1
12003	H	88.03400	46.90580	74.25790	-294.96673	1838.16130	2536.21448	1
12004	C	85.88800	46.98380	73.78190	-514.60994	-676.19537	-330.73772	1
12005	H	85.04600	47.70380	73.87690	2159.55539	2127.79094	840.86413	1
12006	C	86.19700	46.73680	72.27590	513.37198	-390.36037	644.60763	1
12007	H	86.97300	45.94380	72.21590	757.55728	1552.81916	-2629.27478	1
12008	H	86.79000	47.58380	71.86990	-2370.02827	2.51577	2069.10268	1
12009	H	85.32100	46.35980	71.70490	1419.99629	2200.09975	-1743.96039	1
12010	C	85.44900	45.69380	74.43390	-572.82536	-688.13157	172.61823	1
12011	H	86.17400	44.86080	74.31090	-2596.52346	1295.27064	1215.96304	1
12012	H	84.50200	45.40480	73.93090	-2898.30672	-262.72757	-1195.41566	1
12013	H	85.30700	45.81980	75.52790	-2858.06058	-603.19043	1168.70751	1
12014	C	86.58300	49.95080	74.48290	470.41433	35.85679	780.30485	1
12015	O	86.54200	50.31480	75.64190	-588.56167	469.27101	-238.76160	1
12016	N	85.76300	50.38280	73.53390	74.47277	-813.32802	213.59687	1
12017	H	85.97600	50.05580	72.61690	1805.71083	1545.11727	2061.61278	1
12018	C	84.62100	51.21080	73.67290	-165.33727	-443.14724	-779.57367	1
12019	H	84.52300	51.36680	74.73690	-1667.06575	2602.13103	-589.94247	1
12020	C	84.88700	52.61880	73.07790	871.12257	223.68728	-150.20145	1

12021	H	83.94100	53.16780	72.88390	1370.99310	582.96801	2771.05620	1
12022	H	85.25400	52.43280	72.04590	-1938.95471	-86.65666	-2476.12025	1
12023	C	85.88700	53.42880	73.88690	645.13091	-641.00778	66.07680	1
12024	H	86.80800	52.87480	74.16590	-292.94778	2772.15421	-1458.61881	1
12025	H	85.38700	53.70380	74.83990	-220.80937	2915.27530	-1162.17013	1
12026	C	86.28500	54.67180	73.14490	-46.40004	-652.09192	-635.66828	1
12027	H	85.41500	55.31380	72.88890	972.19535	2320.72695	-1888.72678	1
12028	H	86.96800	55.30180	73.75390	1566.75036	2000.37395	1855.26914	1
12029	N	87.02500	54.16280	71.89790	-608.96999	352.30617	466.59212	1
12030	H	86.52100	54.27380	71.04090	2255.82456	2188.50576	-141.15364	1
12031	C	88.26400	53.66480	71.80990	-569.81877	363.39144	-612.13090	1
12032	N	89.10000	53.50980	72.82190	577.68006	610.17971	-81.47856	1
12033	H	88.79100	53.70980	73.75190	-327.84551	2636.03825	1685.83686	1
12034	H	90.04200	53.23980	72.62390	2824.26856	630.69254	1234.48785	1
12035	N	88.74400	53.35480	70.59690	243.88392	-464.76129	661.20335	1
12036	H	88.15000	53.32880	69.79290	593.76744	-1077.70321	-2895.55215	1
12037	H	89.71700	53.20780	70.42090	1555.41710	2697.84599	447.80674	1
12038	C	83.32200	50.61480	73.20590	-627.51682	-478.99942	-456.32576	1
12039	O	83.24600	50.07780	72.10590	158.13124	76.39803	769.92537	1
12040	N	82.30300	50.67980	74.02090	288.65807	-357.90700	-707.99109	1
12041	H	82.47000	51.01780	74.94390	-1317.19795	2080.32748	1958.43135	1
12042	C	80.90500	50.41080	73.69990	213.65388	861.83773	207.45781	1
12043	H	80.90700	49.61780	72.96590	2621.91957	1226.50582	1232.65870	1
12044	C	80.09800	49.91280	74.88890	891.07230	99.44429	165.98792	1
12045	H	80.65700	49.07480	75.35590	-610.32980	2738.34949	-1423.78574	1
12046	H	79.13500	49.50380	74.51390	-1334.15046	-2455.18096	-1445.80609	1
12047	O	79.93000	50.94380	75.84990	404.99634	677.47108	25.26136	1
12048	H	80.78600	51.10580	76.25190	2045.17830	-1934.17400	1405.14871	1
12049	C	80.20200	51.63780	73.09290	-290.77136	460.76193	731.16446	1
12050	O	80.82500	52.67380	72.89290	6.22925	-670.23758	417.57636	1
12051	N	78.90600	51.49280	72.63190	804.15742	-245.13745	76.88145	1
12052	H	78.46200	50.61780	72.45690	1966.48604	2031.87133	1379.36862	1
12053	C	78.10900	52.61380	72.12490	-38.80295	-523.18019	-745.80683	1
12054	H	78.62900	53.02480	71.27190	571.29205	3037.68164	586.80650	1
12055	C	76.74700	52.13880	71.62190	-1.64929	686.49319	600.14613	1
12056	H	76.16900	52.99880	71.21990	960.73814	-1454.63825	2619.01432	1
12057	H	76.18700	51.79780	72.51890	-1762.84482	-2491.16498	-764.65771	1
12058	C	76.84800	51.01580	70.56590	-675.82134	331.44193	514.64820	1
12059	H	75.93000	51.16180	69.95690	965.02650	1592.22819	2536.09138	1
12060	H	77.66100	51.23680	69.84290	2357.70359	464.66706	2030.65126	1
12061	S	76.94200	49.31380	71.19890	341.30531	408.22216	167.55883	1
12062	C	75.79700	48.59480	69.95690	827.16267	245.02624	295.32196	1
12063	H	75.35400	47.67380	70.39290	2064.85392	-2370.72865	-119.37418	1
12064	H	76.40800	48.33680	69.06590	-360.06608	-2325.14734	2088.60443	1
12065	H	75.08300	49.32480	69.51890	1737.04504	1346.82353	-2250.99248	1
12066	C	77.92300	53.80080	73.01490	-216.78428	637.19466	615.17358	1
12067	O	78.11000	54.94380	72.61990	511.66076	-576.12974	-172.93066	1
12068	N	77.71000	53.58280	74.34390	116.26666	-800.05617	243.03183	1
12069	H	77.59800	52.67680	74.74290	-1357.08445	-1232.82351	2556.69596	1
12070	C	77.68700	54.67680	75.33990	-678.35284	-109.41542	-599.43031	1
12071	H	76.94800	55.38980	75.00390	-1206.66008	2905.34747	33.96701	1
12072	C	77.20500	54.32980	76.79390	472.54445	10.69847	-779.76810	1
12073	H	77.72800	53.41580	77.14590	2373.67726	-1298.61513	-1605.45359	1
12074	O	75.76300	54.21780	76.78490	249.98320	-474.61047	-579.55201	1
12075	H	75.63300	53.42280	76.26290	3029.87441	-803.06926	-270.49405	1
12076	C	77.39900	55.42680	77.81890	-565.84948	425.25063	574.82803	1
12077	H	76.81700	55.15480	78.72490	2380.54261	2038.40372	275.95904	1
12078	H	78.42900	55.46880	78.23490	223.84325	3107.75120	-435.89326	1
12079	H	77.11100	56.36280	77.29590	-8.05197	-3029.05317	850.29306	1
12080	C	78.99300	55.41280	75.48290	701.70330	-576.93621	-78.79146	1
12081	O	79.01200	56.64380	75.52890	-59.21911	-775.59247	-136.29617	1
12082	N	80.04200	54.60680	75.54790	-398.63876	510.83580	-541.11571	1

12083	H	79.91100	53.62580	75.42390	-2349.11562	2066.51292	330.76636	1
12084	C	81.45000	55.05880	75.60490	206.95057	637.15206	-618.59495	1
12085	H	81.54600	55.60980	76.52890	632.20188	-642.48221	-3014.26004	1
12086	C	82.49400	53.85080	75.62690	598.64805	397.00326	-561.65820	1
12087	H	83.54200	54.17680	75.80090	-2232.34802	-1661.32334	-1467.94186	1
12088	H	82.40300	53.30880	74.66190	676.89204	2401.68197	-1916.23775	1
12089	C	82.13700	52.85880	76.75290	-370.00610	37.83435	-832.53531	1
12090	O	82.51800	51.66580	76.56390	-351.41515	21.40122	706.87807	1
12091	O	81.53100	53.20380	77.76190	286.97340	74.62546	731.91840	1
12092	C	81.81100	55.96680	74.36290	205.71236	700.87909	-545.80393	1
12093	O	82.31600	57.09180	74.51690	411.41298	417.00731	529.59560	1
12094	N	81.46000	55.58180	73.12090	230.67136	-741.50725	-331.10424	1
12095	H	80.97900	54.71980	72.97790	2577.54806	1047.01609	1469.09140	1
12096	C	81.68400	56.29980	71.95890	389.38357	-169.83255	-806.83848	1
12097	H	82.73300	56.54780	72.03390	-1969.42367	1749.85328	-1719.77037	1
12098	C	81.30300	55.39580	70.72990	-581.59895	323.43404	-623.36513	1
12099	H	81.29600	56.08680	69.85890	-2342.50797	-2032.69013	528.25512	1
12100	H	80.24900	55.09180	70.90490	-2701.29281	1283.89242	976.14733	1
12101	C	82.34400	54.32980	70.40590	45.24449	-679.72194	606.12047	1
12102	H	82.91800	54.03380	71.31090	-1064.36985	1985.27929	2196.36272	1
12103	H	83.11200	54.74680	69.71990	-611.85400	-2639.79983	1598.53612	1
12104	C	81.85800	53.05580	69.67590	660.61407	-567.71870	269.69526	1
12105	H	81.45300	53.35580	68.68590	-2517.02422	-608.94234	1786.61818	1
12106	H	81.02700	52.73880	70.34090	-286.32125	-1820.26254	-2550.07660	1
12107	C	82.96900	51.98280	69.53090	-514.95006	-516.07252	547.67380	1
12108	H	83.51800	51.86480	70.48990	1856.94857	1393.62275	2123.15423	1
12109	H	83.71600	52.20480	68.73890	1301.85931	-1533.97425	2418.74173	1
12110	N	82.51400	50.65680	69.16890	535.25158	528.00295	383.91525	1
12111	H	82.10400	50.74380	68.21690	-169.33332	2201.55980	-2241.13518	1
12112	H	83.32800	50.00980	69.15490	-692.77952	2016.47948	2313.45916	1
12113	H	81.81100	50.26080	69.82490	-1891.10716	-2335.74071	930.72835	1
12114	C	80.96500	57.63780	71.82890	831.35342	-336.52414	164.48099	1
12115	O	81.52700	58.63680	71.43890	528.41780	45.66680	-585.07812	1
12116	N	79.66900	57.69580	72.21290	67.36990	405.06377	-737.60215	1
12117	H	79.23700	56.80280	72.31390	1052.74506	-1323.30612	2653.07651	1
12118	C	78.91900	58.95380	72.34290	673.98104	4.29476	614.15154	1
12119	H	79.04000	59.54580	71.44790	-1796.10232	2269.58137	1233.38685	1
12120	C	77.45800	58.71880	72.77690	817.18460	-349.45788	-203.81249	1
12121	H	76.82600	59.62580	72.87990	-1459.46663	-662.24447	2707.32629	1
12122	H	77.44500	58.21880	73.76890	-2750.54998	1059.53428	1100.04007	1
12123	C	76.64300	57.82380	71.87090	570.71445	-85.92804	705.94079	1
12124	C	76.58300	58.10480	70.48090	196.61060	-845.10815	-280.33459	1
12125	H	77.12200	58.96280	70.10690	-2022.26458	1442.80133	-1930.54307	1
12126	C	75.81100	57.35880	69.59390	-620.67473	-144.62225	652.14898	1
12127	H	75.76500	57.60680	68.54390	-1774.85020	-1785.31973	-1886.99933	1
12128	C	75.22600	56.17080	70.00690	507.99053	-715.82818	246.95473	1
12129	O	74.53900	55.28780	69.16190	636.89690	24.24144	466.26378	1
12130	H	74.41500	54.44180	69.59890	-1229.13574	-2728.82755	-970.02668	1
12131	C	75.90500	56.70580	72.30390	-438.06824	-219.52237	768.99750	1
12132	H	75.83900	56.41280	73.34090	-1389.16845	2304.19206	1630.68580	1
12133	C	75.30900	55.81680	71.36490	-138.47807	486.79549	-758.48862	1
12134	H	74.94300	54.87280	71.74090	1875.29069	1905.15049	-1658.88899	1
12135	C	79.49600	59.91880	73.36590	314.93220	-626.23050	583.18443	1
12136	O	79.75100	61.08780	73.13790	166.40047	34.09026	-771.21720	1
12137	N	79.82100	59.45580	74.55290	-641.07289	-340.81376	-430.74798	1
12138	H	79.68400	58.49580	74.78390	2770.00984	-1453.88336	-333.90849	1
12139	C	80.44200	60.30880	75.56290	-729.93127	358.94081	-412.08353	1
12140	H	79.90500	61.24580	75.55490	-2787.83190	-900.98633	-1146.49167	1
12141	C	80.24100	59.73180	76.98690	332.98027	551.74550	-645.09848	1
12142	H	80.77400	60.48080	77.61190	2466.17135	124.53770	1949.54237	1
12143	H	80.74600	58.75980	77.17490	-1127.69053	2483.20785	-1568.50855	1
12144	C	78.72500	59.53680	77.40490	-655.38688	470.08820	-425.36587	1

12145	H	78.16700	60.42180	77.03090	2662.62756	1561.17670	-609.39974	1
12146	H	78.24300	58.62080	77.00190	-2099.73270	-1947.48585	1302.55430	1
12147	C	78.50600	59.36680	78.91590	31.97752	198.73558	889.34392	1
12148	H	78.94700	58.43680	79.33590	-74.44478	2293.05552	2152.80760	1
12149	H	77.42800	59.16480	79.09190	-1970.42781	-1072.69218	2205.66815	1
12150	N	79.05000	60.55680	79.71390	-229.64616	496.03660	643.33710	1
12151	H	79.41200	61.35180	79.22890	833.13704	-2924.64675	-806.56697	1
12152	C	79.10800	60.62180	81.05290	124.60381	-647.79417	-629.51379	1
12153	N	78.65600	59.79180	81.93890	-677.75721	-278.89576	418.96851	1
12154	H	78.00100	59.08680	81.66790	-1755.95806	-2224.39321	1366.35001	1
12155	H	78.68000	60.11080	82.88590	-1983.36234	-1569.63800	-1871.02555	1
12156	N	79.61200	61.72080	81.54490	-334.65245	-585.25440	-508.09184	1
12157	H	79.92100	62.44280	80.92490	-1562.22485	1491.63732	2287.50909	1
12158	H	79.73600	61.78780	82.53490	-1795.71036	1793.17424	-1859.61734	1
12159	C	81.91100	60.65180	75.26890	616.82672	440.14893	-507.19298	1
12160	O	82.34700	61.74380	75.64890	408.96491	673.97556	-46.17215	1
12161	N	82.63500	59.80580	74.56990	-190.24542	70.08760	-819.49173	1
12162	H	82.35300	58.85480	74.46790	-2529.63481	1462.88648	1165.82036	1
12163	C	83.96700	60.27580	74.06590	580.48783	-682.68440	168.60276	1
12164	H	84.51900	60.58080	74.94290	-2015.52347	-270.18547	2400.60225	1
12165	C	84.76500	59.15580	73.29790	807.44994	-162.97781	-391.04198	1
12166	H	84.27400	58.99080	72.31490	-1304.61225	1425.38317	-2482.84029	1
12167	H	84.62400	58.26080	73.94190	-1610.06251	2701.87052	76.29298	1
12168	C	86.25700	59.33680	73.14890	-736.82847	197.47386	499.53867	1
12169	H	86.42000	60.38280	72.81090	2282.69942	-2080.27261	-599.97954	1
12170	C	86.99400	59.10380	74.43890	-132.79600	758.65012	-488.12522	1
12171	H	88.03400	59.42780	74.21690	2316.28189	2059.60012	539.54772	1
12172	H	86.66200	59.73080	75.29390	1764.69691	-1722.13532	1954.05245	1
12173	H	86.94000	58.03480	74.73590	1618.11774	1947.21808	1867.68921	1
12174	C	86.78800	58.36680	72.08090	-33.05601	290.32281	863.75400	1
12175	H	86.63600	57.36080	72.52590	-1363.19630	2394.79000	-1518.19067	1
12176	H	87.88400	58.53880	72.02790	-262.56333	2650.23136	1674.98074	1
12177	H	86.34700	58.51580	71.07190	-2542.66483	1742.60188	629.61931	1
12178	C	83.83400	61.42680	73.15390	-349.49611	-412.57976	-734.22164	1
12179	O	84.63000	62.37580	73.26490	653.38230	407.13363	-175.95740	1
12180	N	82.85300	61.48880	72.22890	-696.62291	-443.72975	-174.62165	1
12181	H	82.23800	60.70680	72.16490	2557.02351	1717.87314	-639.35033	1
12182	C	82.51100	62.67080	71.40490	-174.66495	893.03350	-58.60317	1
12183	H	83.43700	63.02080	70.97290	2742.09203	936.70899	1225.45248	1
12184	C	81.45100	62.39580	70.30990	654.62704	631.74434	61.75378	1
12185	H	80.52300	61.97280	70.74890	-1124.67376	1215.25919	2675.15986	1
12186	H	81.11100	63.34480	69.84290	-1237.27166	-1033.78453	2701.60593	1
12187	N	83.07400	62.04880	68.49190	-65.61244	-824.28130	170.08128	1
12188	C	81.94000	61.60380	69.18490	553.72523	-722.80060	48.97612	1
12189	C	83.07900	61.30880	67.38090	-156.05578	800.76146	-407.28207	1
12190	H	83.93400	61.31080	66.70590	2707.28651	1600.97032	75.63083	1
12191	N	82.06700	60.43080	67.32990	27.73325	691.53841	-483.40230	1
12192	H	81.96900	59.68080	66.67590	2123.25559	2320.04986	-85.91020	1
12193	C	81.28500	60.67180	68.46190	751.95162	343.93963	-384.35049	1
12194	H	80.30900	60.21780	68.57990	2039.24247	190.54477	2388.18112	1
12195	C	81.99700	63.82580	72.29390	-160.21988	-892.31250	-97.77014	1
12196	O	82.45800	64.95180	72.13090	-742.17490	52.02864	-264.75775	1
12197	N	81.10700	63.58780	73.24290	-506.89933	-356.14508	573.48587	1
12198	H	80.64000	62.70880	73.29990	2261.43733	582.87510	-2108.17079	1
12199	C	80.62600	64.63480	74.15290	540.92378	420.08690	601.97962	1
12200	H	80.25900	65.41980	73.50690	1104.64224	2675.80596	-1232.09343	1
12201	C	79.51400	64.01580	75.02690	487.40404	679.16621	364.17243	1
12202	H	78.93200	63.32680	74.37890	1781.37923	-1451.21758	2149.15839	1
12203	H	80.05900	63.34980	75.72990	2047.54260	2138.23628	-1064.77281	1
12204	C	78.65200	64.92580	75.86790	150.99140	893.23266	-103.86534	1
12205	H	79.32500	65.43280	76.59190	1577.40469	-164.99908	-2717.13010	1
12206	C	77.84300	65.91680	75.11090	402.88510	394.90242	-716.37049	1

12207	H	78.40300	66.58380	74.41990	-2081.17384	-2130.37170	-1014.12924	1
12208	H	77.04300	65.37980	74.55790	1427.12257	-2280.78150	1630.82284	1
12209	H	77.34800	66.57180	75.85890	474.44067	676.84145	-3035.62480	1
12210	C	77.73700	63.96780	76.62590	178.26637	-636.12688	-628.50194	1
12211	H	78.25600	63.31880	77.36390	-2268.84858	-1446.41660	1630.46968	1
12212	H	77.23500	63.24180	75.95090	-2030.35526	-471.07066	-2356.68754	1
12213	H	77.01400	64.60180	77.18190	1036.87980	2968.51869	-104.89656	1
12214	C	81.76100	65.29180	74.99290	343.66896	299.69006	789.63822	1
12215	O	81.80900	66.50180	75.10190	447.19691	528.48600	379.92722	1
12216	N	82.73700	64.49880	75.49490	-433.79278	387.28297	-611.97060	1
12217	H	82.74800	63.51180	75.35190	2667.48998	-1434.27704	-851.80562	1
12218	C	84.02000	64.94880	76.06590	574.89745	-680.42524	194.84716	1
12219	H	83.77900	65.63080	76.86790	-1563.71622	1465.41777	2303.38199	1
12220	C	84.77200	63.73480	76.76590	595.79640	-682.68278	-102.08756	1
12221	H	85.81700	64.05580	76.96690	-1289.96943	2325.87140	1680.63301	1
12222	H	84.71000	62.84780	76.09990	2126.61121	2034.22205	-1112.51591	1
12223	O	84.15300	63.55380	78.01490	486.11575	-42.96009	-620.86483	1
12224	H	84.37800	64.25280	78.63390	-1787.26086	2063.96930	1563.31558	1
12225	C	84.93100	65.67980	75.13190	-663.49168	-288.52248	554.96358	1
12226	O	85.56500	66.64980	75.53790	-588.04176	-513.33378	-119.67683	1
12227	N	85.05100	65.29680	73.86190	-259.51888	742.08221	307.63002	1
12228	H	84.70800	64.42780	73.51290	-2106.68035	-139.62095	2332.51583	1
12229	C	85.69500	66.04380	72.82190	573.02431	366.65430	-607.17277	1
12230	H	86.70800	66.33380	73.05990	2764.78709	-1501.37226	-7.74138	1
12231	C	85.74100	65.15480	71.54090	-133.05896	-869.20207	-241.31740	1
12232	H	84.87900	64.46080	71.44990	148.62272	2088.94663	-2347.85849	1
12233	C	85.79600	65.94080	70.19390	454.61833	-363.57527	701.84486	1
12234	H	84.86900	66.50480	69.95490	2551.92878	-1366.56206	1232.23125	1
12235	H	85.96200	65.21880	69.36590	-1476.37308	-34.90144	-2778.00840	1
12236	H	86.63500	66.66980	70.17690	-1292.00135	2545.19150	1323.23807	1
12237	C	87.01400	64.26180	71.59490	-392.54470	622.82292	538.00676	1
12238	H	86.82200	63.39980	72.26990	-891.72079	-2485.89783	1709.78719	1
12239	H	87.92700	64.84480	71.84190	315.63313	-2973.12995	979.33663	1
12240	H	87.23900	63.84180	70.59090	-3023.59537	-818.79082	292.70952	1
12241	C	84.98600	67.39680	72.55390	-382.12363	-807.35395	-183.33613	1
12242	O	85.69000	68.41580	72.40690	210.25598	-515.88228	559.71879	1
12243	N	83.64700	67.48780	72.47490	216.00212	-314.44842	-753.08536	1
12244	H	83.09500	66.66380	72.57690	1593.33848	328.35976	2692.89409	1
12245	C	82.92000	68.76280	72.32790	-515.80784	257.10074	-706.60632	1
12246	H	83.22900	69.31680	71.45390	2024.47698	1690.93538	-1714.77600	1
12247	C	81.43200	68.40580	72.15790	648.50536	-302.09253	565.35997	1
12248	H	80.91900	69.33580	71.83390	-1725.51672	1315.79795	-2278.04610	1
12249	H	80.92200	68.18880	73.12090	-1757.06882	-1744.11894	1941.38727	1
12250	H	81.28100	67.60480	71.40290	-737.82683	1519.08542	2654.47119	1
12251	C	83.14400	69.72080	73.44490	-395.42291	812.29268	123.58130	1
12252	O	83.43900	70.90080	73.25090	539.79206	559.36134	-139.16412	1
12253	N	83.00700	69.24380	74.69190	-34.22935	573.50717	-618.53873	1
12254	H	82.62000	68.33680	74.84090	2966.83186	973.23497	385.93867	1
12255	C	83.27700	70.00580	75.90190	873.70478	24.39264	259.79983	1
12256	H	82.61000	70.85480	75.90990	-2612.51722	-285.31065	1729.61782	1
12257	C	83.12800	69.09680	77.13590	-189.12856	-631.34043	630.15130	1
12258	H	83.48300	69.52780	78.09690	-429.88148	1737.22478	2587.56221	1
12259	H	83.61800	68.12180	76.92790	552.37381	-3048.72003	-546.27430	1
12260	C	81.58900	68.79880	77.42290	506.34032	746.12677	-135.51871	1
12261	O	80.75700	69.59680	76.91990	634.58558	468.81093	33.83312	1
12262	O	81.33500	67.81580	78.15690	-681.02272	-129.27330	-378.31692	1
12263	C	84.71100	70.58080	75.95190	717.95488	52.30739	559.69253	1
12264	O	84.86800	71.75680	76.30490	-392.94383	-427.35786	535.33880	1
12265	N	85.74100	69.79480	75.67590	-415.04889	265.39372	-685.54568	1
12266	H	85.60700	68.83480	75.43990	2137.04559	-2200.43123	699.54610	1
12267	C	87.13300	70.09780	75.63590	-188.65217	-889.33474	-70.32133	1
12268	H	87.32400	70.52680	76.60790	1091.87028	-2116.68285	2055.65056	1

12269	C	87.91400	68.77880	75.41390	489.60820	-592.84580	490.17207	1
12270	H	87.59900	68.21680	74.50790	700.09827	2650.52625	1543.63184	1
12271	H	87.63200	68.11480	76.25890	-2482.03662	1382.94635	1350.99216	1
12272	C	89.44000	68.82480	75.48290	692.80416	570.40126	-161.60383	1
12273	H	89.72900	69.58180	74.72290	298.18466	-1746.60285	2599.74818	1
12274	C	89.94100	69.29480	76.88690	181.95516	681.49958	577.84223	1
12275	H	89.75800	68.53080	77.67190	2543.27422	1849.91670	-88.26466	1
12276	H	91.05200	69.32680	76.88190	1546.58761	710.38340	2646.06281	1
12277	H	89.44900	70.26980	77.09490	2913.61036	807.48848	870.09380	1
12278	C	89.95100	67.43480	75.03090	-434.95320	-440.02011	669.81267	1
12279	H	89.65900	67.25180	73.97490	-2229.65148	-1205.77526	1863.59505	1
12280	H	91.05800	67.51580	75.08490	-2346.62516	2037.49304	-490.10068	1
12281	H	89.58900	66.62280	75.69590	2317.98498	2115.13878	226.62696	1
12282	C	87.46200	71.14180	74.60090	243.29597	-515.30183	711.84416	1
12283	O	88.19800	72.07180	74.83790	242.16191	-373.73155	652.15762	1
12284	N	86.84400	71.04980	73.39090	-206.19084	-790.70397	212.00203	1
12285	H	86.17000	70.32580	73.26190	-2329.37301	-1645.87292	1327.91187	1
12286	C	87.01800	71.85880	72.20590	-797.26164	-385.05976	-218.06846	1
12287	H	88.03400	71.65880	71.90090	-1368.50983	-1180.41086	-2575.27421	1
12288	C	86.05600	71.26180	71.07990	-544.54715	-641.45881	351.35453	1
12289	H	85.03600	71.30180	71.51890	1898.93754	-2218.42496	1170.83439	1
12290	H	86.42000	70.23180	70.88090	-1156.17871	-2079.34627	2058.59080	1
12291	C	86.06000	71.96180	69.68690	-557.49996	616.60391	-374.75914	1
12292	H	85.52600	72.93580	69.71790	1897.10684	-331.51851	2487.83186	1
12293	C	87.48200	72.28980	69.17990	222.43514	-630.28591	-620.25259	1
12294	H	88.21400	71.45680	69.22790	757.91180	3044.92607	228.51948	1
12295	H	87.92000	73.10780	69.79090	-673.91154	2373.74099	-1951.77436	1
12296	H	87.44600	72.71180	68.15290	1938.39703	1427.72827	2025.44691	1
12297	C	85.20100	71.16880	68.59090	73.40772	-590.80600	690.65952	1
12298	H	85.60800	70.14180	68.47390	358.89761	-2861.34974	1257.81414	1
12299	H	84.15200	71.20580	68.95590	-2358.21230	2029.33669	-467.81789	1
12300	H	85.20300	71.73380	67.63390	1743.93046	-27.50855	-2618.43007	1
12301	C	86.64900	73.30080	72.42790	172.18240	-757.68989	477.18996	1
12302	O	87.45100	74.21280	72.17190	122.55922	-369.80880	-686.91187	1
12303	N	85.50800	73.52580	73.11090	162.34887	-288.33841	-776.64412	1
12304	H	84.97100	72.71180	73.31890	2621.72506	-1513.35586	-857.05191	1
12305	C	85.11500	74.80280	73.59690	627.09744	-477.05513	458.93159	1
12306	H	85.32400	75.60080	72.90090	1530.70822	1534.00608	-2280.78581	1
12307	C	83.55300	74.85180	73.84290	675.88439	204.91434	576.75073	1
12308	H	83.38800	74.05380	74.59790	-1785.28981	-1117.81202	2336.97728	1
12309	H	83.04800	74.70080	72.86490	-1449.53844	-2337.75312	1527.08051	1
12310	C	83.06600	76.20680	74.31390	-316.55822	790.68701	325.66234	1
12311	C	83.49400	77.39480	73.61290	-683.51343	354.64960	488.34830	1
12312	H	84.09300	77.25680	72.72490	-727.13514	2292.88436	-2027.85158	1
12313	C	83.02700	78.64780	74.04590	593.16071	-653.76433	-228.48102	1
12314	H	83.34500	79.53480	73.51790	2491.16766	408.28340	1877.66200	1
12315	C	82.11700	78.73280	75.12690	-66.97421	795.26514	-441.04288	1
12316	H	81.80600	79.73380	75.39090	-2023.60898	283.96525	2392.19495	1
12317	C	82.25700	76.31380	75.36790	516.22629	691.61670	-294.32595	1
12318	H	81.88900	75.42480	75.85690	-283.41445	3128.62409	-172.08652	1
12319	C	81.80600	77.52180	75.83390	161.00809	-648.26628	-620.70785	1
12320	H	81.02300	77.59480	76.57490	1616.68512	1950.46833	1865.53712	1
12321	C	85.85600	75.28680	74.89890	558.42224	-319.32804	646.25476	1
12322	O	86.21200	76.46780	74.94090	-617.03132	-329.65839	366.36720	1
12323	N	86.17100	74.39980	75.83690	365.84895	181.75465	738.77743	1
12324	H	86.02200	73.41680	75.76590	-963.78762	622.65670	2929.44334	1
12325	C	86.82000	74.75980	77.14490	92.88478	-707.91608	567.16686	1
12326	H	86.15300	75.48880	77.57990	-2690.93431	370.99464	1587.28125	1
12327	C	86.94000	73.58780	78.11590	410.88764	701.60620	-412.76033	1
12328	H	87.14500	72.68280	77.50590	2428.38666	1806.31783	859.29061	1
12329	C	88.11000	73.73880	79.17790	432.87521	-784.56392	-168.90679	1
12330	H	89.11200	73.50380	78.75790	-2802.28668	8.86839	-1430.15277	1

12331	H	87.89000	73.00680	79.98390	1689.26299	-2020.98145	1720.53793	1
12332	H	88.01200	74.79180	79.51590	-2365.18424	1456.71194	-1477.20008	1
12333	C	85.60400	73.41880	78.88190	489.21410	391.20761	662.62898	1
12334	H	85.67200	72.50580	79.51190	2305.33576	1919.54368	-948.15892	1
12335	H	85.36200	74.27280	79.54890	1150.20989	-2924.23098	-155.29525	1
12336	H	84.74200	73.40480	78.18090	848.83691	-2268.82709	2007.51732	1
12337	C	88.17300	75.40380	76.92690	269.85313	-698.95484	-519.70416	1
12338	O	88.54300	76.32780	77.61390	222.86699	-474.16548	-590.86769	1
12339	N	88.89700	74.85580	75.91890	-237.45874	-514.82712	-625.49074	1
12340	H	88.53000	74.08180	75.40890	-401.06002	2256.45471	2155.40930	1
12341	C	90.29200	75.32580	75.66290	-228.46060	-244.74551	848.14880	1
12342	H	90.89600	75.29980	76.55790	2246.14420	1860.68591	-1179.36865	1
12343	C	90.95300	74.41080	74.56690	341.32691	764.75637	360.68634	1
12344	H	90.23300	74.14880	73.76190	2554.11733	1652.47885	802.51140	1
12345	C	92.24400	75.00980	73.95790	-637.87628	639.76897	123.53346	1
12346	H	92.97600	75.11480	74.78690	-1452.19126	1638.97488	2259.01043	1
12347	H	92.67300	74.27880	73.23890	1802.54928	-2168.26235	1395.59331	1
12348	H	91.99400	75.90680	73.35290	2254.70122	-2192.03053	-97.72796	1
12349	C	91.30800	73.01580	75.20290	580.51474	-213.05230	-670.12115	1
12350	H	90.39500	72.66380	75.72790	-1253.55495	2442.55631	1536.47157	1
12351	H	92.16300	73.06880	75.90890	-2566.35490	-1170.15823	-1393.83589	1
12352	C	91.58000	71.93880	74.11790	-544.80879	723.46474	105.98658	1
12353	H	92.58900	72.13780	73.69690	-1849.55825	1926.39631	1663.23713	1
12354	H	90.83500	71.82580	73.30090	3081.44701	557.50540	303.47698	1
12355	H	91.68900	70.94580	74.60390	1172.41242	2849.92965	-633.70050	1
12356	C	90.27000	76.76580	75.16090	43.99705	529.99175	-740.69157	1
12357	O	91.26100	77.50980	75.35290	-669.29467	-418.02486	-30.44806	1
12358	N	89.15800	77.21180	74.50990	-185.76579	-545.19233	-617.19420	1
12359	H	88.43600	76.60280	74.19090	1200.96570	1543.34285	2464.54873	1
12360	C	89.12800	78.59280	74.10490	384.61821	503.00683	656.12801	1
12361	H	90.03400	78.84180	73.57190	1476.59375	-1263.13412	-2474.34624	1
12362	C	87.93400	78.86780	73.12990	-21.66292	-737.14628	536.28078	1
12363	H	88.03500	79.86580	72.65290	882.49886	-2368.00120	-1874.03103	1
12364	O	86.60800	78.75480	73.78290	501.75101	-525.68570	309.07555	1
12365	H	86.49900	77.90180	74.21090	3140.14368	27.99916	192.19760	1
12366	C	87.97000	77.75680	72.01390	-713.52948	-542.73673	-166.62390	1
12367	H	87.68400	76.74380	72.36890	1938.00761	2469.06701	-214.61793	1
12368	H	87.16200	78.06680	71.31790	1565.64258	-1314.16470	-2391.64393	1
12369	H	88.96600	77.83780	71.52890	202.51630	-1564.01020	2722.33089	1
12370	C	88.96700	79.58880	75.24390	-546.08792	-598.26994	-418.70284	1
12371	O	89.33600	80.75080	75.13190	-473.21638	-515.99724	-365.29486	1
12372	N	88.46200	79.15180	76.40990	-43.52075	-816.92906	-208.33901	1
12373	H	88.27300	78.17780	76.50590	-1752.13224	-1467.47552	-2162.12267	1
12374	C	88.07500	80.00680	77.54090	-22.34412	188.91236	891.77568	1
12375	H	87.30100	80.66680	77.17790	2302.06814	330.51885	-2118.83595	1
12376	C	87.30500	79.28680	78.65090	-594.77166	183.24338	-666.42294	1
12377	H	87.05400	79.85480	79.57290	-1998.90857	1716.74723	-1719.11887	1
12378	H	87.98500	78.45680	78.93890	48.26060	-2588.39189	1787.77084	1
12379	C	85.94700	78.73980	78.20890	-391.05240	313.85106	761.59473	1
12380	H	86.02600	78.13580	77.27990	-2803.23397	1413.33989	-206.33925	1
12381	C	85.44800	77.83980	79.37790	-895.95207	-10.76464	-169.13015	1
12382	H	86.11200	76.94880	79.37190	227.33190	-2794.30265	-1427.73216	1
12383	H	85.48900	78.35180	80.36290	-2610.76036	1750.12024	-138.69293	1
12384	H	84.39600	77.56880	79.14390	-3046.09747	-127.33998	776.72450	1
12385	C	84.96300	79.87180	77.92290	-896.33437	84.57238	144.51028	1
12386	H	85.05400	80.27480	76.89190	2459.16703	1961.86027	42.75521	1
12387	H	85.04300	80.76780	78.57490	-1997.82917	-1897.36799	-1518.84809	1
12388	H	83.95600	79.43980	78.10290	832.03319	-1456.25588	-2661.81626	1
12389	C	89.17800	80.94580	78.08890	-711.38404	491.58397	289.35955	1
12390	O	88.80600	82.04980	78.42590	650.20613	447.96805	13.55916	1
12391	N	90.47200	80.68380	78.13390	-569.16004	-19.26878	623.18364	1
12392	C	90.96500	79.30680	78.36890	-409.24103	-448.61170	-680.23550	1

12393	H	91.18800	78.92780	77.34790	-1619.60431	1655.05126	2129.76839	1
12394	H	90.26700	78.62680	78.90290	-1439.77459	-1857.19598	-2091.91263	1
12395	C	91.54100	81.64680	78.45690	-29.16890	-449.96339	-792.54850	1
12396	H	91.23900	81.98780	79.43590	1756.31519	-1808.82317	-1881.95163	1
12397	C	92.73700	80.82480	78.49790	-842.40104	144.23372	-317.81774	1
12398	H	93.63600	81.30280	78.94390	415.84241	-1809.51773	2539.87143	1
12399	H	93.12400	80.48380	77.51490	16.29837	-2368.52761	-2070.75773	1
12400	C	92.24000	79.53580	79.14890	-347.10386	-211.95636	816.11544	1
12401	H	92.99800	78.74380	78.96890	-2027.24786	2403.32760	-111.84286	1
12402	H	92.10900	79.69280	80.24090	1908.09932	919.17948	-2326.47637	1
12403	C	91.62700	82.88080	77.58990	248.42227	689.14329	-542.97228	1
12404	O	92.02600	83.95080	78.05690	149.28934	-171.04220	756.36267	1
12405	N	91.29900	82.78080	76.30590	-331.25744	596.28516	-497.37794	1
12406	H	91.10600	81.91780	75.84690	1445.82965	2792.18114	-107.36550	1
12407	C	91.14300	83.99380	75.47590	612.29400	-318.80955	-595.74116	1
12408	H	92.02900	84.60980	75.52090	341.74386	2835.43554	1319.75097	1
12409	C	90.89300	83.53080	73.98690	517.51697	-499.03601	-560.88346	1
12410	H	89.88900	83.05780	73.93690	2128.87328	1637.00740	1639.00321	1
12411	H	90.85600	84.47980	73.41090	-1256.47112	2228.18795	-1831.57992	1
12412	C	92.01000	82.69580	73.39690	-547.41416	493.30768	537.06264	1
12413	C	93.29400	83.19280	73.34590	786.37913	-200.80348	415.61620	1
12414	H	93.55400	84.19180	73.66590	2082.03614	1130.29365	-2070.21448	1
12415	C	94.39900	82.58680	72.68290	-618.47257	-290.02323	604.01093	1
12416	H	95.32400	83.13780	72.59590	655.95752	2022.12489	2319.25783	1
12417	C	94.10100	81.35380	72.07090	600.09640	408.89255	551.49089	1
12418	H	94.80900	80.81280	71.46190	2045.02833	-1258.14154	-2033.01875	1
12419	C	91.83500	81.41480	72.88390	-370.64793	-315.48317	-771.06516	1
12420	H	90.85900	80.95880	72.95990	2820.84396	1337.61107	-389.69505	1
12421	C	92.82900	80.73080	72.21990	278.11087	868.36814	-6.49039	1
12422	H	92.53500	79.82280	71.71490	666.69203	-2802.82065	1264.09824	1
12423	C	90.05300	84.85580	75.95490	652.77190	565.18946	-293.08825	1
12424	O	90.04382	86.12708	75.80982	551.75189	-751.08952	-357.54008	1
12425	N	88.89800	84.23980	76.38290	-68.55996	-686.47804	486.53851	1
12426	H	88.83200	83.24980	76.48090	1531.30311	541.27594	-2694.50503	1
12427	C	87.77100	84.95680	77.05290	-791.18086	69.28925	447.97639	1
12428	H	87.68876	85.71860	76.22213	-4.32545	2646.19084	-211.75168	1
12429	C	86.55800	84.09580	77.20590	170.10671	496.42605	745.70496	1
12430	H	85.74200	84.75480	77.57290	-13.09365	1988.53377	2437.98856	1
12431	H	86.63600	83.28580	77.96190	-1439.65630	-2248.20643	1664.68730	1
12432	C	85.94200	83.48480	75.94290	-435.11005	-533.77840	-597.67121	1
12433	C	86.43200	82.68380	74.93490	-338.30142	779.26114	331.29328	1
12434	H	87.49000	82.51880	74.79890	2684.63309	-1076.73425	1237.58425	1
12435	N	85.42800	82.11980	74.20990	-285.59101	719.79103	336.17099	1
12436	H	85.59200	81.26780	73.76190	-655.80785	1782.74557	-2507.97937	1
12437	C	84.25200	82.63580	74.59690	748.67870	-449.43296	-262.56661	1
12438	C	84.51500	83.48880	75.69290	567.91079	473.39531	533.69019	1
12439	C	83.41000	84.02980	76.41090	-681.13713	147.45827	588.01299	1
12440	H	83.66700	84.57280	77.30890	-3135.43706	-243.59415	-89.00881	1
12441	C	82.13800	83.76480	75.96090	-655.08090	-465.58235	430.75873	1
12442	H	81.32000	84.18880	76.52390	2399.43516	-859.68149	1844.41993	1
12443	C	82.96000	82.40980	74.11690	-616.67597	-657.02197	139.58467	1
12444	H	82.82800	81.82880	73.21690	3104.40561	-417.61983	294.08451	1
12445	C	81.86200	82.98280	74.83290	-43.05539	653.94095	634.00195	1
12446	H	80.85600	82.74780	74.51690	1531.88442	-1265.78041	2439.13024	1
12447	C	88.13266	85.68063	78.48468	421.46270	1341.89035	-82.79167	1
12448	O	87.77254	86.84656	78.75851	96.64544	-454.22717	308.63216	1
12449	N	88.88700	84.89880	79.22090	-38.26233	140.60432	-831.52794	1
12450	H	89.17100	83.95280	79.08290	-2208.21740	-2231.00887	-211.19081	1
12451	C	89.39254	85.43960	80.41420	285.90960	-650.72515	-479.79882	1
12452	H	88.62010	86.00012	80.95697	2005.60584	1428.38417	239.39926	1
12453	C	90.14400	84.27080	81.25390	380.34768	-503.85067	657.96744	1
12454	H	90.98300	83.74980	80.74590	2224.12780	1539.57874	-1606.60483	1

12455	H	89.46800	83.42280	81.49390	-1277.95220	882.25521	-2736.18167	1
12456	H	90.53800	84.71780	82.19190	-2540.64013	-1854.78556	-56.07572	1
12457	C	90.46454	86.67372	80.09553	612.86482	17.34437	321.95628	1
12458	O	91.01738	87.17700	81.04709	-327.98072	-38.68055	-104.89974	1
12459	N	90.70918	86.94281	78.82301	602.17844	120.86078	-396.98466	1
12460	H	90.20806	86.26402	78.24466	-2872.89360	-1690.14412	1046.74332	1
12461	C	91.31575	88.15698	78.32224	-794.05089	-239.06163	162.35325	1
12462	H	91.63957	88.55964	79.27610	1051.17072	548.45034	-603.70724	1
12463	C	92.36897	87.76962	77.23097	281.78538	222.64818	-16.40651	1
12464	H	91.80059	87.57079	76.34403	310.41360	2121.21580	-1158.78356	1
12465	C	93.23977	89.03190	77.07087	-881.96558	-681.90610	848.47989	1
12466	H	93.74850	89.01220	76.07268	-1004.31153	-984.71042	2166.56403	1
12467	H	92.60733	89.90739	77.07508	987.99132	-34.86022	55.86690	1
12468	H	94.04654	89.16440	77.88213	931.50072	2225.75660	1565.01330	1
12469	C	93.22427	86.64411	77.55332	-602.49045	-665.55288	-305.15575	1
12470	H	93.85327	86.35892	76.67925	-28.49928	1563.17898	585.41060	1
12471	H	92.63860	85.67831	77.88920	2308.46298	533.20900	-2958.55561	1
12472	H	93.92428	86.94752	78.35276	-3041.06815	2143.69431	2318.72415	1
12473	C	90.38324	89.15450	77.46361	-309.13347	32.41411	583.12087	1
12474	O	90.39236	90.40464	77.68860	248.18783	-57.67136	-119.03124	1
12475	N	89.53347	88.58471	76.71000	-113.88764	185.83193	-5.43636	1
12476	H	89.53088	87.50031	76.45564	-1344.85052	882.72869	49.91231	1
12477	C	88.58762	89.42839	75.96446	209.79288	318.61737	424.77592	1
12478	H	89.22909	90.24125	75.49579	398.54541	-835.74506	208.02304	1
12479	C	87.92468	88.47275	74.94169	34.49022	-44.90451	30.60544	1
12480	H	88.55343	87.57343	74.80284	211.12861	-745.34354	-584.21100	1
12481	H	86.93620	88.17367	75.28670	-567.68853	353.77062	-437.81733	1
12482	C	87.71140	89.25733	73.58730	-615.02779	-553.43110	-808.75007	1
12483	O	87.35030	88.68992	72.51161	300.61252	319.43422	-135.27365	1
12484	O	87.75379	90.48734	73.66575	261.96608	-273.70168	324.16190	1
12485	C	87.50164	90.10364	77.03409	-348.43488	320.35727	1226.11757	1
12486	O	86.98364	91.16796	76.76672	-277.40784	-1002.68758	132.78945	1
12487	N	87.28471	89.31552	78.02627	-497.35492	-1358.81001	829.36719	1
12488	H	87.64389	88.27674	78.12606	2151.23698	1527.11206	-3150.50481	1
12489	C	86.37797	89.67550	79.06429	832.41363	512.83438	-1.95082	1
12490	H	85.69674	90.42552	78.69028	-1044.24945	-2184.56814	777.11029	1
12491	C	85.86526	88.47082	79.89938	575.65881	298.01353	-155.91740	1
12492	H	85.21659	87.87507	79.20139	-451.15760	-608.26813	1458.14200	1
12493	H	86.65912	87.80939	80.31565	166.35726	1197.13600	-795.04489	1
12494	H	85.19591	88.70979	80.79304	852.73562	-3417.81344	-1396.48802	1
12495	C	87.28267	90.36473	80.30419	1163.14708	304.80842	-83.75883	1
12496	O	87.10485	90.09668	81.49681	197.86614	100.26025	59.12811	1
12497	N	88.32458	91.00807	79.79835	141.58408	751.12205	890.32881	1
12498	H	88.21487	91.13915	78.80227	-1269.31468	794.52918	-3242.10914	1
12499	C	89.04968	91.94052	80.61235	-517.70292	-95.58544	-491.41363	1
12500	H	88.35831	92.19563	81.47857	-108.18851	1282.25492	-5508.22298	1
12501	C	90.26873	91.14750	81.15279	-471.74405	481.41836	178.56037	1
12502	H	91.09055	90.89622	80.42707	1364.63360	-1444.49244	-2284.58820	1
12503	C	90.86576	92.09000	82.28638	348.20003	-678.22616	574.87303	1
12504	H	89.95376	92.12889	82.97642	-1236.18264	2110.71978	1624.06677	1
12505	H	91.79180	91.65227	82.74773	-245.00381	1614.84158	1260.49763	1
12506	H	91.18867	93.09809	81.97738	-1917.59713	2950.86957	258.95719	1
12507	C	89.98064	89.75175	81.78579	-148.22393	329.79114	509.98611	1
12508	H	89.68477	88.95558	81.02536	-1502.56943	-4433.96826	-148.72874	1
12509	H	89.33149	89.81477	82.66909	-247.01519	527.46716	-1892.37899	1
12510	H	90.87869	89.24852	82.21902	2204.35986	2367.17477	767.02874	1
12511	C	89.47309	93.27534	79.76155	767.97488	-235.24695	-11.47387	1
12512	O	89.19199	94.32653	80.23080	1050.03570	948.62731	484.40632	1
12513	N	90.13700	93.02546	78.61364	-603.01862	-186.15632	-110.59265	1
12514	H	90.32077	92.02617	78.30345	-1586.76166	477.02278	1935.43690	1
12515	C	91.26293	93.86673	78.24332	-450.58533	311.44376	-66.18155	1
12516	H	90.99153	94.88471	78.62982	1969.93169	516.90871	1630.18504	1

12517	C	92.58802	93.38522	78.92452	458.01359	399.42698	-672.13354	1
12518	H	92.71009	92.28713	78.97380	2403.00023	3065.11097	352.80324	1
12519	H	93.45596	93.78907	78.33817	-608.29842	691.08343	2431.40796	1
12520	H	92.66941	93.66304	80.02309	-1699.67296	-3118.08163	1112.12524	1
12521	C	91.34328	93.79923	76.61427	-413.05745	-454.81226	496.36330	1
12522	O	91.24849	94.84663	76.01471	1024.23715	-576.80642	-581.88173	1
12523	N	91.66990	92.56544	76.18710	-233.43076	1134.70946	-477.31872	1
12524	H	91.42421	91.71765	76.79243	-3147.52323	1333.41025	517.81623	1
12525	C	91.64980	92.64362	74.69334	-637.34104	-206.49146	1.77623	1
12526	H	90.79713	93.30422	74.36173	-2608.85078	-2106.66949	291.22792	1
12527	C	92.89797	93.32723	74.05079	1011.75876	538.01215	753.89330	1
12528	H	93.52421	93.70575	74.90543	3043.49066	-2191.28001	2859.97668	1
12529	H	93.63728	92.66922	73.51283	-177.73269	-871.86589	922.23930	1
12530	C	92.56818	94.45168	72.96500	-82.47439	-504.99276	553.70587	1
12531	O	93.05275	94.48140	71.85106	150.67444	-282.17470	-248.64851	1
12532	N	91.85445	95.45920	73.46136	-716.01119	-411.06180	-274.10214	1
12533	H	91.54146	95.51184	74.54639	1920.17267	532.73068	-1919.87964	1
12534	H	91.62417	96.33199	73.00580	-656.75405	538.54257	1897.59526	1
12535	C	91.67350	91.14088	74.09348	670.12057	-542.51203	251.95801	1
12536	O	92.43845	90.25722	74.44623	6.70823	-435.90894	-192.08873	1
12537	N	90.88309	91.14317	73.04314	162.19716	402.26487	76.61364	1
12538	H	90.51343	92.04993	72.65382	-1868.14062	1443.06339	442.52027	1
12539	C	91.11414	90.06546	72.08031	255.81491	-112.09453	-111.94846	1
12540	H	91.13954	89.14907	72.77119	-1830.92411	-1632.76510	-1689.52485	1
12541	C	89.89992	90.10770	71.09551	529.43339	-220.55858	-47.74944	1
12542	H	90.06124	91.03435	70.47465	433.55856	22.68571	-1005.32180	1
12543	H	89.02533	90.32178	71.73019	562.07471	-768.09041	-853.31649	1
12544	C	89.84373	88.83129	70.27987	518.51061	538.39116	-201.06466	1
12545	C	90.15786	88.70897	68.90808	-500.78670	-596.21107	-447.40713	1
12546	H	90.34501	89.49046	68.18480	2254.50831	392.72548	-318.78620	1
12547	N	90.09969	87.43655	68.56071	-60.85773	-137.27779	134.81394	1
12548	H	90.32745	87.11911	67.58799	-1191.82052	1306.94709	950.44854	1
12549	C	89.72079	86.55118	69.54521	921.69465	-88.49929	851.43658	1
12550	C	89.56900	87.46685	70.72332	412.96347	-39.88077	-173.17919	1
12551	C	89.17445	86.83452	71.91572	225.65137	-1135.43694	10.35730	1
12552	H	89.01639	87.41870	72.87140	-1690.18655	-390.87836	2680.39243	1
12553	C	88.94516	85.44221	71.88758	164.65726	-1171.02131	594.78334	1
12554	H	88.47080	84.98387	72.77437	2602.06236	642.74086	-579.68113	1
12555	C	89.61569	85.12966	69.59094	-447.23632	-358.99968	304.08451	1
12556	H	89.82687	84.47483	68.74859	-171.95710	367.60334	2427.97537	1
12557	C	89.24690	84.53029	70.81693	-36.70114	-1090.86763	1302.95909	1
12558	H	89.23293	83.41100	71.04404	-386.46190	-1282.54806	-1537.23824	1
12559	C	92.45619	90.37953	71.25535	256.54290	55.78993	-444.45318	1
12560	O	92.47882	90.96519	70.16968	-124.02671	-1239.89170	-705.97119	1
12561	N	93.52852	89.88725	71.89082	351.44286	-174.02105	717.69100	1
12562	H	93.45449	89.47740	72.83443	-3653.47414	-838.85217	-2435.86648	1
12563	C	94.81113	90.08028	71.24636	502.69991	-613.86400	384.62537	1
12564	H	94.69635	91.03827	70.73003	-2049.59347	2515.49578	-2351.64127	1
12565	C	95.90664	90.06849	72.37499	-113.26726	617.97282	-58.96522	1
12566	H	95.81203	89.06514	72.85308	1176.73468	-772.50931	162.03391	1
12567	H	96.97580	90.07926	71.96592	-1589.28478	-786.56241	422.60522	1
12568	C	95.71106	91.11597	73.49787	644.12490	-19.78680	-668.91294	1
12569	C	95.24636	90.61712	74.77010	-845.23297	-368.93051	-386.48019	1
12570	H	95.03971	89.56125	74.84575	854.43170	-2949.35995	952.26328	1
12571	C	95.14648	91.30542	75.95395	-474.85947	-1039.97625	-393.30737	1
12572	H	94.78615	90.88130	76.81261	-1369.25283	2603.55152	-2057.15845	1
12573	C	95.39465	92.70456	75.90139	-227.54658	-209.42683	190.00033	1
12574	O	95.23598	93.57865	77.00542	21.17430	269.33697	-370.69615	1
12575	H	95.03342	92.89038	77.75671	227.12393	-13.46272	3360.11173	1
12576	C	95.98648	92.48954	73.47444	79.34518	256.19032	572.66411	1
12577	H	96.37390	92.89194	72.55948	-3172.32818	1032.21507	-1743.48640	1
12578	C	95.82756	93.25418	74.63019	854.76292	59.11130	172.41260	1

12579	H	96.03239	94.31018	74.53813	-1906.31357	1829.75420	5749.41613	1
12580	C	95.11166	88.91311	70.12279	-710.60377	-717.74138	108.52018	1
12581	O	96.24985	88.47240	69.95030	-489.85232	-221.86761	-330.26894	1
12582	N	94.00103	88.54889	69.46827	-11.60559	106.00108	-5.13403	1
12583	H	93.13520	89.01531	69.77421	359.63336	-991.20028	-283.02095	1
12584	C	94.02730	87.27334	68.81768	-201.54433	15.08555	-76.79505	1
12585	H	95.09112	86.97346	68.71317	-2274.39531	-1340.28627	-506.41260	1
12586	C	93.20986	86.36883	69.85741	-449.97051	-34.46278	-604.84857	1
12587	H	93.42568	85.31213	69.45518	1084.49143	-2385.97426	1463.22463	1
12588	H	92.14338	86.57139	69.80644	1434.55396	-1509.29964	7.71956	1
12589	C	93.64910	86.62473	71.32894	440.15235	-671.53924	-323.86402	1
12590	C	94.95300	86.38388	71.80773	662.71857	533.89205	-312.78732	1
12591	H	95.68749	86.17291	71.05038	2264.48181	831.91806	1557.67480	1
12592	C	95.27784	86.33051	73.17412	-18.34491	-587.06788	-56.73498	1
12593	H	96.35128	86.16555	73.52664	-1829.09043	1443.19809	-2454.65017	1
12594	C	94.24044	86.64066	74.10226	-295.02873	-1354.29241	-574.61833	1
12595	H	94.57891	86.53716	75.19064	656.95353	-2916.45631	1619.33623	1
12596	C	92.59313	86.89360	72.26927	142.80740	-541.77646	919.77600	1
12597	H	91.65328	87.18830	71.91038	-1048.29000	-905.18989	761.49741	1
12598	C	92.90539	86.87696	73.67243	836.21793	-10.31151	-828.75338	1
12599	H	92.16720	87.22557	74.41745	1646.13001	1364.47462	-2638.09606	1
12600	C	93.43519	87.40013	67.30384	333.81899	-13.90955	269.88038	1
12601	O	93.65225	86.55015	66.44853	-27.53369	931.76958	-613.84843	1
12602	N	92.60673	88.48535	67.17386	235.19937	-379.40034	379.17849	1
12603	H	92.90905	89.11704	67.88538	-2646.79917	732.02510	186.65101	1
12604	C	92.53545	88.77874	65.73162	-913.14449	-121.75942	-543.52273	1
12605	H	93.51653	88.34516	65.28926	3556.23307	-571.64783	-2293.14962	1
12606	H	92.43069	89.88196	65.69639	604.01795	104.38601	876.83350	1
12607	C	91.20251	88.02317	65.18702	758.65501	-131.27606	-73.48614	1
12608	O	90.57745	87.11726	65.80473	343.83031	200.23829	-495.24323	1
12609	N	91.02965	88.35823	63.95417	-237.58746	109.48511	-222.42412	1
12610	H	91.58258	89.20328	63.66267	958.24665	-3105.04936	1057.04900	1
12611	C	89.86195	87.88868	63.26411	-267.07206	-165.33449	-918.39408	1
12612	H	89.18782	87.80255	64.14503	-1247.15819	-824.28550	-474.66386	1
12613	C	89.38507	88.97851	62.20763	171.53092	458.97911	90.27361	1
12614	H	89.96054	88.81582	61.23298	-102.51011	134.96865	-19.64861	1
12615	H	89.66777	89.97452	62.53465	-1809.99482	-950.43657	1843.76656	1
12616	C	87.85521	88.95548	61.91316	-17.63690	-344.32024	-241.94738	1
12617	O	87.33727	90.01403	61.65441	814.96813	108.58959	-302.32235	1
12618	N	87.21168	87.72811	62.03912	199.00551	-860.12615	638.51575	1
12619	H	87.74643	86.84140	62.21998	2185.93741	-21.47679	1290.96292	1
12620	H	86.21974	87.53586	62.14080	258.98090	-2266.00480	-842.91740	1
12621	C	90.01296	86.38243	62.77242	-621.10325	-470.15213	-252.73879	1
12622	O	89.05210	85.67993	62.45872	1166.06602	-986.62732	-372.94953	1
12623	N	91.27850	85.98782	62.63810	-847.10457	-217.20434	-1034.89522	1
12624	H	92.01247	86.66062	62.95909	-6806.40419	207.02964	-1013.01983	1
12625	C	91.51800	84.51480	62.52590	-303.85369	327.99406	-794.69732	1
12626	H	90.87200	84.13680	61.74790	653.10532	1475.78820	-2700.69044	1
12627	C	92.98800	84.28580	62.01190	-238.70131	369.43906	798.74118	1
12628	H	93.08100	84.82880	61.04690	1085.24458	-2922.78161	-421.68479	1
12629	H	93.75600	84.78580	62.63890	1128.55225	-2204.32737	1940.49914	1
12630	C	93.37900	82.83780	61.76390	608.72225	-553.81916	-392.67362	1
12631	C	93.09300	82.24380	60.53090	-468.98586	-656.18359	-425.35439	1
12632	H	92.55800	82.73080	59.72890	-1607.52473	-1776.61513	-2039.05104	1
12633	C	93.42400	80.89180	60.32490	-625.83448	-653.59781	112.21452	1
12634	H	93.07600	80.44380	59.40590	-1045.66976	1143.19553	2738.23026	1
12635	C	94.15700	80.14080	61.27890	579.68301	666.09819	-227.44627	1
12636	H	94.35300	79.09980	61.07090	1124.86553	-373.46759	2914.34825	1
12637	C	94.09900	82.07280	62.66490	462.54836	-777.13699	-116.43932	1
12638	H	94.24300	82.65980	63.55990	-85.87457	-3127.46285	331.40295	1
12639	C	94.50800	80.76380	62.47290	675.66046	106.19139	-603.04007	1
12640	H	94.97700	80.15980	63.23490	1560.44302	-1618.92325	-2200.52978	1

12641	C	91.15900	83.68080	63.73290	-511.73531	21.65640	754.39312	1
12642	O	90.49700	82.62580	63.60990	165.21243	358.61325	-683.90688	1
12643	N	91.54500	84.08880	64.97890	410.80864	-705.33174	215.44300	1
12644	H	92.25500	84.78180	65.07190	2449.11558	-1691.15549	1019.82949	1
12645	C	91.05900	83.46380	66.12890	-632.30974	219.01402	-619.40960	1
12646	H	90.97300	82.39880	65.96990	-1278.42454	-1123.25045	-2646.16049	1
12647	C	91.97900	83.68480	67.32190	679.12662	291.88879	533.89041	1
12648	H	92.00800	84.76880	67.56390	105.77246	2278.40069	2167.00916	1
12649	H	91.54900	83.17080	68.20790	2791.06047	1226.09723	-777.74883	1
12650	C	93.41300	83.09980	67.07090	463.97143	782.73025	59.28629	1
12651	H	93.86800	83.56380	66.16990	36.40771	2133.23610	2312.18607	1
12652	C	94.41000	83.62580	68.14990	-600.67703	-670.61488	-144.61603	1
12653	H	94.13600	83.23380	69.15290	1342.01646	-1105.45353	-2622.05846	1
12654	H	94.50000	84.72780	68.25790	-2084.70444	2346.69202	-212.76793	1
12655	H	95.41400	83.22980	67.88390	-2814.07102	-49.33852	-1405.98586	1
12656	C	93.41700	81.60480	66.91190	-587.30337	-417.38709	558.85040	1
12657	H	92.78300	81.17580	66.10690	69.58549	-2208.91414	2239.21469	1
12658	H	93.12900	81.18280	67.89790	-687.56433	1506.23164	-2675.20985	1
12659	H	94.45700	81.21880	66.84390	-1156.29635	-2827.12469	754.03643	1
12660	C	89.61400	83.83780	66.42890	-551.54040	-574.51235	-444.06052	1
12661	O	88.85000	83.03980	67.01290	275.76398	-630.50100	387.36281	1
12662	N	89.15164	84.99011	65.84850	345.49780	-97.67189	106.96102	1
12663	H	89.81756	85.61661	65.38019	-1092.90566	-2219.97629	-2342.34352	1
12664	C	87.80790	85.41022	66.27951	78.55208	-327.43768	20.68235	1
12665	H	87.80867	85.08995	67.37411	395.45919	289.98732	-1053.08973	1
12666	C	87.71714	86.97478	66.08506	510.41089	-362.10339	-121.76844	1
12667	H	88.17140	87.19061	65.08050	288.87275	-1324.45838	-1380.49219	1
12668	H	88.42512	87.46978	66.77608	1229.38135	1627.68022	-377.87877	1
12669	S	85.90407	87.19245	66.39982	-293.42244	-443.17490	224.89229	1
12670	C	86.67300	84.54580	65.53490	468.55176	-778.06349	-80.79270	1
12671	O	85.70400	84.06480	66.09490	-54.92999	-671.22255	412.39570	1
12672	N	86.85900	84.23180	64.25690	66.16328	-769.66710	340.45157	1
12673	H	87.68800	84.53680	63.79390	-135.63952	1068.33728	-2956.09263	1
12674	C	86.09400	83.32380	63.49490	130.49446	-830.37783	-353.40467	1
12675	H	85.03600	83.53880	63.49790	2368.38846	-1149.97036	-1722.36190	1
12676	C	86.54900	83.31080	62.03090	112.81255	636.57212	-643.03987	1
12677	H	86.13700	82.48080	61.41790	-304.47146	-3122.02448	-241.83976	1
12678	H	87.65600	83.22380	61.99490	2937.06650	-918.11379	654.93028	1
12679	C	86.19500	84.62180	61.36690	-497.36283	-287.74757	-708.01311	1
12680	H	86.48533	85.55400	61.93498	2056.79922	227.80555	-1680.52580	1
12681	H	85.09100	84.55380	61.26190	-2298.96645	-1784.27605	1195.54945	1
12682	C	86.79500	84.65480	59.96290	660.26666	303.50348	-550.80358	1
12683	H	86.34400	83.82380	59.38090	2426.74497	-1992.59634	-196.71027	1
12684	H	87.86800	84.41480	60.12190	-1387.40064	-1541.07747	-2366.09931	1
12685	C	86.56896	86.04165	59.28023	-663.38212	-525.34130	212.69577	1
12686	H	86.96342	86.12551	58.31606	-4057.26787	1088.14778	-97.38623	1
12687	H	87.01609	86.81301	59.90644	1049.55862	1651.50254	-1604.09127	1
12688	N	84.98345	86.18479	59.20537	-117.69659	-852.44247	242.69111	1
12689	H	84.43266	86.79026	58.45771	-7.81523	-1251.78969	2611.10668	1
12690	H	84.61953	86.54459	60.18057	2559.67463	2160.55178	-2797.24499	1
12691	H	84.42936	85.21555	59.05079	327.27439	4120.70905	-1660.44421	1
12692	C	86.02200	81.92880	64.05690	-25.20875	-730.95805	544.53269	1
12693	O	84.99900	81.30480	64.09590	-669.60571	-145.24746	392.63036	1
12694	N	87.20100	81.39480	64.42590	664.46358	323.69454	-407.89985	1
12695	H	88.05400	81.83980	64.16690	1874.68390	1570.92865	-1978.88092	1
12696	C	87.36500	80.09380	65.00890	-806.66962	406.06459	-125.88355	1
12697	H	86.88200	79.29380	64.46790	-840.29316	742.92660	-2939.42064	1
12698	C	88.86800	79.76980	65.00690	384.14217	412.45196	716.77694	1
12699	H	89.28500	79.59280	63.99190	242.40516	2840.98077	-1329.77225	1
12700	H	88.98400	78.87080	65.64790	-2622.91723	1509.52797	860.14927	1
12701	H	89.43500	80.62280	65.43790	-671.05250	313.67905	-3057.69852	1
12702	C	86.72700	79.92780	66.35090	447.81818	-666.23100	432.48831	1

12703	O	85.95200	79.01880	66.54290	18.07445	-533.90771	581.58671	1
12704	N	86.90000	80.80780	67.33590	52.24553	-1.42966	-842.57976	1
12705	H	87.40500	81.66380	67.25290	-635.55545	3074.58441	-203.04230	1
12706	C	86.19000	80.52680	68.62890	-45.17959	-746.01266	522.37431	1
12707	H	86.32400	79.48480	68.87990	2489.32848	-1413.08181	-1305.63002	1
12708	C	86.84000	81.26180	69.83390	897.64650	-110.01010	-116.53127	1
12709	H	86.44200	80.90480	70.80790	1408.17935	2475.00587	1337.76048	1
12710	C	88.33400	81.07680	69.72290	-582.43885	632.82097	-302.90858	1
12711	H	88.48300	79.98080	69.82890	-1210.19525	2649.47509	1189.09016	1
12712	H	88.82500	81.27280	68.74590	-2159.66932	-2208.90610	595.64124	1
12713	H	88.77100	81.69980	70.53290	-2075.46351	-2104.57188	1077.70805	1
12714	C	86.58200	82.78080	69.82590	-583.50057	-481.36666	509.17996	1
12715	H	86.96400	83.25980	70.75290	2213.50099	-179.52086	-2228.54478	1
12716	H	85.55100	83.08380	69.54390	624.68477	2755.71629	1383.48217	1
12717	H	87.13100	83.11580	68.91990	-244.60913	3125.03068	-269.39903	1
12718	C	84.70900	80.73080	68.63990	-624.07646	-121.06114	653.70006	1
12719	O	84.02200	80.17280	69.49290	-238.44104	571.68688	489.84406	1
12720	N	84.24600	81.55880	67.65790	-151.63758	-810.04598	183.04056	1
12721	H	84.91200	81.97480	67.04290	1977.50723	1873.26611	1574.34604	1
12722	C	82.80800	81.69580	67.40890	499.75622	-247.95496	721.25797	1
12723	H	82.37200	81.78180	68.39290	-348.33637	-218.96637	-3119.12515	1
12724	C	82.41500	82.92780	66.52990	742.69846	-31.02271	528.09810	1
12725	H	81.41600	82.87480	66.04590	896.14559	-2284.10859	-1969.26312	1
12726	H	83.13300	83.04280	65.69090	-1146.78510	1807.43618	2305.70697	1
12727	N	83.05488	85.39562	67.42495	-758.86066	-363.66507	-575.09653	1
12728	H	83.82195	85.64829	66.78882	-2352.77402	647.38171	-14.21466	1
12729	C	82.39900	84.15480	67.43290	902.00239	-124.80661	-47.60248	1
12730	C	82.67891	86.33990	68.24494	164.51503	-254.15872	297.22412	1
12731	H	82.97405	87.37578	68.26264	869.53167	-4281.94418	3174.36846	1
12732	N	81.79687	85.69668	69.03402	-402.81311	1028.23774	710.44540	1
12733	C	81.65600	84.41580	68.51590	145.69151	-483.20267	-759.43411	1
12734	H	80.87200	83.84280	68.99590	-3021.51565	347.01583	-805.13936	1
12735	C	82.16700	80.46780	66.77990	725.62175	110.67695	-540.99418	1
12736	O	81.09700	80.01880	67.19390	479.04239	-454.87964	432.70097	1
12737	N	82.89000	79.89280	65.78590	188.12333	734.94736	-370.31646	1
12738	H	83.69400	80.36680	65.43590	1914.81718	-549.16846	2435.18283	1
12739	C	82.59700	78.59880	65.20790	54.12027	769.66613	-485.93832	1
12740	H	81.57800	78.58580	64.84890	-1049.03304	2426.50211	1705.82632	1
12741	C	83.57500	78.33080	64.01290	596.97102	-687.01777	55.52647	1
12742	H	84.59400	78.72480	64.21390	-496.89337	2038.51344	-2344.30931	1
12743	C	83.59900	76.78780	63.77490	232.22169	-880.38005	-49.54850	1
12744	H	84.31500	76.28780	64.46290	246.70180	201.97220	-3129.94755	1
12745	H	83.98300	76.51480	62.76890	-2337.88053	281.78683	2086.41728	1
12746	H	82.64600	76.27180	64.01990	-2667.66253	262.47740	-1647.09090	1
12747	C	83.00400	79.04680	62.75690	-678.67608	258.77949	551.25580	1
12748	H	81.91100	78.88580	62.63890	3119.82534	-308.84410	-263.68804	1
12749	H	83.47200	78.73680	61.79890	-191.64151	3022.17448	-853.20641	1
12750	H	83.14800	80.14080	62.88390	1772.08540	-2410.22431	-974.04228	1
12751	C	82.54300	77.54080	66.30590	-631.12913	145.22344	641.90122	1
12752	O	81.51500	76.91780	66.54690	-130.07486	580.52320	519.32704	1
12753	N	83.59100	77.46180	67.16990	126.88737	-117.38196	826.31311	1
12754	H	84.39600	78.01380	66.96890	1956.94730	-1116.92560	-2195.69140	1
12755	C	83.61000	76.47880	68.21290	172.84335	-885.22278	-134.00303	1
12756	H	83.48300	75.48980	67.79590	2001.37120	-2191.18902	-1044.71538	1
12757	C	85.03500	76.38780	68.80890	-548.43571	-706.59961	-177.16170	1
12758	H	85.44800	77.41780	68.87090	-1703.84352	1680.71119	2042.14431	1
12759	C	85.07400	75.72080	70.18590	-539.66435	-539.81379	498.81306	1
12760	H	86.10000	75.62280	70.60190	-2611.82489	1740.15603	-220.12259	1
12761	H	84.55100	76.30080	70.97590	-496.85295	-1171.17159	2877.45034	1
12762	H	84.66100	74.69080	70.12890	2368.40023	-2056.67944	242.85024	1
12763	C	85.97700	75.72480	67.76590	-89.73891	-245.42260	873.59354	1
12764	H	85.69100	74.65480	67.67490	-1508.14052	2268.84120	-1573.56220	1

12765	H	85.74100	76.16480	66.77290	1471.34731	1867.64784	2060.40163	1
12766	C	87.47200	75.97180	67.95890	398.49030	399.48319	716.28881	1
12767	H	88.05300	75.45780	67.16290	1584.70168	-2599.63602	-792.99393	1
12768	H	87.73000	75.66880	68.99590	1408.83570	-3.37167	2813.07605	1
12769	H	87.69600	77.04780	67.79490	1761.32265	-1730.37664	-1949.81164	1
12770	C	82.51700	76.61280	69.28290	-612.13101	80.81315	-670.98127	1
12771	O	81.96700	75.61980	69.76790	-700.48536	235.55583	278.31806	1
12772	N	82.13600	77.82380	69.67790	-397.17551	-497.81979	554.16546	1
12773	H	82.59400	78.62980	69.31090	651.88955	2517.34254	1770.94686	1
12774	C	81.05000	78.07380	70.56590	654.19916	-590.42628	-234.24616	1
12775	H	81.27600	77.50580	71.45590	-377.49390	-3116.51217	-207.54877	1
12776	C	81.05200	79.58980	71.00790	-114.37893	862.88896	271.64518	1
12777	H	80.98000	80.15680	70.05590	943.25906	-572.63602	-2946.28182	1
12778	H	82.02300	79.80180	71.50490	-1748.26127	656.72251	-2531.90132	1
12779	C	79.92200	80.03280	71.97990	452.51212	528.19214	589.65825	1
12780	C	79.38500	79.12780	72.88490	754.59482	199.91169	-471.24620	1
12781	H	79.82100	78.13980	72.84190	2344.68839	-2090.15074	178.69654	1
12782	C	78.46300	79.55580	73.85390	-193.29632	798.69741	-395.18348	1
12783	H	78.13700	78.88380	74.63390	509.82928	2843.38580	1246.37776	1
12784	C	77.98700	80.85580	73.88990	709.78619	190.32186	-539.84457	1
12785	O	76.96700	81.12580	74.81990	334.16104	-638.41461	-323.09504	1
12786	H	77.08100	82.02380	75.14090	1606.67949	-1710.99670	2095.06505	1
12787	C	79.47200	81.38480	72.01490	-504.04825	738.87999	177.32097	1
12788	H	79.94600	82.09480	71.35290	2005.67626	-799.99938	2288.11931	1
12789	C	78.48900	81.79280	72.93090	691.47901	405.71107	-434.40339	1
12790	H	78.06400	82.77980	73.03490	51.16103	757.40718	-3053.18574	1
12791	C	79.67300	77.54080	70.07190	-591.54483	-271.63962	-638.54337	1
12792	O	78.96500	76.79380	70.76590	480.63820	-472.80926	-411.17582	1
12793	N	79.39400	77.68380	68.75890	-742.13666	-402.33044	5.97397	1
12794	H	79.95300	78.19680	68.11190	-1152.78188	-985.56835	2756.44249	1
12795	C	78.20500	77.02080	68.19390	61.86485	795.84696	440.73955	1
12796	H	77.43900	76.92980	68.94890	2957.23336	311.72141	1027.53435	1
12797	C	77.48800	77.80880	67.07390	365.22154	-641.60525	-535.17000	1
12798	H	76.97700	77.12180	66.36490	1489.23193	-2376.00632	1426.53721	1
12799	O	78.48200	78.54080	66.33890	-429.72842	-403.07271	-525.82612	1
12800	H	77.96600	79.06380	65.71990	-574.08783	2164.89805	2209.49448	1
12801	C	76.51200	78.84980	67.67590	697.50266	558.61072	181.37007	1
12802	H	76.14500	79.53180	66.87990	2249.53106	-1717.20658	-1374.42272	1
12803	H	77.06600	79.47580	68.40790	2634.55936	-1601.01892	627.74326	1
12804	H	75.64300	78.39980	68.20290	-713.51949	1849.88532	2442.75264	1
12805	C	78.36700	75.56380	67.75190	-7.02825	-797.23219	442.51829	1
12806	O	77.49200	74.70580	67.73790	240.06474	726.04181	-197.12798	1
12807	N	79.64800	75.13880	67.41590	-408.58583	723.26836	150.37549	1
12808	H	80.37000	75.81880	67.31490	490.41974	-2731.32403	-1482.42496	1
12809	C	79.99100	73.68980	67.21490	96.94854	903.87318	-71.17058	1
12810	H	79.38000	73.32380	66.40290	1636.03180	79.93332	2686.11929	1
12811	C	81.38900	73.44280	66.61790	753.31258	-143.30555	493.39100	1
12812	H	82.10200	74.18380	67.03690	1.26167	-3129.15480	326.51929	1
12813	C	81.96200	72.04380	66.97190	590.03942	163.45730	675.71162	1
12814	H	82.88300	71.83080	66.38890	1734.49980	-1908.04658	-1802.52460	1
12815	H	81.18600	71.31880	66.64490	2503.40734	-883.74296	-1688.24652	1
12816	H	82.34400	71.99180	68.01390	424.99352	-1858.61728	-2502.62833	1
12817	C	81.32400	73.80080	65.10990	471.76441	434.85651	647.91139	1
12818	H	80.97800	74.84980	64.98990	2747.00389	-1517.00860	-225.56764	1
12819	H	82.37400	73.66580	64.77390	-1751.98534	1436.13269	-2183.18495	1
12820	H	80.63300	73.08980	64.60990	682.85022	-2983.27233	729.40251	1
12821	C	79.75400	72.79980	68.47990	-611.60228	619.69360	-270.87543	1
12822	O	79.20000	71.70380	68.33390	539.82664	389.62199	424.74596	1
12823	N	80.08100	73.22380	69.70090	180.51449	-501.80127	654.43280	1
12824	H	80.50800	74.12280	69.76890	-623.22305	-2689.20612	-1509.30106	1
12825	C	79.61600	72.58280	70.91190	-758.21121	77.84343	-500.50691	1
12826	H	79.83700	71.53080	70.80090	-2388.70021	-667.93170	1935.51150	1

12827	C	80.32000	73.15880	72.15090	173.62257	886.27264	125.80548	1
12828	H	80.52000	74.24680	72.04990	-487.35254	2917.52556	-1071.80145	1
12829	H	81.33400	72.70680	72.18690	-1942.63109	-1104.31059	-2214.70287	1
12830	C	79.57500	73.06880	73.50490	0.53602	-710.39638	571.65348	1
12831	O	78.59100	73.73680	73.79790	503.15830	-70.38296	-604.57025	1
12832	N	80.05400	72.13480	74.36090	397.13462	-702.76268	247.14571	1
12833	H	80.91400	71.64380	74.22290	2443.43042	1919.69813	-492.57803	1
12834	H	79.62900	72.06180	75.26290	-1603.97196	-1825.56446	1998.20284	1
12835	C	78.06400	72.62880	71.06090	-123.19949	902.26504	-46.80486	1
12836	O	77.44500	71.63380	71.38190	-387.17212	282.86592	627.46462	1
12837	N	77.42000	73.74480	70.75490	-507.13097	-667.59190	-99.05314	1
12838	H	77.98600	74.52280	70.49790	-2034.56775	-2307.93209	657.42663	1
12839	C	76.00300	73.97580	70.88590	-846.11252	99.95548	-324.88999	1
12840	H	75.75900	73.92180	71.93690	1782.92205	-2460.45939	815.81541	1
12841	C	75.56400	75.38480	70.54190	-253.18701	-871.19825	91.43828	1
12842	H	75.41200	75.53680	69.45190	2147.36810	1424.51941	1804.93239	1
12843	H	76.35700	76.10880	70.82590	2127.62731	-2289.29574	-361.32158	1
12844	C	74.25900	75.91580	71.28290	-525.10873	544.33656	509.32263	1
12845	H	73.50300	75.10180	71.26190	-1666.29387	-2300.37864	1352.75610	1
12846	C	74.54200	76.24980	72.74990	-617.90918	-485.30478	462.72943	1
12847	H	74.82100	75.38380	73.38690	-351.36839	2865.56617	-1250.31876	1
12848	H	73.69400	76.78080	73.23390	-1920.77585	2242.40229	1086.49821	1
12849	H	75.40100	76.95280	72.71390	-589.63127	-2948.43239	925.90908	1
12850	C	73.71700	77.15380	70.58690	-87.72335	480.98790	769.67932	1
12851	H	72.74800	77.35680	71.09090	-1276.29460	2225.82568	1820.71370	1
12852	H	73.66100	76.90080	69.50690	-2203.76964	934.25333	2041.76304	1
12853	H	74.31300	78.05480	70.84590	-1234.75030	-2563.91468	1341.62567	1
12854	C	75.09600	73.04480	70.08690	-823.19531	386.69312	-65.33692	1
12855	O	74.19500	72.43780	70.57690	526.45364	454.78628	-373.68869	1
12856	N	75.58000	72.79280	68.84390	443.93448	-712.83705	-86.35858	1
12857	H	76.37800	73.29880	68.52390	601.87010	1445.94777	-2728.59188	1
12858	C	75.03800	71.79380	67.92590	40.82754	-550.16236	-726.02031	1
12859	H	73.97500	71.68380	68.08490	-943.64116	2265.16292	1968.96027	1
12860	C	75.21300	72.27780	66.44590	0.42648	-911.21787	-33.65742	1
12861	H	74.68000	71.57580	65.76990	-390.88671	2219.09751	2195.68669	1
12862	H	76.30400	72.25780	66.23490	1252.60414	1664.08903	-2357.96879	1
12863	C	74.58800	73.64280	66.30190	26.48589	860.96915	299.13478	1
12864	C	73.40500	74.05580	66.90090	-621.48891	167.06086	-645.98236	1
12865	H	72.87400	73.31580	67.48090	2145.74123	2086.75121	-969.27303	1
12866	C	72.89700	75.36980	66.79290	-857.74780	244.13350	-190.04880	1
12867	H	72.03100	75.61380	67.39190	1603.14685	2173.95579	1613.09101	1
12868	C	73.59500	76.30480	66.07290	-539.21799	452.23959	-579.80541	1
12869	O	73.11000	77.58880	66.04690	460.31102	-255.30135	588.69535	1
12870	H	73.77800	78.08480	65.56790	2107.07791	-2267.33556	563.59415	1
12871	C	75.25300	74.59480	65.48390	-684.91077	80.98427	-596.48118	1
12872	H	76.17700	74.26580	65.03190	52.89202	-2929.72220	1145.49398	1
12873	C	74.76400	75.91180	65.39090	335.61882	465.96907	708.29643	1
12874	H	75.26000	76.67480	64.80990	2047.39318	-735.56354	-2272.74144	1
12875	C	75.55000	70.36280	68.08790	-730.70072	225.96520	-496.45462	1
12876	O	74.98700	69.48580	67.47890	492.52319	-467.35595	-403.26983	1
12877	N	76.64500	70.10980	68.85690	332.02813	-574.83824	-521.52719	1
12878	H	77.20900	70.81580	69.27890	-332.30311	-1613.18258	2680.56763	1
12879	C	77.21400	68.74780	68.93090	-683.50515	-67.23577	-599.79252	1
12880	H	76.76200	68.11280	68.18290	-2599.98571	1610.27686	738.45040	1
12881	C	78.76800	68.59680	68.72990	603.28981	448.25783	516.29190	1
12882	H	78.91700	68.76980	67.64290	2145.86021	-2299.79467	66.74314	1
12883	H	79.12100	67.55780	68.90390	-2639.78228	-698.79261	1562.51867	1
12884	O	79.43400	69.45380	69.61290	760.86385	211.04121	13.23026	1
12885	H	79.36600	70.29480	69.15390	-3047.61140	-664.88082	410.15176	1
12886	C	76.83600	68.12980	70.21990	505.51926	593.75309	-472.60824	1
12887	O	76.31600	67.01880	70.22490	-305.41886	529.60808	-499.86181	1
12888	N	76.90800	68.88580	71.39690	82.91860	470.09816	-696.27905	1

12889	H	77.09200	69.86380	71.34290	-1866.32202	2134.50234	1363.43982	1
12890	C	76.65900	68.29280	72.72790	499.97309	463.04944	-605.85735	1
12891	H	77.37300	67.49480	72.86990	-351.75708	-47.79780	-3126.05319	1
12892	C	76.99100	69.27280	73.89690	725.69444	72.90043	-547.26969	1
12893	H	78.08900	69.43780	73.90890	367.04990	3123.02768	-100.98865	1
12894	H	76.72300	68.86880	74.89590	2930.09636	78.26983	1143.08153	1
12895	O	76.37400	70.60180	73.75590	279.79270	520.02189	-524.32862	1
12896	H	76.99100	71.20580	73.33690	534.48385	2596.34613	-1694.56189	1
12897	C	75.22200	67.71180	72.98090	202.29665	-549.82311	698.72857	1
12898	O	75.04700	66.54180	73.22690	544.77936	-309.00250	-480.99910	1
12899	N	74.23400	68.54880	72.77190	-752.15878	-381.67568	-35.39965	1
12900	H	74.49300	69.49780	72.60890	1268.04132	2607.15182	1221.90704	1
12901	C	72.81700	68.20780	72.84690	710.04538	-428.18661	-379.39792	1
12902	H	72.69700	67.79180	73.83690	-686.59231	-1500.55204	-2678.64907	1
12903	C	71.92400	69.42580	72.75590	209.06955	-36.19039	886.80955	1
12904	H	72.28100	70.22380	73.44090	-2085.32984	2284.08993	576.67919	1
12905	C	71.88500	70.06880	71.32090	499.76581	-492.78721	-582.10471	1
12906	H	72.95400	70.30580	71.12690	2779.33005	739.84867	1275.21553	1
12907	H	71.46800	69.35080	70.58190	1524.64378	-1888.52651	-2001.78800	1
12908	H	71.31100	71.01980	71.33190	2637.64247	-1630.49978	-531.54386	1
12909	C	70.59100	69.04780	73.37790	-372.81460	-735.77503	388.70989	1
12910	H	69.91400	69.92780	73.42990	1625.06971	2261.93045	1463.23112	1
12911	H	70.01500	68.20180	72.94690	-864.21140	-2007.22371	2263.27592	1
12912	H	70.85600	68.68180	74.39290	-469.47901	2020.33590	2365.59898	1
12913	C	72.36900	67.11980	71.85690	629.43342	358.41755	-553.89659	1
12914	O	71.52900	66.26080	72.13090	-589.69875	363.08965	-379.53724	1
12915	N	72.91100	67.09180	70.61690	-449.40910	168.04409	-694.59696	1
12916	H	73.50900	67.85780	70.39290	1964.75811	-654.85447	-2368.35754	1
12917	C	72.45400	66.06380	69.71790	468.66728	-462.33048	630.91402	1
12918	H	71.39000	65.90280	69.80790	2191.61940	1245.69789	-1882.35688	1
12919	C	72.66000	66.54280	68.23090	-170.29364	-613.54213	652.69988	1
12920	H	72.52100	65.61380	67.63890	-2061.86786	-957.50340	2174.88261	1
12921	H	73.68700	66.96680	68.24990	2005.53283	408.55536	-2389.38210	1
12922	C	71.72500	67.59780	67.72090	128.59630	-727.81848	534.03582	1
12923	C	71.74100	68.95780	67.92090	894.52228	-29.63960	174.36279	1
12924	H	72.58600	69.44280	68.38690	2030.21511	2058.12856	1241.19285	1
12925	N	70.70500	69.55680	67.31790	727.30233	420.89478	-80.93944	1
12926	H	70.35400	70.42880	67.57890	-1973.75192	-1651.95424	1809.30284	1
12927	C	69.94900	68.58180	66.73890	243.32934	-63.35365	-876.48625	1
12928	C	70.55000	67.30580	66.99790	-190.94289	172.77976	874.72223	1
12929	C	69.90800	66.17080	66.61990	-93.85484	-660.48461	621.61271	1
12930	H	70.39900	65.26380	66.93990	2048.96375	-2016.74493	1277.77684	1
12931	C	68.76100	66.27480	65.85090	-377.12460	-617.76491	554.61208	1
12932	H	68.26800	65.37480	65.51390	1730.73166	-2328.72526	1216.48379	1
12933	C	68.83000	68.69180	65.97190	730.54797	-304.43379	-452.84736	1
12934	H	68.33200	69.62280	65.74690	-2320.43694	1339.02085	1649.49137	1
12935	C	68.20200	67.49880	65.54590	-244.50619	-641.80439	599.79567	1
12936	H	67.29300	67.52580	64.96390	-1265.65520	2117.35612	-1952.72789	1
12937	C	73.19300	64.74780	69.88990	-482.85355	-411.10843	-655.20478	1
12938	O	72.67800	63.69780	69.58190	-227.20677	516.73750	-552.25598	1
12939	N	74.40600	64.73880	70.51790	306.62036	443.17883	-649.80671	1
12940	H	74.96100	65.55880	70.63090	541.35490	-2263.20012	-2117.33000	1
12941	C	74.94700	63.53980	71.09390	211.47599	668.35783	583.11810	1
12942	H	75.05800	62.74180	70.37490	1193.44186	-1526.63374	2478.57059	1
12943	C	76.44200	63.74480	71.56290	-164.41428	-877.45988	-185.69629	1
12944	H	76.37000	64.76080	72.00790	-1630.38460	2144.49160	1625.18554	1
12945	C	76.85300	62.73380	72.62490	-608.62513	-648.12263	202.39444	1
12946	H	77.96400	62.74180	72.63890	2696.28003	-1620.77259	-37.36905	1
12947	H	76.59800	61.68380	72.36590	1179.64944	2730.85172	1024.25695	1
12948	H	76.41300	62.97180	73.61690	-1478.26273	1604.74732	-2266.66089	1
12949	C	77.39100	63.63880	70.36590	8.20750	265.60563	872.25987	1
12950	H	76.79400	64.06380	69.53090	462.68468	-2934.50414	-1035.77727	1

12951	H	77.58600	62.57880	70.09590	-1516.21961	1468.85257	2332.76155	1
12952	C	78.55700	64.57680	70.48490	839.58786	-355.09175	-21.28559	1
12953	H	79.21500	64.35480	71.35190	-436.62506	-2985.91408	-889.88870	1
12954	H	78.21700	65.63480	70.49190	2176.02064	-1949.66633	1167.03110	1
12955	H	79.23400	64.48180	69.60890	-331.58476	2196.46751	2227.96055	1
12956	C	74.09700	62.96180	72.24090	649.57505	638.24844	46.28366	1
12957	O	73.82900	61.77480	72.30290	-138.42758	177.31496	-756.98378	1
12958	N	73.51000	63.84680	73.06590	356.39596	-536.86647	545.37015	1
12959	H	73.79600	64.80180	73.04790	604.44629	2816.39918	1265.21403	1
12960	C	72.53000	63.56280	74.09690	-367.57465	819.53089	157.19097	1
12961	H	72.92800	62.80480	74.75590	-2230.80755	-2203.91626	-253.92325	1
12962	C	72.31300	64.68880	75.09590	-713.56169	533.97940	-192.73483	1
12963	H	71.43000	64.41080	75.70990	737.94673	-1447.00282	2694.40971	1
12964	H	71.98400	65.56780	74.50090	988.30864	-2623.77034	1427.34070	1
12965	C	73.46500	64.97780	76.06990	315.59796	810.29507	-274.35532	1
12966	H	74.37300	65.14780	75.45290	-1407.76648	-148.86095	2809.67261	1
12967	C	73.19900	66.08480	77.11390	-686.19111	-497.15689	-336.79043	1
12968	H	74.07700	66.31080	77.75590	175.12160	-2544.02273	-1842.69015	1
12969	H	72.87400	67.00380	76.57990	-2609.81228	-1501.90045	911.81200	1
12970	H	72.38300	65.70780	77.76590	1615.89084	-2455.22836	-1122.04132	1
12971	C	73.79100	63.67480	76.88490	651.44052	173.93095	-613.86015	1
12972	H	74.66400	63.90280	77.53190	1930.19295	-2010.98147	1458.94995	1
12973	H	72.87900	63.35080	77.43090	-537.77902	2884.37451	1135.51911	1
12974	H	74.16100	62.87780	76.20390	843.70987	-2804.94804	-1148.32328	1
12975	C	71.22700	62.91880	73.51690	187.75238	-389.88903	-802.61235	1
12976	O	70.71800	61.98380	74.14690	577.28224	-43.37584	537.11357	1
12977	N	70.70300	63.40180	72.34790	128.20291	632.22047	544.54896	1
12978	H	71.10300	64.26580	72.05290	186.89101	98.28880	-3139.05038	1
12979	C	69.73400	62.58180	71.58590	654.06218	-578.57456	-262.49789	1
12980	H	68.87900	62.38480	72.21590	1298.20440	-2813.05665	-547.36078	1
12981	C	69.26800	63.38280	70.33890	-409.82423	454.41187	676.02141	1
12982	H	68.28800	62.96680	70.02090	2106.20782	-2278.35270	520.79157	1
12983	H	69.96100	63.29480	69.47590	-2163.36909	25.16517	-2284.16881	1
12984	H	69.03900	64.45180	70.53990	1007.43167	948.51124	-2825.53253	1
12985	C	70.21000	61.21680	71.12590	491.19168	598.24155	-481.96346	1
12986	O	69.50700	60.27980	71.39790	-532.73410	-403.46037	-420.76280	1
12987	N	71.39700	61.10080	70.48690	-225.28400	-777.07639	240.98069	1
12988	H	71.96500	61.91780	70.43290	2166.94562	691.93797	-2173.42926	1
12989	C	71.91600	59.80780	70.10590	-126.00536	575.75589	695.75772	1
12990	H	71.21400	59.26580	69.48990	-690.27769	-1789.79050	-2493.67057	1
12991	C	73.26300	60.01580	69.27590	224.21008	184.41705	-864.39065	1
12992	H	73.86400	59.08180	69.30890	-1619.40231	-2123.66932	-1663.06675	1
12993	H	73.85400	60.81780	69.76790	1913.52656	-1741.36255	-1790.05552	1
12994	C	73.07700	60.37180	67.86290	-622.17021	-263.70164	612.22274	1
12995	C	71.99300	61.12680	67.38390	-153.95335	-692.81968	-572.49477	1
12996	H	71.19200	61.52980	67.98490	-1051.61428	-1867.79130	2302.97401	1
12997	C	71.80300	61.37380	66.02090	-108.51949	-460.74910	-779.34895	1
12998	H	70.93800	61.91180	65.66190	-2696.83752	568.12273	-1517.40904	1
12999	C	72.70500	60.88880	65.10690	558.68542	-586.75041	418.38447	1
13000	H	72.48900	61.01780	64.05590	-1393.58512	1798.98202	-2172.51247	1
13001	C	73.97600	59.87980	66.90290	-668.38031	-292.36310	-547.03070	1
13002	H	74.74700	59.17780	67.18090	-519.74511	-1949.36202	-2414.14145	1
13003	C	73.75000	60.08480	65.52790	345.24016	-765.15780	356.08113	1
13004	H	74.35200	59.44180	64.90390	1616.51876	-2429.04107	1176.79770	1
13005	C	72.12500	58.72180	71.18490	-303.75585	855.95742	-80.74823	1
13006	O	71.74000	57.56280	70.96290	-445.51117	517.35292	-396.85386	1
13007	N	72.61100	59.07480	72.37390	624.43315	-41.74067	566.58030	1
13008	H	72.89000	60.02280	72.50490	-2034.23856	-302.64010	-2380.86301	1
13009	C	72.68100	58.14080	73.49390	713.61045	-433.99477	365.86837	1
13010	H	73.09600	57.19180	73.18990	-1633.72734	654.31360	-2607.87939	1
13011	C	73.64600	58.74880	74.51190	260.21211	-18.29780	873.73100	1
13012	H	74.62300	58.87080	73.99490	-2067.64718	-1943.85280	-1358.12284	1

13013	C	73.16700	60.07580	75.15390	440.04924	-542.59235	-586.00444	1
13014	H	72.36900	59.90880	75.90790	-1735.24072	-1838.97854	-1872.25100	1
13015	H	72.74200	60.71680	74.35090	2076.29169	1145.42748	-2067.66413	1
13016	H	73.98700	60.55380	75.73090	61.29541	-2003.23385	-2425.18520	1
13017	C	74.00800	57.66680	75.58290	-407.78799	564.90514	-588.25347	1
13018	H	74.22300	56.72280	75.03790	-1794.03469	1567.45159	-2054.93583	1
13019	H	73.10600	57.48480	76.20490	-1525.73716	1839.86572	-2045.78750	1
13020	C	75.17000	58.18180	76.40990	765.16157	229.69992	-439.56423	1
13021	H	76.07100	58.47080	75.82890	2386.89484	-203.53102	2039.49366	1
13022	H	74.83000	59.07680	76.97390	-1837.93490	2218.18707	-1264.85874	1
13023	H	75.49500	57.43180	77.16290	2558.80596	729.98521	1678.64822	1
13024	C	71.27200	57.86480	74.12990	-473.64884	546.29694	-555.57847	1
13025	O	71.00500	56.75880	74.66690	-269.51525	338.64344	660.53719	1
13026	N	70.33700	58.79980	73.99790	646.29447	534.45494	96.61090	1
13027	H	70.55600	59.61580	73.46790	781.07339	-2098.00231	-2210.55127	1
13028	C	68.93700	58.59380	74.35490	593.35796	568.41995	-395.31771	1
13029	H	68.88800	58.26980	75.38390	207.37911	2077.34144	-2353.69341	1
13030	C	68.03700	59.88580	74.21290	-217.45794	-817.13132	341.26157	1
13031	H	66.94500	59.71580	74.32590	-659.08708	-2535.99944	1741.41819	1
13032	H	68.26200	60.32580	73.21790	-1033.35935	-2156.23168	-2044.76396	1
13033	O	68.38100	60.83480	75.21390	-253.99409	745.99177	51.09315	1
13034	H	69.14200	61.29780	74.85590	803.33209	3021.09575	-354.77355	1
13035	C	68.26600	57.55280	73.49690	-30.08678	-625.98435	-662.33630	1
13036	O	67.62400	56.66180	74.00890	-147.26451	764.27598	-133.50141	1
13037	N	68.41900	57.71580	72.14690	-287.87827	-29.02419	-793.06745	1
13038	H	68.91000	58.48880	71.75390	1145.58148	-2423.08517	1647.58234	1
13039	C	68.00800	56.73880	71.10290	159.68382	-403.84943	-801.78409	1
13040	H	66.93000	56.69380	71.05990	-2629.37076	1715.92865	-200.56050	1
13041	C	68.42200	57.32980	69.74790	-560.24413	-688.18695	-209.70514	1
13042	H	68.40100	56.60980	68.90190	705.45967	2170.66254	-2165.35841	1
13043	H	69.46400	57.71380	69.75790	-2176.69301	979.14654	2049.75751	1
13044	C	67.53700	58.48480	69.21390	-503.21823	77.51028	756.44866	1
13045	H	67.35400	59.16180	70.07590	1502.90016	-2763.10212	69.16678	1
13046	C	68.30300	59.44180	68.21290	-889.39703	87.46079	-181.03738	1
13047	H	67.50000	60.12880	67.86990	-467.28716	2715.87637	-1517.85523	1
13048	H	68.58400	58.83980	67.32290	3139.17701	-199.59344	-62.89984	1
13049	H	69.13000	60.00380	68.69590	-2149.99199	625.97437	-2209.95854	1
13050	C	66.27600	58.00980	68.50990	-855.61590	268.32927	-165.44437	1
13051	H	66.46300	57.26280	67.70990	-2981.96851	-570.26593	825.15865	1
13052	H	65.65900	58.82780	68.07890	802.82144	-1280.83377	-2759.19713	1
13053	H	65.59800	57.65380	69.31590	1210.31431	2486.21506	-1500.69990	1
13054	C	68.65300	55.42080	71.41890	391.22034	-381.16090	-730.14657	1
13055	O	67.96100	54.39280	71.36790	455.71177	545.16498	-344.59999	1
13056	N	69.99700	55.34680	71.65690	351.48327	563.15960	521.51995	1
13057	H	70.50300	56.19780	71.54090	-1979.51661	-2341.54775	704.90735	1
13058	C	70.66600	54.11680	71.95390	435.66842	173.61348	-781.98618	1
13059	H	70.37400	53.43580	71.16790	863.62376	2358.74427	-1894.38795	1
13060	C	72.21100	54.42880	71.99990	391.20592	677.24236	-468.77683	1
13061	H	72.41300	55.16980	72.80390	351.82945	-486.90668	-3088.26232	1
13062	H	72.52700	54.79380	70.99990	-2874.21529	-490.39723	-1181.78815	1
13063	C	72.99600	53.16680	72.28990	-158.05239	897.39430	33.96919	1
13064	O	73.09800	52.74080	73.45190	-319.86522	-36.92665	721.07551	1
13065	O	73.42800	52.48280	71.30890	21.67933	-572.38710	543.62693	1
13066	C	70.16900	53.41580	73.19190	746.88087	11.67975	522.95655	1
13067	O	70.09800	52.19680	73.28190	-322.11435	-301.26398	655.06457	1
13068	N	69.80300	54.19280	74.24790	-534.60853	-443.75660	479.52694	1
13069	H	69.85400	55.18780	74.23790	-98.47031	2179.77530	2266.51924	1
13070	C	69.17300	53.66180	75.45390	489.20023	634.45007	435.43913	1
13071	H	69.73600	52.83980	75.86990	-2529.30393	-1780.19729	-575.97347	1
13072	C	69.09800	54.71380	76.61790	-508.57795	603.74851	-456.38494	1
13073	H	69.19700	55.75280	76.23590	-2706.36543	520.13211	-1517.65444	1
13074	H	68.12200	54.60580	77.13890	1669.27123	1344.82401	-2302.86955	1

13075	C	70.26100	54.47080	77.66490	628.80261	-236.01511	616.72940	1
13076	H	70.11000	55.20080	78.48890	-1946.14455	1913.91686	1564.50308	1
13077	H	70.18700	53.40880	77.98390	-1769.25170	-2205.48983	1379.77870	1
13078	C	71.68300	54.73580	77.10590	323.18171	728.31266	443.35680	1
13079	H	72.30700	54.92680	78.00490	1725.79829	1879.44631	1840.52385	1
13080	H	71.52300	55.67780	76.53890	1230.80889	-706.21838	2807.95144	1
13081	N	72.29500	53.58780	76.26790	-646.18371	-481.90583	250.77015	1
13082	H	72.33300	53.71780	75.27790	-2297.33232	1210.76458	-1776.10235	1
13083	C	72.51900	52.36480	76.67390	661.82706	237.93006	580.36647	1
13084	N	72.45100	51.90980	77.92390	523.04594	587.03562	307.38317	1
13085	H	72.43900	52.51280	78.72190	-1787.39077	2469.37472	778.23451	1
13086	H	72.53400	50.92280	78.06190	619.34052	36.08832	3084.37047	1
13087	N	72.86300	51.48580	75.77490	-499.76751	365.50436	573.85650	1
13088	H	72.93300	51.87680	74.85690	428.56464	-2759.31526	-1449.39224	1
13089	H	73.24600	50.61580	76.08390	2888.30830	25.41442	-1247.09883	1
13090	C	67.78400	53.02580	75.23090	419.40290	-701.88434	403.62183	1
13091	O	67.57600	51.90080	75.66890	739.58384	-7.74335	-276.73636	1
13092	N	66.94800	53.66880	74.42790	272.18759	-526.80115	-600.88830	1
13093	H	67.26800	54.51680	74.01190	-114.68577	570.29813	3091.89803	1
13094	C	65.70600	53.17180	73.94890	802.44318	-342.17193	-265.43233	1
13095	H	65.24000	52.91680	74.88890	-773.61628	2935.24407	827.09510	1
13096	C	65.01600	54.39180	73.21590	-514.19369	-573.38898	-488.14028	1
13097	H	65.75700	55.08780	72.76690	586.04189	-1171.70827	-2860.39872	1
13098	H	64.48300	54.96280	74.00590	-1918.41273	-1950.05892	-1554.08784	1
13099	C	63.96000	54.00580	72.20890	589.46538	-651.03714	-245.21870	1
13100	C	62.81500	53.27380	72.56890	82.15858	-902.01760	105.19132	1
13101	H	62.64500	52.99980	73.59990	-1367.78945	-1996.15587	2010.65660	1
13102	C	61.86200	53.00680	71.55590	-399.62295	295.36783	764.53276	1
13103	H	60.98800	52.51080	71.95090	-292.73603	-3089.36869	-518.00862	1
13104	C	62.07000	53.38380	70.23690	-273.52043	79.29525	866.22736	1
13105	O	61.17200	53.02380	69.23190	495.62397	-74.81991	-610.23446	1
13106	H	61.57000	53.06280	68.35890	851.61547	-2247.43352	2030.27581	1
13107	C	64.22300	54.25280	70.86090	650.27815	-305.94784	-561.23547	1
13108	H	65.19200	54.70680	70.71490	1349.63683	2773.39621	-620.46766	1
13109	C	63.28000	53.95980	69.85490	-277.81554	535.08939	684.06789	1
13110	H	63.50300	54.29180	68.85190	1275.25847	-1228.78225	-2600.39156	1
13111	C	65.83400	51.91380	73.11590	574.02176	142.30897	-694.04480	1
13112	O	65.14200	50.94680	73.39390	552.31917	520.35186	-218.64288	1
13113	N	66.72600	51.85580	72.13990	422.02364	574.53356	-452.19411	1
13114	H	67.18100	52.70080	71.86790	1203.14880	-1030.59614	2718.18520	1
13115	C	67.06100	50.73780	71.34590	790.22595	424.03887	-164.87872	1
13116	H	66.18800	50.37980	70.82090	-2262.06129	-451.42444	-2139.51418	1
13117	C	68.18900	50.95680	70.27890	613.00707	645.78500	196.55807	1
13118	H	68.49600	49.97580	69.85790	1447.96023	1574.31117	2307.20215	1
13119	H	69.07300	51.42780	70.75990	-522.29934	3100.87838	99.91442	1
13120	C	67.74500	51.90280	69.18490	-391.16536	-815.71745	114.21783	1
13121	H	67.22000	52.78380	69.61290	-1776.43918	1361.34034	2211.16316	1
13122	C	68.90400	52.46280	68.26490	510.25515	640.32723	-401.33741	1
13123	H	69.21300	51.65180	67.57190	-814.81842	2419.76861	1838.21028	1
13124	H	69.81900	52.69180	68.85290	2307.23219	-1576.31507	-1445.73049	1
13125	H	68.67000	53.44480	67.79890	-512.84722	2259.63912	2128.20229	1
13126	C	66.79800	51.18780	68.16290	113.62520	245.58611	-870.76276	1
13127	H	67.28100	50.33580	67.63890	-1961.02823	-2100.52277	-1280.78047	1
13128	H	66.50300	51.92080	67.38290	-1866.41494	477.41028	-2487.32807	1
13129	H	65.90400	50.68680	68.59190	-1249.88407	1244.38661	-2605.28655	1
13130	C	67.57100	49.59980	72.22890	-510.18512	-755.64773	12.59556	1
13131	O	67.16500	48.45580	72.05690	170.02894	-395.46220	-662.06271	1
13132	N	68.39700	49.92080	73.24090	644.36919	409.26202	-360.50692	1
13133	H	68.72700	50.85680	73.34190	1479.30347	-47.64056	2776.25969	1
13134	C	69.08400	48.91580	74.02090	-270.91730	-767.29334	411.47996	1
13135	H	69.46000	48.13080	73.38090	1797.65204	435.01954	2545.07983	1
13136	C	70.26000	49.50580	74.88190	468.22097	-770.57178	135.79122	1

13137	H	69.96200	50.21280	75.68490	2054.26700	1367.04935	1951.76572	1
13138	H	70.89000	50.10780	74.19090	-2146.73375	1282.63419	-1909.08616	1
13139	H	70.83600	48.64580	75.28590	1459.47504	2739.95025	-510.71662	1
13140	C	68.12500	48.26380	75.04290	756.15586	506.05180	-59.92406	1
13141	O	68.45400	47.23480	75.64590	296.21782	-703.34129	202.96123	1
13142	N	66.89700	48.82080	75.37790	97.57007	399.55034	737.23259	1
13143	H	66.81100	49.74780	75.01990	-1511.28522	28.39929	-2759.24568	1
13144	C	65.93700	48.35880	76.39690	-624.55313	501.03365	-436.29082	1
13145	H	66.38800	47.45080	76.76890	-1511.13383	-1840.62939	2055.91445	1
13146	C	65.75500	49.42180	77.42890	-341.69308	-696.41013	479.28047	1
13147	H	65.76800	50.45180	77.01090	-1462.77981	1153.28881	2535.43416	1
13148	C	64.37800	49.29580	78.19190	-248.81438	762.72529	-433.35037	1
13149	H	64.35700	50.15180	78.89890	1472.39796	2763.45699	305.90179	1
13150	H	63.54600	49.42280	77.46690	1387.58266	-2563.18625	-1184.44790	1
13151	H	64.34900	48.32980	78.73890	2105.62272	-2040.34506	1140.86423	1
13152	C	66.94300	49.36980	78.37390	601.89979	-537.61864	424.42177	1
13153	H	67.87300	49.13980	77.81290	1558.10070	2341.21922	-1410.40454	1
13154	H	66.93800	48.50780	79.07490	1414.57683	694.44056	-2723.04075	1
13155	C	67.20200	50.71380	79.14890	-595.51929	367.18638	584.79222	1
13156	H	68.24400	50.65780	79.52990	-1747.67030	852.83322	-2473.16604	1
13157	H	66.39500	50.70680	79.91290	1661.18725	-1989.41852	1783.50697	1
13158	H	67.23000	51.56080	78.43090	2692.93388	-1447.99748	741.37483	1
13159	C	64.68400	47.94480	75.66090	12.54828	-908.34415	78.76834	1
13160	O	64.12400	46.89680	75.93190	-369.21429	-539.63082	-442.83926	1
13161	N	64.12500	48.67480	74.69190	88.43404	127.31748	829.84454	1
13162	H	64.58500	49.51780	74.42290	1222.07498	2313.77896	-1746.76440	1
13163	C	62.87300	48.23880	73.93890	700.69683	574.78948	-100.45899	1
13164	H	62.32800	47.76380	74.74190	1626.40524	-736.02938	2590.61633	1
13165	C	62.19700	49.49980	73.38790	-825.74470	64.46257	381.36763	1
13166	H	62.95800	50.04680	72.79190	30.59940	2226.53833	2222.56990	1
13167	C	61.03600	49.08980	72.50190	-498.83728	-243.21960	-723.50301	1
13168	H	61.35600	48.76480	71.48890	-2526.11441	1854.13627	-281.33770	1
13169	H	60.40500	48.31080	72.98290	-2242.58347	-1795.54235	1282.60410	1
13170	H	60.31000	49.90180	72.28490	2313.48785	-1447.36120	-1565.61354	1
13171	C	61.82500	50.37880	74.60090	-591.38656	-661.95142	208.64624	1
13172	H	61.06500	51.09380	74.21890	1955.52936	-432.03524	2426.41231	1
13173	H	62.72800	50.86480	75.02890	1190.10654	-2493.82458	1504.23124	1
13174	H	61.21500	49.71080	75.24590	-2259.28048	2110.24103	-583.74717	1
13175	C	63.20100	47.23580	72.87290	417.80222	307.40444	749.92988	1
13176	O	62.38700	46.38080	72.49590	-492.71843	595.46477	-162.10330	1
13177	N	64.47400	47.13380	72.43890	-193.69306	672.65699	-471.89815	1
13178	H	65.23300	47.65180	72.82590	470.99995	-1159.54275	-2886.49370	1
13179	C	64.77200	46.31680	71.22390	-609.91446	214.90419	-642.86199	1
13180	H	64.08400	45.51580	70.99690	-2480.15667	1231.58407	-1493.40210	1
13181	C	64.96500	47.11680	69.95990	-646.88090	640.06767	57.52811	1
13182	H	65.19000	46.42980	69.11690	790.08686	-2387.03599	-1891.04420	1
13183	H	65.80000	47.84180	70.06290	-1996.62865	-1793.95742	-1641.16332	1
13184	N	62.80000	47.30780	68.67190	248.17708	-160.52799	-790.76620	1
13185	H	62.85700	46.39880	68.25890	-1772.11809	2275.94912	1256.13665	1
13186	C	63.74700	47.92880	69.43990	-677.71136	604.87165	79.30073	1
13187	C	61.90700	48.23880	68.29190	398.74466	-522.32628	632.16213	1
13188	H	61.02100	47.93880	67.73390	-685.14795	487.19339	-3031.73896	1
13189	N	62.23400	49.43580	68.75890	414.44244	-668.32608	-307.00163	1
13190	C	63.35500	49.21480	69.53490	-529.59590	698.22968	-251.90175	1
13191	H	63.91700	50.02480	69.98390	-1320.23936	1001.53031	2674.34689	1
13192	C	66.09300	45.60480	71.41390	748.32666	-202.42896	-480.08408	1
13193	O	67.00800	45.60980	70.60490	549.98168	-566.01703	27.78668	1
13194	N	66.26200	44.96680	72.58690	-401.93304	-341.53202	659.14945	1
13195	H	65.54000	44.88280	73.26990	-1650.61831	1008.01634	2481.44887	1
13196	C	67.55100	44.53680	72.97490	-444.39073	536.63254	-588.21204	1
13197	H	68.36100	45.24380	72.87890	2748.24951	-1450.17862	492.27311	1
13198	C	67.54100	44.11380	74.52790	684.43262	130.49388	-588.19583	1

13199	H	67.20500	45.01580	75.08290	1852.05488	-1067.55999	-2308.34023	1
13200	H	66.79700	43.31280	74.72290	2410.20495	595.60692	-1932.45718	1
13201	H	68.52800	43.74880	74.88590	-1383.08883	-911.40774	-2674.81353	1
13202	C	68.08100	43.25480	72.25790	-398.17893	100.57878	814.11821	1
13203	O	69.24900	42.90780	72.37290	636.46954	-463.33057	-62.11712	1
13204	N	67.23100	42.50780	71.53190	4.30664	598.47252	595.38591	1
13205	H	66.32800	42.91980	71.44090	2912.59593	-475.07240	1090.55829	1
13206	C	67.54800	41.26580	70.93090	-335.31234	258.58779	807.55742	1
13207	H	68.32300	40.86780	71.56890	-2010.33196	1752.49858	-1668.99382	1
13208	C	66.43900	40.21380	70.95290	658.31779	513.60753	-366.43690	1
13209	H	66.01200	40.24680	71.97790	-1852.94001	1355.80876	-2150.95843	1
13210	O	66.96200	38.92080	70.87490	550.85539	82.34729	559.82541	1
13211	H	67.72100	38.72880	71.43090	-1576.56453	-1211.14979	2438.39839	1
13212	C	65.34400	40.37980	69.88590	749.87638	-35.58720	-517.56156	1
13213	H	64.40400	39.92280	70.26290	1715.98814	2070.02727	-1633.58441	1
13214	H	65.72800	39.97280	68.92590	-218.60340	-3067.59484	663.55156	1
13215	H	65.10900	41.45680	69.74290	1934.06509	1985.81936	-1487.99863	1
13216	C	68.04700	41.39180	69.50990	-678.69371	-598.30908	113.36708	1
13217	O	68.49600	40.41480	68.88190	293.00025	-344.02636	-647.62948	1
13218	N	67.97800	42.58880	68.90590	-98.72521	-227.23125	807.02638	1
13219	H	67.40400	43.31080	69.28390	1231.01158	1517.88517	2465.53469	1
13220	C	68.25700	42.84080	67.50690	-681.96376	472.33319	378.52053	1
13221	H	69.24300	42.47480	67.26390	1563.84161	-1931.99102	-1928.73957	1
13222	C	67.21300	42.10680	66.52190	757.31941	496.00431	109.07811	1
13223	H	67.50300	42.52180	65.53290	-2122.92264	366.82424	2292.78557	1
13224	H	67.39400	41.01280	66.44490	1704.69488	-133.87949	-2640.89339	1
13225	C	65.73100	42.38580	66.82990	-606.63431	-671.11848	-114.21820	1
13226	O	65.28300	43.17080	67.69590	700.57820	200.82518	304.11620	1
13227	N	64.85100	41.84280	65.95390	-470.70949	144.07806	685.81803	1
13228	H	65.23300	41.18080	65.30890	1897.93127	-1554.74088	-1969.48317	1
13229	H	63.87600	42.02380	66.07990	-976.37974	-1779.46187	-2403.83533	1
13230	C	68.28700	44.37280	67.28890	603.54252	251.75734	635.45705	1
13231	O	67.32600	45.05080	66.84790	-283.11668	71.34098	-733.74562	1
13232	N	69.42800	45.01480	67.51390	-509.83989	439.26624	509.68691	1
13233	H	70.29900	44.54280	67.62790	3073.41697	96.42858	665.60942	1
13234	C	69.59800	46.39680	67.30590	-250.56010	-750.92999	-452.52049	1
13235	H	69.34300	46.64780	66.28690	2380.22491	527.76585	1988.52176	1
13236	C	68.81800	47.28080	68.35890	-751.25610	368.83109	-361.97915	1
13237	H	67.74200	47.08880	68.15690	-1135.32986	1162.85284	2693.88671	1
13238	H	68.95200	48.36380	68.15390	2621.79742	1598.95014	683.93200	1
13239	O	69.09100	46.87480	69.72790	82.97477	577.35857	-532.35279	1
13240	H	68.34100	46.30280	69.90690	-994.29190	-1709.16046	2447.11674	1
13241	C	71.05900	46.81080	67.33990	-598.58095	-246.29948	-642.25262	1
13242	O	71.31200	47.99080	67.04890	-119.88413	-416.63787	660.05144	1
13243	N	72.08300	46.00080	67.59690	-235.47629	186.73699	-788.89321	1
13244	H	71.88000	45.04780	67.80590	-1941.52766	367.00668	2448.26523	1
13245	C	73.48600	46.44780	67.59790	-117.31300	808.07841	405.82995	1
13246	H	73.52400	47.26880	68.29890	-94.15309	555.56409	-3095.27219	1
13247	C	74.37500	45.29980	68.15590	349.24143	-694.52830	476.56255	1
13248	H	74.02300	44.33880	67.72490	2187.56157	1734.49200	-1450.63369	1
13249	H	74.17000	45.24680	69.24690	-462.21592	-675.52413	3037.80345	1
13250	C	75.92100	45.26480	67.94090	-688.34064	-188.53166	-567.53325	1
13251	H	76.30900	44.56380	68.70990	900.64859	2483.23659	1708.97465	1
13252	H	76.31100	46.28280	68.15790	2722.79775	917.21387	1281.91941	1
13253	C	76.47700	44.90180	66.52690	-694.39980	62.00798	587.72011	1
13254	O	77.48800	45.40880	66.06490	-583.38469	-402.96791	-347.71597	1
13255	N	75.84000	43.91380	65.89590	677.82138	-414.44226	-285.42615	1
13256	H	75.05300	43.46880	66.32490	1601.33989	2239.89573	1522.10510	1
13257	H	76.20200	43.57880	65.02690	1908.02434	-180.88731	-2494.98479	1
13258	C	74.06300	47.03080	66.32090	522.08630	-575.61216	-477.01944	1
13259	O	74.69700	48.06380	66.27790	244.51640	-347.06706	665.87042	1
13260	N	73.75600	46.55480	65.10790	-757.58830	144.48831	-343.30071	1

13261	H	73.25200	45.70380	64.98290	-484.25524	488.11033	3070.09306	1
13262	C	74.08400	47.23980	63.86290	-161.53046	-750.43013	492.15193	1
13263	H	75.12800	47.51180	63.92690	-1065.13115	-2932.33163	406.39032	1
13264	C	74.06800	46.20880	62.72890	-731.28525	-469.71222	275.75953	1
13265	H	73.13500	45.60880	62.79690	-2009.06986	-1599.06496	1817.92623	1
13266	H	74.85700	45.42680	62.72790	-416.58161	-528.78603	3073.28347	1
13267	C	74.06200	46.76480	61.27790	-776.95958	-436.42055	193.18882	1
13268	H	73.11700	47.30680	61.06290	1417.32230	2737.90974	-627.11560	1
13269	H	74.90400	47.46680	61.10090	-1647.08289	868.00982	-2536.11970	1
13270	C	74.25100	45.71380	60.15490	787.69201	-432.25438	-155.39769	1
13271	H	75.13100	45.04580	60.27290	-2340.97760	1034.54472	1829.69051	1
13272	H	73.41700	44.99080	60.02890	-276.37492	2903.44781	1179.76013	1
13273	N	74.37500	46.45680	58.85890	-541.96141	-484.39141	429.31933	1
13274	H	73.83000	47.27780	58.68890	439.68406	2676.96414	1593.35092	1
13275	C	74.66200	45.80580	57.73890	412.49453	602.72693	-545.91163	1
13276	N	75.21300	44.60980	57.67290	343.28745	-484.01684	600.46125	1
13277	H	75.14000	43.94180	58.41390	1066.64886	1702.06179	-2421.46073	1
13278	H	75.29600	44.15880	56.78390	-2741.62249	591.53017	-1425.42078	1
13279	N	74.43800	46.41980	56.59390	-652.77470	441.51959	-302.68453	1
13280	H	74.35200	47.41580	56.55990	-366.14760	-834.01819	-3011.40761	1
13281	H	74.81700	46.00380	55.76690	-2089.51111	-2352.02812	-11.54432	1
13282	C	73.45900	48.66280	63.65890	367.37472	-648.97084	524.71294	1
13283	O	74.22500	49.62080	63.25590	591.72685	-305.57477	-424.39443	1
13284	N	72.19600	48.93680	63.88290	-569.87937	557.90511	-276.86041	1
13285	C	71.15200	47.91380	63.64390	554.89815	314.54020	651.61607	1
13286	H	71.01200	47.26380	64.53490	-408.21656	-2507.78575	1855.42343	1
13287	H	71.30300	47.24080	62.77290	2314.20547	-2085.90791	437.79846	1
13288	C	71.58800	50.28980	63.86990	223.43296	-572.17464	673.90274	1
13289	H	71.84300	50.86080	62.98890	2443.94981	-1878.97436	628.32388	1
13290	C	70.07700	50.06480	63.96190	-439.81422	-571.98101	557.54119	1
13291	H	69.46100	50.84980	63.47390	-2705.05160	792.16700	1397.63854	1
13292	H	69.73700	49.93580	65.01190	-1616.19085	-411.24491	-2667.77641	1
13293	C	69.87000	48.68880	63.34890	-607.08387	-680.02370	21.63219	1
13294	H	69.82900	48.81780	62.24590	2001.62042	2191.28034	-1044.04615	1
13295	H	68.94600	48.19980	63.72390	-1180.94778	-2507.16573	1489.19729	1
13296	C	72.06400	51.10980	65.08690	418.51034	-615.39546	-526.86671	1
13297	O	72.36800	52.25980	64.91690	-310.85032	-687.91968	231.87457	1
13298	N	72.14200	50.58980	66.34490	-289.32400	-596.50411	522.63444	1
13299	H	71.85400	49.64680	66.48990	1363.66697	2593.04601	-1146.62592	1
13300	C	72.81900	51.31980	67.35990	357.30677	628.45541	555.72176	1
13301	H	72.31400	52.25080	67.56990	2502.65950	1397.91440	1296.44011	1
13302	C	72.89600	50.49980	68.67390	-257.51074	-482.49481	-729.61495	1
13303	H	73.60400	51.00680	69.36290	-2483.46327	1672.50487	966.10759	1
13304	H	73.30500	49.50780	68.38590	-1677.63239	2346.91290	1255.29902	1
13305	C	71.62900	50.31280	69.43890	-163.66395	-590.59331	-675.17750	1
13306	H	70.76200	49.92680	68.86190	-554.84535	2989.57813	-807.95758	1
13307	H	71.29200	51.26680	69.89990	481.09859	-1476.23941	-2736.32739	1
13308	C	71.72500	49.24180	70.58390	446.76018	-774.28284	-179.84001	1
13309	H	70.75000	48.93880	71.02290	1486.63614	-1571.06313	2284.71002	1
13310	H	72.23500	48.32680	70.21490	-1807.91618	1953.25876	1677.63092	1
13311	N	72.53600	49.96180	71.58390	-293.05361	786.60279	-89.71019	1
13312	H	72.73100	50.93480	71.46790	-1194.06061	2648.21785	-1208.05119	1
13313	C	73.24800	49.36280	72.44790	810.67973	-416.96001	19.84276	1
13314	N	73.02000	48.12780	72.87290	-787.41695	-159.99390	258.93781	1
13315	H	72.19900	47.67380	72.52690	-2513.64235	-426.69839	1843.30052	1
13316	H	73.73800	47.68480	73.40890	1844.99598	1762.05733	1841.02417	1
13317	N	74.05500	50.13280	73.16390	-11.35797	841.95718	60.42671	1
13318	H	74.03900	51.12880	73.07790	-990.59967	-2636.73108	1401.63752	1
13319	H	74.58500	49.72780	73.90890	-1576.76848	1001.33361	2531.67106	1
13320	C	74.26400	51.75680	67.03390	490.81175	-88.58160	-763.35321	1
13321	O	74.70400	52.87880	67.34290	-97.63868	-781.84572	53.02065	1
13322	N	74.99000	50.84080	66.43790	391.45388	-416.25300	-621.42545	1

13323	H	74.53700	50.00780	66.12990	-2434.88356	1263.10961	-1540.81873	1
13324	C	76.32900	51.05180	65.91890	755.75258	424.99039	282.26265	1
13325	H	76.92000	51.30980	66.78590	2383.14925	975.35757	1807.62371	1
13326	C	76.94900	49.70280	65.47390	-127.10057	449.84396	-782.90284	1
13327	H	76.30500	49.24080	64.69590	-1462.01769	-776.97564	2675.26435	1
13328	H	76.96900	49.10280	66.40990	2351.35848	2038.64845	-461.79218	1
13329	C	78.38400	49.85180	64.90690	507.13821	429.47325	624.35131	1
13330	H	78.99800	50.42380	65.63490	1539.25316	2178.00992	-1668.89147	1
13331	H	78.48000	50.46080	63.98190	497.81871	1585.92457	-2671.18813	1
13332	C	79.08600	48.50880	64.76090	-465.49210	-579.50324	-528.15158	1
13333	H	80.13800	48.65880	64.43590	-1798.56283	2098.41842	-1503.34231	1
13334	H	79.13800	48.00180	65.74790	-1712.44281	2016.17196	1703.17835	1
13335	C	78.42400	47.54480	63.73590	-276.83746	-461.54264	736.06414	1
13336	H	77.43900	47.19580	64.11290	2062.78229	-900.72626	2198.14641	1
13337	H	78.43800	48.07180	62.75690	-581.77017	-1296.54614	2806.90894	1
13338	N	79.19100	46.31480	63.58490	668.80042	-48.88060	512.82451	1
13339	H	79.15700	45.54480	64.28290	-1455.35871	2733.96206	-552.81890	1
13340	H	78.84600	45.88880	62.70090	2802.27857	696.03767	-1249.39690	1
13341	H	80.20700	46.41180	63.38790	-1395.14776	167.54165	-2814.91008	1
13342	C	76.45600	52.09780	64.76190	-340.64362	379.01610	-756.14795	1
13343	O	77.33400	53.00380	64.73790	480.83886	274.14261	-563.26464	1
13344	N	75.49900	52.07180	63.80890	474.66355	163.46394	-678.70932	1
13345	H	74.82500	51.33980	63.87890	-1343.72188	-1828.90196	-2178.93446	1
13346	C	75.37200	53.05880	62.72290	505.86493	-644.58825	-400.07208	1
13347	H	76.24900	53.07880	62.09390	1996.30797	-1795.19527	1640.19958	1
13348	C	74.08200	52.69580	61.93290	467.02505	-635.74028	-457.35423	1
13349	H	73.19500	52.54980	62.58490	2992.05203	-698.08008	677.15216	1
13350	H	74.18000	51.73280	61.38690	-2643.66720	-1378.09349	1005.04144	1
13351	C	73.59900	53.60380	60.75090	746.41321	-148.09729	502.37985	1
13352	H	73.51200	54.61580	61.20090	-2259.59392	2000.75123	888.51342	1
13353	C	74.75200	53.70080	59.70190	392.86651	818.16838	-87.79179	1
13354	H	75.73100	53.99880	60.13390	973.97142	-2231.00409	-1993.04456	1
13355	H	74.40100	54.35980	58.87990	-2807.57231	-610.77700	-1281.68460	1
13356	H	74.77600	52.72380	59.17190	461.01885	-2966.66190	940.53442	1
13357	C	72.26900	52.99980	60.24790	145.82257	-611.60754	-660.39609	1
13358	H	72.31900	51.91280	60.01990	-2677.86183	717.21180	-1487.57839	1
13359	H	71.53100	53.17380	61.05890	2811.05797	716.38731	-1217.77196	1
13360	H	71.90400	53.53280	59.34390	-582.05890	1814.68262	-2503.26999	1
13361	C	75.26700	54.48680	63.29190	864.36087	-210.32899	-200.23236	1
13362	O	75.99400	55.39780	62.81990	-722.97101	-65.10869	-310.96785	1
13363	N	74.42500	54.77980	64.32690	56.26413	662.10682	-520.69299	1
13364	H	73.71000	54.13580	64.58490	1481.70092	2723.79880	-532.64312	1
13365	C	74.40000	55.99780	65.09690	135.32019	888.85078	151.93334	1
13366	H	74.15100	56.75380	64.36690	1816.38195	-1659.32307	1961.02774	1
13367	C	73.31000	55.86980	66.17990	147.39433	803.00974	-406.08038	1
13368	H	73.30000	56.73880	66.87090	-1879.52770	558.27214	2460.47436	1
13369	H	73.61800	54.94780	66.71790	-124.36038	1122.47502	2936.46225	1
13370	C	71.87600	55.65080	65.62390	-292.57289	-459.05976	-731.51640	1
13371	H	71.83700	54.60480	65.25090	853.61981	-51.96252	-3027.68217	1
13372	C	70.97400	55.48080	66.86590	-262.24589	276.38742	-828.42506	1
13373	H	71.23100	54.55980	67.43290	-35.86831	1339.43061	-2846.55324	1
13374	H	71.08600	56.36480	67.52890	690.15356	-2302.03786	2030.40291	1
13375	H	69.94100	55.32880	66.48690	789.05455	-2499.06386	1740.77540	1
13376	C	71.25800	56.61480	64.56090	507.07240	560.70252	-509.84435	1
13377	H	70.17700	56.37880	64.46190	-1746.50458	-1860.64461	1840.09500	1
13378	H	71.83700	56.72880	63.61990	1435.80627	2799.35657	17.01108	1
13379	H	71.32500	57.64680	64.96790	-602.34540	-2187.68669	-2179.31943	1
13380	C	75.73500	56.27280	65.77590	449.23342	690.57438	-390.82908	1
13381	O	76.34600	57.33580	65.63190	98.01944	-737.45968	-264.90119	1
13382	N	76.31200	55.24680	66.49890	474.00165	695.72037	62.99122	1
13383	H	75.88100	54.35180	66.58390	-2128.34693	2169.62168	813.08508	1
13384	C	77.48200	55.40080	67.33590	-188.92237	684.46151	-572.07673	1

13385	H	77.32600	56.29280	67.92390	-2248.40509	1524.77759	-1586.80624	1
13386	C	77.62100	54.17580	68.29490	656.69761	-251.44449	580.49541	1
13387	H	78.49700	54.34580	68.95590	-1355.25345	2557.13823	1233.91994	1
13388	H	76.75900	54.12480	68.99390	-186.38175	-699.89618	-3061.63901	1
13389	H	77.70900	53.20180	67.76690	763.93062	-1527.50127	2642.22938	1
13390	C	78.78300	55.65680	66.64290	-504.56942	517.63806	555.79811	1
13391	O	79.62000	56.37780	67.15490	-520.37260	-556.13294	208.70012	1
13392	N	78.96700	55.15180	65.41590	-170.22067	783.12437	-265.35529	1
13393	H	78.26300	54.58880	64.98890	-2830.38522	295.52187	-1341.57092	1
13394	C	80.24300	55.01480	64.81890	-742.71501	-319.79120	-421.37752	1
13395	H	80.93500	55.54480	65.45490	-1284.08264	1406.65318	2504.13355	1
13396	C	80.74100	53.60680	64.68090	369.62887	-790.28411	-265.09721	1
13397	H	81.54200	53.50280	63.91790	1367.07050	2829.87709	-145.39652	1
13398	H	79.93900	52.99380	64.21490	-1230.72456	-447.92394	-2860.57817	1
13399	C	81.19200	53.07180	66.00590	-439.81834	431.09233	672.43604	1
13400	H	80.21400	52.97080	66.52290	822.31980	-2077.29909	2215.13992	1
13401	H	81.98500	53.67880	66.49090	2425.71536	1965.56947	-388.15957	1
13402	C	81.80000	51.67080	65.81990	-194.87544	641.85926	-617.64978	1
13403	O	82.54700	51.38680	64.86090	490.51294	511.21769	348.82770	1
13404	O	81.46400	50.77080	66.62690	586.86452	97.56209	519.32543	1
13405	C	80.24800	55.64180	63.46990	-393.60719	-299.78151	765.93435	1
13406	O	81.28400	56.18180	63.05390	185.46925	-763.79646	-76.44188	1
13407	N	79.10300	55.73680	62.73990	1.18328	620.27752	-572.64884	1
13408	H	78.21300	55.39680	63.03490	-2991.28572	-323.39887	919.70058	1
13409	C	79.08500	56.37380	61.44790	456.82388	-551.93061	564.03506	1
13410	H	80.07800	56.57180	61.07090	2080.94848	-158.14349	2354.33011	1
13411	C	78.41800	55.43180	60.43790	595.38611	-262.83251	-638.65911	1
13412	H	77.80000	55.86380	59.62190	-1201.22448	1916.78934	-2186.59658	1
13413	H	77.61800	54.90880	61.00490	-2339.72894	2080.30056	-310.23263	1
13414	C	79.39200	54.30580	59.96390	523.91545	550.26969	-504.14965	1
13415	H	80.20100	54.78780	59.37390	1632.38826	612.06032	2618.95341	1
13416	H	79.81400	53.79280	60.85490	3082.36072	-630.18896	-11.85261	1
13417	C	78.69400	53.25980	59.05890	535.32051	-553.97053	-487.85204	1
13418	H	78.18300	53.69880	58.17490	-2896.45892	-1228.09288	-23.23467	1
13419	H	77.89200	52.86580	59.71890	574.79550	-3068.48749	-390.15494	1
13420	C	79.52300	52.08780	58.64990	119.91645	-217.39813	-877.38766	1
13421	H	78.88900	51.18480	58.52290	1550.97321	-136.94496	2733.85340	1
13422	H	80.17100	51.87080	59.52690	-1835.80481	76.09568	-2553.87086	1
13423	N	80.41500	52.29680	57.45590	-340.75312	-238.62309	734.58738	1
13424	H	81.01600	53.14280	57.39090	2077.51361	1710.64734	1629.67761	1
13425	H	80.99800	51.45480	57.27390	2036.95678	-1679.36001	-1711.36882	1
13426	H	79.79000	52.30380	56.62490	-136.84474	-2232.74320	2212.31949	1
13427	C	78.36900	57.66680	61.44790	-436.04995	495.04796	-629.47515	1
13428	O	78.89200	58.71780	61.08490	-87.52700	-612.14327	491.16888	1
13429	N	77.09500	57.58980	61.86190	607.50853	527.28763	-256.07310	1
13430	H	76.77100	56.72180	62.22990	1458.51518	-1997.19696	-1944.77865	1
13431	C	76.09900	58.66480	61.66090	133.28248	-784.46330	445.31350	1
13432	H	76.35500	59.15680	60.73390	-2975.33665	-993.06191	243.77466	1
13433	C	74.63500	58.10880	61.42090	-235.67123	686.81576	-551.53802	1
13434	H	74.40700	57.32080	62.17090	-2592.77985	286.31803	-1758.90331	1
13435	C	73.63900	59.25180	61.53490	412.54753	67.66444	810.35613	1
13436	H	73.66300	59.64980	62.57190	1124.66712	1030.89139	-2751.47470	1
13437	H	72.61900	58.85480	61.34290	-2442.61912	-1685.69764	1044.15588	1
13438	H	73.85800	60.07080	60.81690	1055.85425	-1531.17459	2537.49924	1
13439	C	74.54200	57.54180	59.97590	-322.67470	385.89947	760.53510	1
13440	H	75.40900	56.88280	59.75790	1220.58053	-2103.52528	1995.89348	1
13441	H	73.71200	56.81880	59.81990	2015.11253	1366.60431	1992.47093	1
13442	H	74.61300	58.32480	59.19190	301.43086	-2515.68369	1865.12768	1
13443	C	76.21100	59.84480	62.65990	-12.43828	6.78298	-911.72928	1
13444	O	75.93300	60.98580	62.30390	576.43795	213.03201	-495.94745	1
13445	N	76.85000	59.71980	63.88290	-395.10264	459.78809	-587.50414	1
13446	H	76.85700	58.81880	64.30890	-1745.59768	-2615.25319	-107.54412	1

13447	C	77.20900	60.88380	64.76190	682.57926	-366.07454	481.17147	1
13448	H	76.28000	61.42980	64.83790	-1968.94770	1636.93714	1828.08861	1
13449	C	77.73400	60.39280	66.08790	-528.03511	-107.94521	-735.51190	1
13450	H	77.00500	59.71580	66.58190	2074.08785	1543.57762	1792.69461	1
13451	C	79.03700	59.53180	65.95890	-159.07311	-559.93267	-701.87047	1
13452	H	79.91700	60.21080	65.96790	3081.88190	-14.18254	632.47849	1
13453	H	79.30200	58.94780	65.05190	-1119.62649	-2552.41944	-1459.38951	1
13454	H	79.18400	58.75480	66.73890	-2398.91850	585.98352	-1949.36902	1
13455	C	77.96200	61.63780	66.98490	237.71013	-728.35172	494.41751	1
13456	H	78.82900	62.29580	66.75890	2530.62891	1755.47006	-642.23704	1
13457	H	78.00300	61.31880	68.04790	-1566.25258	1835.16075	2019.22364	1
13458	H	77.05900	62.28480	66.98290	-1195.10023	2422.04621	-1613.58416	1
13459	C	78.17500	61.78680	63.99590	591.43949	297.00416	-627.24705	1
13460	O	78.09900	62.98780	64.12390	-680.00288	401.52001	-2.23548	1
13461	N	79.04000	61.27880	63.15690	461.53381	222.71467	-670.86288	1
13462	H	79.21600	60.30180	63.07090	-351.47570	1952.59601	2441.73297	1
13463	C	79.83300	62.16880	62.23990	-743.29342	-451.56983	273.95362	1
13464	H	80.38500	62.91080	62.79690	-567.46054	2257.40796	2116.67760	1
13465	C	80.87800	61.35180	61.53590	247.62975	876.88086	-34.79164	1
13466	H	81.46900	62.00780	60.86190	1668.15668	-2662.34459	165.53182	1
13467	H	80.48200	60.49880	60.94490	3032.26998	320.36756	775.19650	1
13468	C	81.78800	60.76180	62.55890	-542.31176	452.41814	-576.77273	1
13469	C	81.47900	59.48980	63.13990	610.43304	80.23188	-672.59598	1
13470	H	80.54500	58.99280	62.92390	2094.09441	-2307.64190	-433.34013	1
13471	C	82.33100	58.99680	64.14690	-627.84855	-285.72860	596.33579	1
13472	H	82.11600	58.00880	64.52490	1288.86116	-2499.37535	-1410.73952	1
13473	C	83.50600	59.67180	64.52090	597.32487	558.50971	-403.38680	1
13474	O	84.34300	59.10380	65.48790	784.82525	-16.16578	-86.11168	1
13475	H	85.16400	59.59980	65.50190	1989.31837	2340.00078	-682.08136	1
13476	C	82.96400	61.42180	62.94590	-743.72146	-227.65914	-475.92091	1
13477	H	83.22800	62.37680	62.51590	-1601.44261	-1953.72382	-1875.25225	1
13478	C	83.79600	60.81880	63.85490	-646.60004	642.81176	-12.34635	1
13479	H	84.68400	61.36680	64.13590	-1077.47896	1761.32941	2373.81213	1
13480	C	79.07200	63.01480	61.18490	755.97992	-504.10201	76.33172	1
13481	O	79.35300	64.19780	61.05590	305.27495	532.93805	496.39850	1
13482	N	78.11400	62.42880	60.51990	-330.48286	752.95759	-191.07130	1
13483	H	77.89300	61.46280	60.63090	-1800.74236	-2418.28065	-898.59439	1
13484	C	77.45200	63.00280	59.37490	-171.02718	887.28241	122.19095	1
13485	H	77.88600	63.93180	59.03590	1745.28610	-293.13041	-2601.20688	1
13486	C	77.51400	62.02580	58.15990	496.29923	423.73091	-636.85963	1
13487	H	78.58700	61.74980	58.07590	-1987.58359	1594.16214	1845.63940	1
13488	C	76.64800	60.74380	58.20490	-838.08345	59.05954	354.37142	1
13489	H	76.89000	60.04880	57.37290	1950.03968	-933.72632	-2285.54733	1
13490	H	75.57900	61.03780	58.26890	-1395.33314	2687.81368	852.60148	1
13491	H	76.88300	60.24480	59.16990	-855.71685	683.96007	2949.26661	1
13492	C	77.07000	62.83080	56.90790	-570.77126	-609.60883	366.12599	1
13493	H	77.53500	63.83980	56.88090	476.65632	-683.53386	3033.77759	1
13494	H	77.24600	62.12980	56.06390	-2189.15145	-1811.11047	1351.19245	1
13495	H	75.98500	63.07180	56.90790	-1330.65511	-1417.88160	2473.29638	1
13496	C	75.96700	63.43180	59.71690	-272.22670	-592.10152	-637.77693	1
13497	O	75.23100	63.95280	58.88690	-83.50511	410.59184	-669.37917	1
13498	N	75.55600	63.14580	60.96990	-150.57332	825.49864	92.47680	1
13499	H	76.07500	62.48980	61.51290	504.16011	2415.79102	1951.41040	1
13500	C	74.24300	63.52480	61.53090	-523.91201	361.70244	-652.79288	1
13501	H	73.64800	62.66780	61.80990	-1282.59050	2670.70883	1058.53775	1
13502	H	73.74100	64.17580	60.82990	-2164.17609	-669.96139	-2183.05287	1
13503	C	74.39400	64.47380	62.76890	667.40836	-593.81190	-182.76899	1
13504	O	73.38900	65.08080	63.16490	213.44088	492.89450	578.90002	1
13505	N	75.62000	64.65580	63.34290	407.76159	-528.08353	517.23356	1
13506	H	76.40600	64.05980	63.19790	-1565.45391	-724.90537	2630.98698	1
13507	C	75.80700	65.65780	64.37690	248.54503	560.24445	675.13149	1
13508	H	74.96800	66.32780	64.49790	-134.98160	2855.56669	-1313.67617	1

13509	C	76.01200	64.93380	65.67590	278.61279	-370.56758	785.17870	1
13510	H	76.89500	64.26080	65.65490	2093.60022	-2303.69237	-456.14232	1
13511	C	76.30800	65.94080	66.83790	659.81054	-153.30146	-610.40947	1
13512	H	77.32300	66.35880	66.66890	2604.30123	1417.98064	-1051.27172	1
13513	H	76.23100	65.35680	67.77990	1842.88595	1275.58512	2207.91308	1
13514	H	75.48500	66.68680	66.80890	2557.02413	-1828.61020	-126.64340	1
13515	C	74.73100	64.15080	66.04990	-260.84914	590.19267	-644.26807	1
13516	H	73.85200	64.82480	66.13390	-1559.89301	-2590.09786	-869.68563	1
13517	H	74.86500	63.63880	67.02690	-1583.21081	890.33354	-2568.84720	1
13518	H	74.49800	63.28680	65.39090	-1477.86579	-1563.69327	-2295.43074	1
13519	C	76.98200	66.54980	64.00090	-311.36156	-663.92101	541.95376	1
13520	O	76.81300	67.75280	63.82890	493.09283	-568.06205	240.40009	1
13521	N	78.17500	65.95380	63.88490	669.45657	322.63646	-400.50705	1
13522	H	78.34800	64.98480	64.04090	-1952.26483	-1901.95370	1571.45169	1
13523	C	79.38000	66.79380	63.80390	275.33721	269.64065	-826.39842	1
13524	H	79.33300	67.52180	64.60090	435.59070	-1565.41234	-2694.06221	1
13525	C	80.72500	65.95580	63.88190	783.96094	-408.45164	-223.65934	1
13526	H	81.57500	66.47980	63.39390	952.56650	2545.70453	1584.37108	1
13527	H	80.62700	65.05980	63.23190	-935.60924	-1361.43225	-2677.56677	1
13528	C	81.07600	65.46380	65.23690	756.59391	-502.07413	-83.29604	1
13529	C	81.17800	64.13780	65.68490	-792.75719	-351.50764	-281.83227	1
13530	H	81.15400	63.23580	65.09090	409.44274	1620.97532	-2665.14950	1
13531	N	81.54500	64.11680	67.03990	-628.07833	249.30732	-505.99977	1
13532	H	81.89000	63.41080	67.61890	-799.53679	1852.52640	-2413.94140	1
13533	C	81.67300	65.44380	67.41590	799.83290	-399.14944	-179.99461	1
13534	C	81.36600	66.28480	66.35090	-261.53011	-603.09923	631.92114	1
13535	C	81.43800	67.69780	66.49390	449.92375	-625.12954	-488.09085	1
13536	H	81.35400	68.36680	65.64990	2137.35506	1826.49301	1412.04209	1
13537	C	81.95200	68.19480	67.67890	795.64160	-402.47773	190.83272	1
13538	H	82.20600	69.23880	67.78590	-1100.00132	2894.86718	554.94806	1
13539	C	81.95100	65.96580	68.65390	-476.80441	764.53960	139.95628	1
13540	H	82.12500	65.34080	69.51690	2152.14988	774.02491	2160.40796	1
13541	C	82.16800	67.36880	68.71590	112.25910	-691.74216	-583.38811	1
13542	H	82.68500	67.67280	69.61390	-1251.40173	-1419.70961	2513.29357	1
13543	C	79.54100	67.60780	62.56990	-662.04951	-398.77358	-483.86060	1
13544	O	79.68900	68.83180	62.62190	-72.69763	683.15442	389.41279	1
13545	N	79.43900	66.98780	61.39490	234.11088	-475.89358	-656.80263	1
13546	H	79.52900	65.99580	61.36090	-1658.50736	-143.70214	2669.63092	1
13547	C	79.40100	67.72880	60.09790	664.72391	-587.29714	211.36507	1
13548	H	80.27400	68.36380	60.06790	816.95783	600.97156	-2978.19397	1
13549	C	79.57800	66.71580	58.97690	-89.51908	129.76712	898.10792	1
13550	H	79.06400	65.76680	59.23990	1520.52353	1979.92785	1914.71150	1
13551	C	79.02300	67.18080	57.59490	-566.26586	586.52737	408.38661	1
13552	H	79.08700	66.33780	56.87390	-745.45430	-1568.61513	2623.35104	1
13553	H	77.97200	67.53780	57.64990	2928.32411	1084.36958	-383.77957	1
13554	H	79.57700	68.09680	57.29790	2043.77050	-2084.93708	-1172.29081	1
13555	C	81.08100	66.50980	58.92390	388.43729	695.20120	444.14273	1
13556	H	81.56100	66.51280	59.92590	2721.90919	-1233.68186	983.59831	1
13557	H	81.53800	67.31980	58.31590	1799.36522	2401.52655	945.08269	1
13558	C	81.48100	65.22680	58.17990	554.61258	-314.94345	-651.66442	1
13559	H	82.58100	65.23080	58.01990	-548.99997	-2333.92582	-2037.06051	1
13560	H	81.14600	64.38880	58.82690	-1062.72655	1845.77819	2315.58662	1
13561	H	81.07500	65.34680	57.15190	-2526.76737	-1845.25930	-329.68320	1
13562	C	78.20300	68.68480	59.97390	-169.06395	509.15556	737.31201	1
13563	O	78.39300	69.81780	59.50690	-730.96421	-163.19824	250.36949	1
13564	N	76.94300	68.38580	60.25590	382.34420	-450.46081	602.96788	1
13565	C	76.40600	67.04980	60.23790	101.55111	39.63848	-905.29949	1
13566	H	76.84500	66.50280	61.09990	-35.26389	-2364.76667	-2074.81596	1
13567	H	76.61900	66.55080	59.26890	-2215.49163	1831.81047	-1278.39488	1
13568	C	75.89100	69.36780	60.47890	-503.71622	-382.96712	-656.54944	1
13569	H	75.63800	69.83980	59.54090	2410.32531	1718.91546	-1064.84167	1
13570	C	74.79500	68.58480	61.07990	322.65296	-422.80851	740.66121	1

13571	H	74.84900	68.53780	62.18890	-1040.70574	-1901.65108	-2280.10547	1
13572	H	73.81200	69.09380	60.98690	2242.03676	-2148.05451	-507.30583	1
13573	C	74.91000	67.23780	60.38990	-325.40783	-656.23778	-543.05867	1
13574	H	74.48000	66.36180	60.92190	2405.11862	197.92356	2018.52840	1
13575	H	74.36300	67.34880	59.42990	-56.49788	846.00936	3029.73636	1
13576	C	76.27700	70.60180	61.32290	703.01954	-46.61631	-578.82766	1
13577	O	75.93900	71.65980	60.85690	-723.71387	-201.97021	-243.05039	1
13578	N	76.98300	70.49280	62.53090	441.73769	351.29978	627.79660	1
13579	H	77.22900	69.59880	62.89790	-998.57522	-2127.28062	2091.82956	1
13580	C	77.34300	71.60280	63.34590	51.77988	707.65465	-572.70825	1
13581	H	76.43300	72.10680	63.63490	2898.13603	-1172.21801	-353.46674	1
13582	C	78.07100	71.11780	64.56590	-253.11347	659.10138	-577.03548	1
13583	H	77.40400	70.42680	65.12390	-1411.15697	-2314.43961	-1596.94444	1
13584	H	78.32800	71.98480	65.21090	-2709.75096	367.84358	1555.68861	1
13585	H	79.06500	70.67980	64.33290	-3067.13397	137.45548	-687.03816	1
13586	C	78.26200	72.58380	62.57290	682.49780	447.18425	407.03071	1
13587	O	77.99600	73.79480	62.52490	-478.25785	550.39124	303.25920	1
13588	N	79.28600	72.04380	61.88190	-190.06427	-631.23312	-527.34487	1
13589	H	79.45000	71.06180	61.82190	1714.14310	1948.78440	-1778.25167	1
13590	C	80.16600	72.83480	60.97290	-481.45767	-367.76633	681.46712	1
13591	H	80.56600	73.62780	61.58790	1.92333	3141.55384	-169.88815	1
13592	C	81.26100	71.99780	60.26490	-642.24492	-600.79952	240.85763	1
13593	H	80.87300	71.21680	59.57690	1253.90065	-2877.67719	-211.97497	1
13594	H	81.86300	72.79880	59.78490	1351.93614	-2410.42112	-1503.45100	1
13595	C	82.21600	71.17680	61.14290	37.20441	698.82925	584.55497	1
13596	H	81.67600	70.33280	61.62390	-1335.69003	-1079.49409	-2636.06731	1
13597	C	83.30900	70.67280	60.22790	-647.67314	-293.02833	571.05596	1
13598	H	82.82200	70.02180	59.46990	-334.40520	1911.46601	2476.42829	1
13599	H	83.81700	71.51980	59.71990	-1094.50796	2151.03179	2018.25192	1
13600	H	84.03400	70.09680	60.84190	2169.42575	-2232.25064	-457.02871	1
13601	C	82.83200	72.00880	62.34890	-734.31262	-29.66428	-539.77404	1
13602	H	81.97800	72.18080	63.03890	1618.46271	2641.76034	547.63768	1
13603	H	83.61500	71.40980	62.85990	1034.92887	1218.91969	-2709.49871	1
13604	H	83.28400	72.93580	61.93590	904.06768	2719.56616	1298.01685	1
13605	C	79.39800	73.56380	59.85490	-412.89558	811.61597	-47.41066	1
13606	O	79.60700	74.74080	59.58190	-265.26780	686.81507	285.56135	1
13607	N	78.44400	72.86480	59.19490	630.45625	456.03448	-327.45955	1
13608	H	78.25100	71.91980	59.44990	-2228.30596	1238.06642	1843.92796	1
13609	C	77.51900	73.42580	58.26290	466.52900	-601.72352	501.72752	1
13610	H	78.15500	73.93980	57.55690	1337.24937	-2722.63665	-835.00899	1
13611	C	76.60000	72.37380	57.56490	309.95694	430.93829	-741.39725	1
13612	H	75.90000	72.97980	56.94990	342.40933	-2245.93785	2176.40650	1
13613	H	76.05600	71.96080	58.44090	1084.66154	928.89903	-2803.36979	1
13614	C	77.41200	71.39580	56.68990	866.46906	252.80207	129.51252	1
13615	H	78.23700	70.92380	57.26490	-1870.34412	-1592.98019	1965.31250	1
13616	C	76.51500	70.32580	56.03890	-579.50716	-525.10325	468.92328	1
13617	H	75.79800	70.79480	55.33190	1948.98959	-2450.34638	308.97967	1
13618	H	77.06300	69.52180	55.50390	935.83366	-2836.40874	988.54796	1
13619	H	76.02800	69.82180	56.90090	-2204.04567	997.94039	-2011.10017	1
13620	C	78.08700	72.20080	55.55590	-548.67517	-215.89980	695.55290	1
13621	H	78.93000	72.84180	55.89090	2446.53965	-890.45067	-1766.28638	1
13622	H	77.35600	72.90380	55.10290	-19.42709	-3080.31590	-639.92405	1
13623	H	78.47800	71.55980	54.73690	-1972.30071	-1450.31055	1976.07071	1
13624	C	76.65800	74.51080	58.81890	231.98561	562.33357	-679.27508	1
13625	O	76.44500	75.53780	58.13990	714.06837	-40.17815	-334.84222	1
13626	N	76.13800	74.39180	60.04090	617.36970	286.62132	-499.37476	1
13627	H	76.10800	73.55980	60.58990	2165.59712	-1853.48418	-1331.54487	1
13628	C	75.18900	75.41980	60.53390	701.13198	-525.05250	253.34724	1
13629	H	74.52600	75.63580	59.70990	942.78482	-2944.10920	584.46903	1
13630	C	74.32700	74.98880	61.72290	-449.78881	-343.47278	-714.95978	1
13631	H	73.68700	75.85480	61.99690	2635.01368	188.31622	1708.64454	1
13632	H	75.08200	74.73680	62.49790	-2836.22068	1121.91519	771.61179	1

13633	C	73.43400	73.79580	61.37990	-400.29774	366.91327	732.52125	1
13634	H	73.87200	73.05280	60.67990	-2481.98041	-1112.62012	1581.16285	1
13635	C	73.20600	72.96180	62.64590	524.56692	373.61649	-645.51628	1
13636	H	72.47500	72.15780	62.41390	-135.19921	1449.58460	-2789.02347	1
13637	H	72.89900	73.58880	63.51090	-219.67440	-1200.96979	2899.59324	1
13638	H	74.09900	72.35780	62.91390	1564.87649	1580.78756	-2224.97157	1
13639	C	72.04600	74.18280	60.80190	-273.69235	416.04256	763.84036	1
13640	H	71.38500	73.30880	60.62390	749.99034	-2806.24561	1208.60509	1
13641	H	71.56400	75.00680	61.36990	1626.87072	-1973.16836	-1832.51863	1
13642	H	72.15400	74.59180	59.77490	-2157.38483	-596.93883	-2210.78741	1
13643	C	75.85100	76.71480	60.91390	422.05272	-388.77636	-708.64338	1
13644	O	75.24100	77.76980	61.06290	-536.29828	147.64734	560.54585	1
13645	N	77.17700	76.61080	61.06990	435.26067	426.40441	-584.29420	1
13646	H	77.61500	75.74080	60.85690	3076.65370	-173.31295	634.34286	1
13647	C	78.06900	77.62580	61.56690	-385.31104	623.44216	-542.50003	1
13648	H	77.44900	78.34180	62.08490	1219.20639	2253.68843	1825.55484	1
13649	C	79.05700	77.17280	62.62790	-209.66098	-676.59296	574.20837	1
13650	H	79.78300	77.96780	62.90290	-2046.86423	791.12563	2254.48293	1
13651	O	79.81600	75.99880	62.30490	-537.29814	487.37630	-312.09339	1
13652	H	79.18000	75.28680	62.20490	1726.20155	-1706.24308	2001.79644	1
13653	C	78.13500	76.76780	63.83490	244.30263	-860.47520	177.05836	1
13654	H	77.36500	77.55080	64.00490	-1786.84574	-1433.28235	-2156.64328	1
13655	H	78.74600	76.71880	64.76190	-1218.63170	2026.93918	2074.77241	1
13656	H	77.51500	75.84680	63.79690	-466.71224	-692.76123	3033.23059	1
13657	C	78.80100	78.28280	60.43990	-665.85034	456.81807	-423.57004	1
13658	O	79.82000	78.91780	60.65690	-552.27533	557.56958	87.95085	1
13659	N	78.35900	78.17880	59.20190	-162.28026	-574.47720	596.91989	1
13660	H	77.57900	77.59780	58.98190	-367.52315	-1901.80390	-2479.17222	1
13661	C	78.86300	79.05080	58.16390	-14.04506	-447.73381	-794.22174	1
13662	H	79.93700	78.96980	58.24790	-1992.67779	-1609.82420	1826.45216	1
13663	C	78.55500	78.55580	56.73090	655.95336	-529.40855	-347.71078	1
13664	H	77.45400	78.54380	56.58590	-2215.42451	2227.87174	-163.42572	1
13665	C	79.23400	79.47680	55.69190	-159.48417	502.42681	744.03166	1
13666	H	79.23300	79.06580	54.66090	2879.15674	-1266.80384	62.37558	1
13667	H	78.67300	80.41380	55.48890	3132.71444	-55.29409	-285.07721	1
13668	H	80.26600	79.78080	55.97290	-366.21256	-1156.54205	-2902.84775	1
13669	C	79.06900	77.10780	56.54390	-394.22383	621.10379	-538.76587	1
13670	H	79.00500	76.45980	57.44390	-2499.35262	-1550.88304	1116.34425	1
13671	H	80.15200	77.14780	56.29690	700.62728	2262.72359	-2070.61093	1
13672	C	78.26600	76.33080	55.51690	-565.96897	-633.65471	-331.07678	1
13673	H	78.23500	76.94280	54.59090	-1800.90823	-2245.03912	-1270.73015	1
13674	H	77.16900	76.27180	55.68190	2418.72941	-1963.84501	437.36376	1
13675	H	78.74700	75.33680	55.39290	667.24415	-2148.85118	2198.96568	1
13676	C	78.55300	80.52180	58.35990	641.49862	-13.07469	-647.88856	1
13677	O	79.45400	81.34280	58.28290	429.95962	-391.11820	-534.59191	1
13678	N	77.30800	80.94280	58.79090	-701.89462	110.25088	455.91773	1
13679	C	76.06600	80.31780	58.47990	-458.25423	444.20150	-651.25962	1
13680	H	75.80500	79.49080	59.17390	1834.49021	2545.03429	235.94993	1
13681	H	76.09400	79.92480	57.44090	-2289.01874	1680.45934	1354.50206	1
13682	C	77.11200	82.34380	59.28390	685.39954	588.08551	125.83284	1
13683	H	77.25900	83.06080	58.48990	-2803.66106	-1131.60613	-870.16002	1
13684	C	75.62100	82.35380	59.68890	265.07419	809.50247	-325.41118	1
13685	H	75.54600	82.00980	60.74290	-1970.85200	2004.33411	-1413.01571	1
13686	H	75.08500	83.32580	59.65190	-1975.54576	246.85397	2436.08462	1
13687	C	75.00600	81.34580	58.64290	-729.52436	511.26967	-194.54699	1
13688	H	74.62200	81.75380	57.68290	27.38355	2677.86276	1651.21997	1
13689	H	74.09500	80.94680	59.13790	-1442.41782	-2487.04692	-1277.59722	1
13690	C	78.03700	82.78180	60.40490	-288.39612	-864.61200	-26.92155	1
13691	O	78.48700	83.90380	60.44290	71.24541	-687.37751	-382.18253	1
13692	N	78.30300	81.91980	61.40090	198.69635	742.53901	349.03850	1
13693	H	77.87300	81.02280	61.32790	-2899.48114	1090.08704	550.40495	1
13694	C	79.25100	82.16380	62.47790	-722.98745	417.40509	-366.76032	1

13695	H	78.89200	83.09180	62.89790	1628.09794	-2323.51493	-1359.70648	1
13696	C	79.28600	81.04580	63.50590	819.55453	342.94851	205.34772	1
13697	H	80.16800	81.03780	64.18090	-2671.41909	1114.04009	-1233.15082	1
13698	H	79.41000	80.13580	62.87990	-1620.82808	-1182.19392	2423.54288	1
13699	C	78.00000	80.97680	64.30490	482.25145	637.00377	-439.44368	1
13700	O	77.75200	81.96580	65.02190	-547.32903	563.75195	79.00572	1
13701	O	77.25500	79.98480	64.24790	471.88587	-373.17630	511.55685	1
13702	C	80.65900	82.48880	61.91190	-606.37378	-460.62791	501.58127	1
13703	O	81.35100	83.42380	62.34390	426.03667	-539.98626	387.98817	1
13704	N	81.09300	81.65880	60.95190	222.40387	228.73368	781.59434	1
13705	H	80.60900	80.81980	60.71590	878.16134	-204.40596	-3014.17934	1
13706	C	82.35100	81.84880	60.18090	-65.79329	-908.34534	45.06656	1
13707	H	83.14500	81.81080	60.91190	960.33334	-2233.31578	-1997.06954	1
13708	C	82.61200	80.57680	59.36790	656.24266	-411.00044	-481.53422	1
13709	H	81.68500	80.38480	58.78690	2137.83445	256.08662	-2293.97248	1
13710	H	82.65500	79.66680	60.00390	1811.37974	2258.80147	1230.83126	1
13711	C	83.86900	80.51280	58.43890	592.11703	-547.29352	-425.81478	1
13712	C	85.11900	81.10280	58.74990	458.80924	-635.21661	-466.30992	1
13713	H	85.29600	81.67880	59.64590	-1969.18704	-1703.49115	1765.96900	1
13714	C	86.16200	81.10780	57.83790	-577.35659	-705.72029	-8.32061	1
13715	H	87.06200	81.63480	58.11890	917.19045	2209.95698	-2042.81131	1
13716	C	85.98200	80.43580	56.65890	-883.29316	208.07235	89.16331	1
13717	H	86.69700	80.46980	55.84990	-1065.22346	-984.63313	-2791.77772	1
13718	C	83.79600	79.72480	57.31990	462.88303	622.13985	-479.72107	1
13719	H	82.86100	79.25980	57.04390	-888.21074	1701.64388	-2492.73264	1
13720	C	84.80600	79.76980	56.36290	531.78267	-487.63267	-557.55948	1
13721	H	84.81800	79.17080	55.46490	-2241.90357	-1139.90078	-1890.16423	1
13722	C	82.49700	83.11280	59.39990	-4.58079	-673.93494	-614.20006	1
13723	O	83.51000	83.80280	59.50090	289.26115	-607.22467	413.80360	1
13724	N	81.49500	83.40680	58.56490	-483.96202	-633.02836	-278.79768	1
13725	H	80.75700	82.74780	58.43890	-2093.70205	-2006.71631	1219.72440	1
13726	C	81.46900	84.64280	57.71890	451.47373	-784.39792	111.09623	1
13727	H	82.41100	84.77380	57.20590	-1818.09101	-1530.39103	-2061.71642	1
13728	C	80.38000	84.70980	56.67890	591.42356	-262.21945	-642.58084	1
13729	H	79.41800	84.79380	57.22890	-1933.84250	-1014.42248	-2264.82372	1
13730	C	80.25793	86.02367	55.81110	152.05830	286.49608	5.03143	1
13731	H	79.30471	86.07443	55.21362	-2701.44667	-3313.63133	973.14526	1
13732	H	81.10588	86.03791	55.08126	1804.05332	1807.51652	-2381.84338	1
13733	H	80.40477	86.92900	56.47901	590.04437	-2553.56804	-2216.63615	1
13734	C	80.27800	83.41680	55.77490	71.22585	-730.26392	541.38017	1
13735	H	80.08400	82.53880	56.42690	1881.30631	2002.94117	-1532.03769	1
13736	H	81.26700	83.29280	55.28390	586.69067	2093.17112	2274.34715	1
13737	C	79.15000	83.46480	54.79990	521.37426	-376.54092	-646.40298	1
13738	H	79.31000	82.70080	54.00990	-857.53232	1957.92398	2308.54895	1
13739	H	79.14200	84.43280	54.25390	1805.22892	-574.56076	-2511.82299	1
13740	H	78.13300	83.27280	55.20590	1499.02114	-2753.28145	-265.71247	1
13741	C	81.29435	85.95993	58.66052	-390.22823	-578.25712	299.80814	1
13742	O	81.89151	86.94172	58.29162	-6.60191	449.95666	-513.31653	1
13743	N	80.41537	85.80258	59.66654	364.71777	-488.14600	287.00339	1
13744	H	79.83920	84.96741	59.94694	-2753.72157	-1335.81653	1386.98916	1
13745	C	79.97046	87.02145	60.34127	1214.40645	-492.49888	-160.94696	1
13746	H	80.32923	87.84327	59.63239	-1237.54963	451.72784	764.24661	1
13747	C	78.35519	86.93138	60.43238	-1146.07183	236.42253	340.45094	1
13748	H	77.91407	86.01865	60.90249	-881.06880	-1694.12530	-616.81141	1
13749	H	77.95487	87.82723	61.03258	-312.13728	-970.42000	-1300.71558	1
13750	C	77.79842	86.98275	59.00642	124.12464	331.04572	-398.19970	1
13751	C	77.92140	88.13552	58.15426	279.58209	-271.13171	-279.05140	1
13752	H	78.62129	88.99292	58.30965	186.35609	340.40999	-183.77102	1
13753	C	77.16761	88.12173	57.01139	-272.25838	246.31376	888.09348	1
13754	H	77.30293	89.01223	56.34801	-3861.05286	2241.08160	1098.58271	1
13755	C	76.28779	87.05424	56.56855	-397.78120	425.90058	-300.50926	1
13756	H	75.61827	87.11137	55.73109	4620.57658	2625.41654	-800.62205	1

13757	C	76.98858	85.86382	58.67400	-94.04236	-860.37524	-309.92622	1
13758	H	76.72968	85.00935	59.26013	945.61834	-1090.94890	1755.48046	1
13759	C	76.37144	85.89302	57.38579	-903.64696	56.38484	-99.25184	1
13760	H	75.78178	85.04604	57.10891	-3130.98711	2364.19423	1100.31398	1
13761	C	80.68025	87.14561	61.75012	206.31539	410.31805	178.03756	1
13762	O	80.28711	87.97060	62.60202	271.78208	-583.03061	-336.56969	1
13763	N	81.67938	86.28424	62.05618	128.40062	-629.98501	577.96186	1
13764	H	82.08217	85.84994	61.19803	-1110.78105	1889.71553	3708.19309	1
13765	C	82.47920	86.74128	63.15249	-222.02422	629.66839	718.55145	1
13766	H	81.76878	87.20451	63.93093	-2173.26376	-1278.86691	2222.48081	1
13767	C	83.18066	85.43270	63.72016	-618.94000	401.05419	10.38351	1
13768	H	83.99242	85.58321	64.45376	2371.72654	826.85817	340.83449	1
13769	H	83.68000	84.87680	62.92990	-2797.18605	-1173.47946	834.81879	1
13770	H	82.44800	84.78880	64.16490	741.18275	1458.74523	-2687.18007	1
13771	C	83.76004	87.61644	62.65060	-98.21619	1134.53698	-889.64057	1
13772	O	84.35293	87.29911	61.60448	-34.26165	-754.21393	775.31920	1
13773	N	84.08339	88.59608	63.47357	164.17466	-612.97198	545.79879	1
13774	H	83.66431	88.66293	64.38778	2004.50951	-3477.41028	-1842.50398	1
13775	C	84.63693	89.86638	63.11578	-444.38399	-473.46763	478.87003	1
13776	H	85.30494	89.68176	62.29422	-1968.17386	-1574.68950	-507.83829	1
13777	C	83.59925	90.96228	62.61223	-30.98287	93.12932	-191.02613	1
13778	H	83.16035	90.52913	61.71960	1388.60028	1507.95988	54.92656	1
13779	H	84.24385	91.81706	62.31844	-102.01177	20.07114	-1692.39431	1
13780	C	82.53574	91.24399	63.73787	483.76293	416.75690	-201.04841	1
13781	O	82.32141	92.35334	64.15342	11.57749	182.31595	-294.95203	1
13782	N	81.75757	90.13219	64.02115	244.71723	114.28038	118.99073	1
13783	H	81.70092	89.31338	63.44789	518.41530	1560.74323	-4433.04225	1
13784	H	80.92930	90.26089	64.57133	4083.31629	-819.33372	40.44073	1
13785	C	85.10155	90.48922	64.54881	-1204.20372	-406.77630	440.81798	1
13786	O	84.43821	90.19666	65.57844	397.53133	-294.81116	-86.52722	1
13787	N	86.24913	91.08130	64.44759	501.53053	858.18479	317.67063	1
13788	H	86.85425	91.30843	63.63504	3786.20782	815.10454	-1190.80684	1
13789	C	86.61197	91.75782	65.62988	210.56494	-190.83085	-48.34686	1
13790	H	85.79658	91.34270	66.32626	-2584.28099	-997.96794	237.38297	1
13791	C	88.15304	91.37745	65.91771	-545.78515	-226.05921	222.25244	1
13792	H	88.76741	91.87305	65.12183	-3332.85581	4948.54741	1028.77705	1
13793	C	88.45888	91.78325	67.41398	588.25888	77.80743	57.29265	1
13794	H	89.44196	91.33868	67.78258	198.38172	-3126.65912	-361.37154	1
13795	H	87.64811	91.45676	68.14113	1478.55607	-1201.50283	1961.85493	1
13796	H	88.56085	92.86583	67.66639	-321.66120	-2998.52293	2333.10099	1
13797	C	88.20650	89.83539	65.85210	-1277.98494	-512.49220	-139.17996	1
13798	H	87.39790	89.41262	66.54247	-335.37658	487.63297	1312.88896	1
13799	H	87.99500	89.43616	64.81481	-3396.75012	1342.10122	-1987.91895	1
13800	H	89.18269	89.44240	66.17054	1172.30064	-1718.15149	-3010.81853	1
13801	C	86.23052	93.39100	65.56741	1081.94507	-624.56753	-412.30269	1
13802	O	86.70543	94.22920	64.83266	-313.63384	441.30314	425.29857	1
13803	N	85.26369	93.39286	66.50999	472.92943	70.40719	-72.47908	1
13804	H	85.08038	92.55817	67.16013	-2594.92729	-2947.68339	936.16404	1
13805	C	84.63604	94.61790	66.76159	112.65458	-420.50054	-469.85325	1
13806	H	84.93359	95.16721	65.80356	-58.26690	3842.82686	-780.99220	1
13807	C	83.08769	94.33753	66.87164	-411.31152	-122.14401	447.83415	1
13808	H	83.06990	93.49416	67.62064	-2136.91643	1529.88850	1468.94241	1
13809	H	82.68370	93.90251	65.92429	809.43220	-3942.73502	2264.45261	1
13810	O	82.08013	95.48237	67.20170	-784.78492	211.48561	-189.93261	1
13811	H	81.66656	95.07434	67.95154	-2088.78625	2771.13716	2261.35533	1
13812	C	85.27131	95.14918	68.21520	-501.95710	102.88246	745.94236	1
13813	O	86.40385	94.85537	68.54619	-0.30646	-483.20548	-672.20373	1
13814	N	84.32698	95.79688	68.92599	-334.66801	80.17726	-437.52633	1
13815	H	83.42916	96.05743	68.50606	1340.25544	1845.84127	752.57755	1
13816	C	84.85954	96.66255	69.90330	431.26815	1137.86817	-400.53202	1
13817	H	85.66897	96.16383	70.38492	-3081.00602	-1336.20587	-580.58205	1
13818	C	85.21801	98.11703	69.20364	214.16633	841.05239	62.51854	1

13819	H	84.46664	98.88393	69.47873	-1008.15524	-1872.12058	-907.57401	1
13820	H	85.12111	98.10544	68.09640	-2309.92687	-82.90843	-1383.16708	1
13821	C	86.59361	98.69145	69.53667	-881.67244	-1080.44986	-632.31648	1
13822	H	86.47466	99.76758	69.63215	-676.11804	-841.44896	-2021.55685	1
13823	H	86.88485	98.34915	70.55372	4331.20222	1497.04376	-1020.88408	1
13824	C	87.60506	98.19042	68.28484	101.36738	34.95869	-238.65941	1
13825	O	88.72763	97.82844	68.61874	-73.92511	366.33439	-16.12614	1
13826	O	87.23475	98.25456	67.10765	320.99322	-421.02995	-325.03561	1
13827	C	83.57589	96.83848	70.83590	619.32610	206.10760	-1346.72166	1
13828	O	82.47745	97.14854	70.47331	-378.20383	330.56636	222.23510	1
13829	N	83.97472	96.62628	72.12168	-327.08154	118.82115	-338.85577	1
13830	H	84.97987	96.27628	72.41781	-1256.70126	-57.42501	72.19580	1
13831	C	82.95302	96.81220	73.14552	866.75144	291.80368	34.04728	1
13832	H	82.33766	97.70080	72.77315	1866.18357	53.91338	874.16402	1
13833	C	82.10956	95.55223	73.41097	439.38785	147.74684	-426.24477	1
13834	H	81.56413	95.59773	74.37700	2188.26633	-48.14329	-1914.11467	1
13835	H	82.75591	94.63314	73.47517	630.85216	2598.32969	2683.39043	1
13836	H	81.42190	95.39235	72.63287	-766.66350	2237.07381	-2697.90445	1
13837	C	83.69938	96.97051	74.58027	-330.18957	-77.31721	-437.62154	1
13838	O	84.63730	96.25694	74.78810	411.36312	-383.38989	874.17113	1
13839	N	83.12476	97.81517	75.49926	152.58612	-358.47878	-762.18327	1
13840	H	82.15302	98.17070	75.35562	508.86774	-2440.44904	-418.23736	1
13841	C	84.00948	98.63231	76.25728	653.82990	2.66434	180.85428	1
13842	H	83.39411	99.35706	76.78559	5004.44898	-217.72382	-1173.26984	1
13843	C	84.82637	97.72259	77.28442	959.96019	2.21559	94.47996	1
13844	H	85.03756	96.76464	76.87409	-410.37105	-402.61115	1733.81981	1
13845	H	85.76942	98.31722	77.32357	-90.07469	1349.66446	2367.11496	1
13846	C	83.94494	97.72346	78.62320	-68.44274	-340.31864	-467.13575	1
13847	O	83.80673	96.78695	79.35507	539.37811	-153.73789	37.43074	1
13848	O	83.30060	98.99011	78.95600	-655.59873	81.13477	-861.20575	1
13849	C	84.94886	99.46318	75.26400	-760.51575	173.59273	-271.85630	1
13850	O	86.08213	99.69553	75.70452	406.46738	1130.21747	-776.48921	1
13851	N	84.50086	99.69667	74.03077	442.21739	-751.87914	-1307.29913	1
13852	H	83.48402	99.61419	73.75585	12.30853	-1388.16587	477.71456	1
13853	C	85.34719	100.39754	73.11586	-716.33433	786.75319	-344.41980	1
13854	H	84.56615	100.65659	72.38967	-321.26123	1509.88195	609.69574	1
13855	C	85.93221	101.60970	73.89625	411.16964	-124.18927	-399.20586	1
13856	H	86.67327	101.38821	74.66375	-2050.10370	-4650.28200	-1477.15550	1
13857	H	85.08124	102.10855	74.38495	-1081.92182	1489.70307	-2459.80768	1
13858	C	86.48419	102.89989	73.09342	-959.70328	-108.61541	-605.86053	1
13859	O	85.61176	103.67450	72.60272	495.66420	-93.38016	166.48195	1
13860	O	87.68324	103.06755	73.00285	303.21840	-495.80901	-469.75606	1
13861	C	86.58548	99.69560	72.34855	-454.93520	1185.24083	520.51014	1
13862	O	87.37085	100.32188	71.68344	-225.50221	-369.32503	-507.96594	1
13863	N	86.57680	98.32367	72.48879	-13.68555	-572.88299	231.45362	1
13864	H	85.69066	98.14712	73.07271	-2357.09550	-1350.39284	-3441.43993	1
13865	C	87.88097	97.70034	72.50469	-496.31329	344.33225	583.42639	1
13866	H	88.27670	98.18646	71.59290	-1353.70532	-1796.64561	3559.74555	1
13867	C	88.65237	97.96703	73.87080	-502.10001	-785.79656	629.37919	1
13868	H	89.57763	97.40877	73.82796	-574.62586	1109.30206	93.49506	1
13869	H	88.80266	99.02212	74.22599	-1587.20925	-1177.02545	373.23829	1
13870	C	87.69483	97.29434	74.94572	498.38319	-668.11310	684.82398	1
13871	H	86.87348	96.76146	74.36787	-2716.16265	-1500.53377	1131.00619	1
13872	H	87.29206	98.09117	75.62804	4286.10869	-2045.74677	1379.86050	1
13873	C	88.68418	96.32836	75.77004	116.02189	1116.43263	-139.81510	1
13874	H	88.43124	96.08339	76.83194	2419.70832	2183.06291	-47.96691	1
13875	H	89.72956	96.63097	75.60072	-3112.59461	-621.23437	-1288.32281	1
13876	N	88.67617	95.22846	74.90769	-310.11762	919.25012	73.28263	1
13877	H	88.84784	95.32374	73.86587	845.45189	126.65650	907.75531	1
13878	C	88.38669	94.03428	75.22549	-927.12403	-547.85440	324.33256	1
13879	N	88.46097	93.16146	74.07471	-1026.16378	-608.83530	-1447.51037	1
13880	H	88.67699	93.44034	73.10545	-263.78223	2773.62611	1512.72221	1

13881	H	88.02945	92.24967	74.10522	1861.31934	1903.43004	-561.79253	1
13882	N	88.05736	93.74256	76.57720	-194.67461	-600.71995	-1511.83616	1
13883	H	88.02449	94.51285	77.29563	-836.24045	3938.34056	3301.00828	1
13884	H	87.40796	92.92061	76.71669	-2031.34268	-28.16775	1617.71950	1
13885	C	87.70738	96.16059	72.12662	401.76951	448.06707	-384.30041	1
13886	O	86.70005	95.53423	72.27762	-316.00537	-596.66323	75.50397	1
13887	N	88.93420	95.65473	71.79711	-600.37593	-28.88860	77.14660	1
13888	H	89.67132	96.38106	71.63854	-1919.25485	407.57311	618.75497	1
13889	C	88.93640	94.94791	70.51906	-272.80274	-420.68161	-545.72759	1
13890	H	88.21178	95.37476	69.81381	-414.91228	406.33785	-815.88404	1
13891	C	90.47536	95.02250	70.00015	-863.90342	250.30750	-297.35425	1
13892	H	91.15388	94.45818	70.75276	2005.55337	-1974.84724	-151.82399	1
13893	H	90.86072	96.05327	69.92908	1391.84048	381.23818	1298.06500	1
13894	C	90.57496	94.33815	68.61678	-1499.53570	696.22398	-444.36374	1
13895	C	91.18904	93.04604	68.48084	100.08141	-699.99235	351.55211	1
13896	H	91.67293	92.55069	69.29710	18.91776	583.73820	-666.62404	1
13897	C	91.34854	92.71756	67.13198	-223.87238	287.59402	-353.33051	1
13898	H	92.01818	91.90202	67.01986	1485.95092	1671.66295	-1025.05158	1
13899	C	90.80299	93.30546	65.94948	-569.07238	564.84599	182.82441	1
13900	O	91.05951	92.76854	64.65174	283.29883	17.14560	-525.14573	1
13901	H	91.18247	93.68492	64.13719	-661.96878	373.80981	-257.56897	1
13902	C	90.02156	95.03557	67.51856	54.94295	-111.04484	264.06090	1
13903	H	89.57855	96.00174	67.59052	28.09133	445.09580	-626.54392	1
13904	C	90.09709	94.52416	66.23953	-377.05579	-621.76598	299.12365	1
13905	H	89.61590	95.05674	65.44710	81.48547	803.64714	-1382.53719	1
13906	C	88.60399	93.43672	70.90913	23.89656	-470.64377	956.83059	1
13907	O	89.40775	92.79416	71.59711	-547.69643	-13.00531	-229.03881	1
13908	N	87.43258	93.04269	70.42415	945.36093	-328.12729	492.66798	1
13909	H	86.88892	93.73251	69.91833	546.98814	1069.32735	-68.06762	1
13910	C	86.79860	91.92394	71.04922	45.70728	927.63975	-242.75731	1
13911	H	87.54096	91.34198	71.69769	25.90074	1115.76036	-1585.12590	1
13912	C	85.68809	92.59587	71.96640	-435.58465	44.31811	380.34168	1
13913	H	86.24417	93.31999	72.68685	1616.68142	-357.86455	258.86956	1
13914	C	84.62890	93.38046	71.13302	419.89237	278.90816	-404.50939	1
13915	H	85.11957	94.08511	70.49336	-2213.24333	324.45250	2350.34775	1
13916	H	83.92746	92.74832	70.45385	113.11504	-3178.43949	-3130.44738	1
13917	H	83.95649	93.92160	71.82699	2402.20294	-2844.87350	-961.61891	1
13918	C	84.89011	91.51747	72.86616	-1.32535	-366.87155	601.96392	1
13919	H	85.39433	90.54706	72.77432	1373.88061	-4.78398	-301.43636	1
13920	H	83.88845	91.37825	72.47040	-571.04103	-380.15567	451.26380	1
13921	C	84.84920	92.13690	74.29614	282.47733	-781.41388	-969.70246	1
13922	H	83.94052	91.74615	74.84687	-629.73359	886.76447	-2415.19054	1
13923	H	85.75783	91.90875	74.87440	1053.90242	155.20685	2408.25465	1
13924	H	84.71621	93.22006	74.23208	640.91256	-3816.42151	-909.36362	1
13925	C	86.24158	91.06899	69.77310	-778.16312	-975.72115	-623.35126	1
13926	O	85.70473	91.57020	68.81357	-931.39523	-411.45015	-60.09687	1
13927	N	86.33304	89.76469	70.10138	-68.55402	290.51663	-117.42854	1
13928	H	86.79272	89.40877	71.04978	-1658.93993	3852.67520	-3350.62536	1
13929	C	85.75082	88.90623	69.04051	160.72181	-370.81040	101.30368	1
13930	H	85.92206	89.17277	68.05634	-661.17454	349.85384	-673.04815	1
13931	C	86.52262	87.57832	69.33640	230.86293	82.34845	-189.58570	1
13932	H	87.61508	87.69893	69.08556	-676.79378	5086.05869	1494.50617	1
13933	H	86.48323	87.41247	70.43421	-2018.09246	2801.76106	-348.80071	1
13934	S	85.67117	86.34068	68.28809	312.95724	-453.72978	-199.72691	1
13935	C	84.14240	89.00197	69.21804	459.28204	168.81372	121.92130	1
13936	O	83.56176	88.71894	70.22613	246.34708	245.34057	18.62210	1
13937	N	83.52166	89.26058	67.98026	-253.61831	65.05695	15.64268	1
13938	H	83.97964	89.57280	67.06940	1219.60499	352.25740	-1038.66016	1
13939	C	82.13472	89.69410	68.14434	-876.05743	-749.61842	117.24861	1
13940	H	81.70226	89.13154	69.02498	-539.92743	243.28496	-1194.92968	1
13941	C	82.35716	91.22581	68.32634	129.06750	-40.53911	712.41951	1
13942	H	82.78988	91.62548	67.41035	-857.85192	4876.06962	-2934.47315	1

13943	H	83.19562	91.32435	69.10418	-2615.08493	1860.51486	-480.93573	1
13944	C	80.94164	91.89904	68.83685	826.68310	866.07857	-334.51309	1
13945	O	79.83405	91.53720	68.37754	-450.50408	690.49790	-970.76118	1
13946	O	81.07240	92.69249	69.75181	431.36244	-721.06697	-210.52493	1
13947	C	81.43291	89.05558	66.80581	190.59663	415.43774	19.24115	1
13948	O	81.94768	88.19773	66.16393	-435.74705	-553.59519	174.10552	1
13949	N	80.17240	89.52918	66.65602	48.48485	435.14972	-83.59656	1
13950	H	79.79021	90.22141	67.39136	-1305.70347	-1493.46367	-1281.66318	1
13951	C	79.38487	88.74202	65.73086	484.66722	-78.72887	-89.06425	1
13952	H	80.06598	88.33724	64.93685	-1752.45557	-1548.91631	7.78866	1
13953	C	78.82358	87.61814	66.74712	253.13399	501.21655	-516.08216	1
13954	H	77.99774	88.02670	67.46009	1082.85916	-1664.18491	-683.81075	1
13955	H	79.66883	87.32854	67.47812	-407.31378	-2332.32829	2673.06997	1
13956	C	78.36337	86.36580	66.00389	37.70900	1078.81614	-750.36254	1
13957	H	78.38607	86.45437	64.89361	42.29258	2601.50001	156.81562	1
13958	H	77.28676	86.07211	66.21489	1439.47571	-1579.07227	1441.17753	1
13959	C	79.38247	85.17999	66.45591	163.78601	172.35096	-54.47748	1
13960	H	80.16137	84.93367	65.66073	-805.19118	-557.67664	-789.73091	1
13961	H	79.76649	85.28940	67.49385	-1980.57573	578.27411	219.54551	1
13962	N	78.71300	83.93980	66.64390	139.49274	632.25749	541.72366	1
13963	H	78.51800	83.39480	65.82790	1546.00063	1711.60222	-2139.74908	1
13964	C	78.40500	83.36480	67.75690	-660.28185	376.69649	-503.56592	1
13965	N	78.10900	83.97080	68.86490	784.59473	306.33082	-56.96336	1
13966	H	78.26600	84.95480	68.95690	-1717.42843	1638.68264	-2064.79661	1
13967	H	77.74400	83.35480	69.56290	-1352.92526	1935.42880	-2078.92637	1
13968	N	78.05200	82.10080	67.70790	-565.40399	528.41277	-337.29892	1
13969	H	78.04200	81.66580	66.80690	-1268.65259	2583.95523	1269.61498	1
13970	H	77.44800	81.87880	68.47390	-1851.91353	1823.05462	-1773.44702	1
13971	C	78.16178	89.68052	65.18531	-408.79671	-583.76897	-611.63275	1
13972	O	77.39907	90.27184	65.90131	435.50664	327.25821	-253.02711	1
13973	N	78.09246	89.64981	63.80734	39.82565	75.19617	802.10226	1
13974	H	78.78988	89.03990	63.31835	78.60113	-1059.68893	-964.87466	1
13975	C	77.53751	90.76850	63.13660	-180.10114	-97.42520	-493.52497	1
13976	H	76.78820	91.01785	63.92243	1971.33856	-2059.42211	2612.32715	1
13977	C	78.43795	92.11741	63.13888	-189.55747	-581.20128	-1008.44059	1
13978	H	79.25077	92.22569	63.90324	2657.43301	992.82722	1282.74026	1
13979	H	78.95990	92.07429	62.19045	-1876.78807	-2489.51632	111.86145	1
13980	C	77.46662	93.30423	63.29053	391.63366	-276.48602	233.16243	1
13981	C	77.03929	93.51381	64.64162	-847.49313	971.13181	-342.44919	1
13982	H	77.49769	92.88228	65.44828	81.35612	28.29992	-85.73287	1
13983	C	75.96549	94.43265	64.83004	233.00818	-309.08721	-161.85015	1
13984	H	75.69974	94.84966	65.83242	142.03968	2054.76708	672.30761	1
13985	C	75.30444	95.06668	63.75852	419.96716	19.14397	347.13331	1
13986	H	74.43592	95.61884	64.00364	589.23210	517.35577	2171.97151	1
13987	C	76.85517	93.87015	62.14846	-538.62070	348.61843	637.52979	1
13988	H	77.12140	93.54894	61.17135	1711.26519	2354.46408	45.19968	1
13989	C	75.80561	94.74912	62.43572	638.11478	356.32972	-329.44377	1
13990	H	75.33132	95.27556	61.58840	-2148.63612	301.82023	-2887.26722	1
13991	C	77.24374	90.29380	61.63510	-374.13222	-459.99714	-563.86591	1
13992	O	78.13604	89.79364	60.96180	862.28553	611.62435	-90.47274	1
13993	N	76.04837	90.76006	61.20383	-275.83096	757.55934	558.36813	1
13994	H	75.62717	91.41065	61.82038	1785.73026	2430.20223	-3416.16492	1
13995	C	75.26527	89.98134	60.30707	-50.55588	639.51885	396.85819	1
13996	H	75.80826	89.06022	60.08106	-1195.43381	962.17787	3418.74556	1
13997	C	74.02403	89.62450	61.29607	248.28846	-351.38164	104.08048	1
13998	H	73.09139	89.25917	60.83176	2374.27984	-69.20717	1126.27955	1
13999	H	73.72138	90.55411	61.78293	1850.47715	1631.99325	-1856.75117	1
14000	C	74.58041	88.61192	62.30953	-85.54345	401.85168	689.93699	1
14001	C	74.74223	87.21310	62.05831	-263.20937	643.59442	-693.25774	1
14002	H	74.54379	86.93804	61.01395	3678.85736	-2835.37052	-1258.92967	1
14003	C	74.99065	86.30691	63.03467	13.95167	99.99647	-627.90731	1
14004	H	75.16492	85.28743	62.67876	7.17441	821.19348	1260.23579	1

14005	C	75.20200	86.59432	64.39091	487.48073	848.68338	-63.98404	1
14006	O	75.51503	85.62287	65.44030	391.98589	1096.05662	664.21609	1
14007	H	75.54600	84.77580	64.99090	11.90255	-1173.96099	2918.88680	1
14008	C	74.84338	88.96595	63.65584	-577.21055	-506.75654	171.78594	1
14009	H	74.89781	90.05825	63.77310	-2111.17063	-1359.00240	-571.86904	1
14010	C	75.20052	87.98080	64.60002	-690.05292	42.16870	-53.07005	1
14011	H	75.44283	88.25573	65.66592	-1369.95235	193.68095	642.99877	1
14012	C	74.74964	90.92617	59.11233	-182.19769	354.85429	-336.31221	1
14013	O	74.66135	92.10794	59.30672	488.70566	189.92761	481.24031	1
14014	N	74.27388	90.23559	58.05756	257.09348	-924.58507	-449.67404	1
14015	C	74.14569	88.77777	58.17785	-1032.41590	479.05627	-174.07575	1
14016	H	75.20560	88.47976	58.07490	-1184.23622	444.65710	-711.25046	1
14017	H	73.75294	88.51527	59.19826	-415.56757	-1370.38304	1031.97020	1
14018	C	73.74310	90.86257	56.90709	180.52976	-181.25740	602.56904	1
14019	H	74.49028	91.60010	56.51483	523.34970	2153.78062	391.12519	1
14020	C	73.56668	89.66523	55.90845	-362.55473	255.01935	347.58257	1
14021	H	72.63857	89.92243	55.35088	2698.32985	-1948.93495	1115.03575	1
14022	H	74.41804	89.44218	55.30924	1862.36980	-2826.00558	2215.80648	1
14023	C	73.31540	88.44003	56.89003	396.79335	-956.31403	956.16276	1
14024	H	72.24735	88.27093	57.02854	-1469.73174	-690.43831	650.87693	1
14025	H	73.67303	87.47644	56.36447	-668.52776	182.73151	5.27969	1
14026	C	72.24520	91.54862	57.17918	-168.49310	182.32882	3.75861	1
14027	O	71.71603	92.15776	56.28914	-601.39786	-717.54229	153.48497	1
14028	N	71.67987	91.14826	58.34706	-214.14881	558.62083	-503.38954	1
14029	H	72.34730	90.46749	58.69433	4365.25968	474.55124	-766.25779	1
14030	C	71.28833	92.22006	59.27791	121.57431	-305.66526	147.78023	1
14031	H	72.25031	92.73103	59.31970	-2802.48550	-2123.60669	3784.91824	1
14032	C	70.21517	93.13362	58.54424	364.68363	-456.15191	399.71780	1
14033	H	70.57783	93.30701	57.43790	542.31364	402.73093	-2805.06701	1
14034	H	69.24172	92.67219	58.58107	861.97005	-959.63480	-2750.60334	1
14035	C	69.91060	94.50513	59.29432	802.27883	707.90941	-588.42304	1
14036	O	69.12428	94.63193	60.20905	-386.42188	-418.07591	366.75864	1
14037	N	70.81485	95.37278	58.81857	636.30750	-226.03511	399.65377	1
14038	H	71.56012	94.91675	58.20906	631.61411	-186.98609	340.82060	1
14039	H	71.17507	96.33050	59.14258	-16.95256	-2554.63019	-1898.98756	1
14040	C	70.79739	91.56565	60.62216	-169.56745	-23.07196	229.18709	1
14041	O	71.14036	90.41142	60.92792	375.47705	-171.70011	-11.35829	1
14042	N	69.87100	92.31498	61.27231	576.25861	-870.24652	467.04367	1
14043	H	69.50670	93.31857	61.14202	1340.52577	-56.61552	-1014.37191	1
14044	C	69.56419	91.73799	62.56720	917.41719	-302.86189	-393.24583	1
14045	H	70.27377	90.93392	62.64823	-1436.22803	455.96798	573.74853	1
14046	C	69.95867	92.89116	63.55788	1186.18925	-788.03106	709.23420	1
14047	H	69.83769	93.90444	63.11767	1683.40553	5679.63519	-3128.67563	1
14048	H	69.32302	92.90718	64.47457	2662.28085	-3927.52739	-1181.49027	1
14049	C	71.53237	92.68050	63.98434	785.53623	-83.81291	370.77771	1
14050	O	72.20624	91.69765	63.57129	-210.98842	-662.65087	840.71784	1
14051	O	71.99749	93.58473	64.67684	183.32837	147.42686	390.17059	1
14052	C	67.95046	91.34012	62.60424	-271.57057	392.74043	-555.53965	1
14053	O	67.43069	91.05139	63.64606	56.24349	289.58403	134.45446	1
14054	N	67.36709	91.33103	61.40859	287.56015	-471.29209	-299.71061	1
14055	H	67.95703	91.75046	60.62256	469.92768	2529.81568	-913.06289	1
14056	C	66.31934	90.41578	61.20445	-302.04252	11.00499	286.59142	1
14057	H	65.78837	90.31663	62.23385	685.42608	3011.47063	794.17801	1
14058	C	65.34575	91.03669	60.07416	310.81221	496.25801	-891.81213	1
14059	H	64.97170	92.07637	60.39493	1525.80228	-393.20583	1968.40601	1
14060	H	65.90197	91.30211	59.14953	-2808.97742	-1391.60202	1829.70569	1
14061	C	64.19033	90.09560	59.85625	-554.62368	-88.26727	887.19054	1
14062	H	64.54779	89.12863	59.65681	-392.38452	3149.35206	-12.16608	1
14063	C	63.30014	90.06723	61.08698	124.36620	-146.77964	365.42342	1
14064	H	62.69961	89.15272	61.08288	1510.34514	215.19984	3717.91580	1
14065	H	62.62819	91.02345	61.16328	1495.77102	1163.21751	1814.22002	1
14066	H	63.99004	89.95864	61.98295	409.47358	339.45447	-653.97273	1

14067	C	63.34688	90.52361	58.64097	91.76991	874.12700	445.30672	1
14068	H	63.92327	90.30716	57.69875	48.74815	472.14338	-915.74562	1
14069	H	62.43007	89.91836	58.36957	-2433.56751	-746.57861	-1203.89242	1
14070	H	62.93857	91.57504	58.68282	-138.96610	-710.57094	443.35888	1
14071	C	66.89239	89.00440	60.62658	413.65970	1154.98388	-256.27195	1
14072	O	66.12565	88.06851	60.30801	295.88352	195.29568	-663.93966	1
14073	N	68.22470	89.05352	60.41407	-679.08332	266.72424	149.89871	1
14074	H	68.51337	89.94540	60.86072	-1040.92882	188.51639	-238.64444	1
14075	C	68.97556	87.98522	59.90292	-169.34417	388.01783	905.67004	1
14076	H	68.25475	87.33235	59.42611	-831.75328	400.36129	-2468.84425	1
14077	C	70.14952	88.48028	58.89020	776.37179	44.05328	-233.28297	1
14078	H	71.10096	87.99123	59.19126	-2205.26679	1309.19603	-1110.70595	1
14079	H	70.37171	89.50593	59.00690	1614.42487	739.03914	32.66978	1
14080	C	69.95070	88.22034	57.43685	-566.11007	-142.05862	821.61992	1
14081	C	69.82151	89.03672	56.30152	391.66663	301.45252	738.43434	1
14082	H	70.05315	90.08301	56.20112	-788.81485	-2237.43777	2165.00990	1
14083	N	69.53598	88.29303	55.21088	116.09016	301.11147	-67.10785	1
14084	H	69.39777	88.87459	54.34975	2843.04304	-2739.68159	1614.25998	1
14085	C	69.56073	86.95395	55.43279	-13.17607	-613.20837	43.43489	1
14086	C	69.88804	86.85595	56.89548	223.80128	1226.42458	-330.31272	1
14087	C	69.97267	85.55018	57.40095	593.94380	259.91232	-171.05693	1
14088	H	70.05454	85.30758	58.46891	187.59258	744.13465	680.23551	1
14089	C	69.68000	84.43180	56.55090	-249.17678	520.15760	706.25633	1
14090	H	69.73600	83.43380	56.95890	1509.78763	463.94103	2720.94217	1
14091	C	69.41924	85.85046	54.53743	255.20052	1475.00728	447.40393	1
14092	H	69.39528	86.04228	53.45878	517.28370	-2030.79955	2627.55641	1
14093	C	69.46400	84.55980	55.13790	-726.02323	-516.91701	192.71243	1
14094	H	69.43900	83.61780	54.60990	-1237.27372	2881.62697	252.20224	1
14095	C	69.70376	87.11172	61.01788	-370.88860	-364.43154	708.49524	1
14096	O	69.53443	85.88388	61.18224	-222.52823	-205.96057	-17.33432	1
14097	N	70.38360	87.90454	61.83059	730.42373	-254.48810	197.87973	1
14098	H	70.60358	88.85740	61.41650	2121.04765	-1901.86087	18.47931	1
14099	C	70.43330	87.76247	63.22048	-129.39239	-81.67978	-553.78176	1
14100	H	70.97345	86.78676	63.44706	-975.29685	643.75869	-2893.24297	1
14101	C	71.09529	89.06919	63.82369	392.01006	-143.20793	0.36304	1
14102	H	71.45867	89.83372	63.08539	-1490.01080	2452.63868	2589.13068	1
14103	C	70.25980	89.73078	64.97019	707.47100	1306.70138	151.49765	1
14104	H	70.56849	89.42351	65.98187	-3178.03610	-3596.25468	1020.55690	1
14105	H	69.11376	89.64867	64.82236	-3045.09365	-1832.07941	-1757.64413	1
14106	H	70.36901	90.82693	65.08744	2867.16850	1861.76586	1517.56439	1
14107	C	72.32539	88.45993	64.55990	689.61169	-446.52440	463.50726	1
14108	H	72.89319	89.29780	65.03973	-1109.21805	-2051.54454	1455.30382	1
14109	H	71.99861	87.74327	65.32995	-3917.46447	-1743.44734	2868.01900	1
14110	H	73.04110	87.86520	63.93786	-682.23652	283.36395	-794.91119	1
14111	C	68.96101	87.24255	63.86695	-116.44350	-230.69373	-687.60400	1
14112	O	69.17820	86.59430	64.90934	1100.46677	-362.73233	-722.40992	1
14113	N	67.83301	87.64973	63.44045	-16.66745	-285.71353	122.58057	1
14114	H	67.96038	88.05796	62.47950	-2571.54056	2975.40350	3047.41287	1
14115	C	66.66130	86.92684	63.89340	-321.44217	-297.08748	1082.49319	1
14116	H	66.85006	86.95062	65.02533	201.21966	-1267.33614	308.23474	1
14117	C	65.34729	87.63173	63.34339	313.05436	-343.76533	-373.90061	1
14118	H	65.39247	87.96143	62.30595	3454.34323	1905.08844	-320.74339	1
14119	C	64.05969	86.74937	63.65734	-93.83819	-36.52620	70.20924	1
14120	H	64.07744	85.78560	63.07443	2065.91999	5487.36447	-553.57438	1
14121	H	64.00680	86.54498	64.76147	-1064.24762	-1240.95980	-2068.36805	1
14122	H	63.12395	87.31056	63.40648	-1723.26171	-1691.26670	971.98353	1
14123	C	65.21191	88.94926	64.22575	20.74464	53.42926	22.15231	1
14124	H	65.28481	88.69125	65.34335	624.73886	-1602.69254	-2518.42020	1
14125	H	66.12111	89.52317	64.07296	2694.04171	-2532.50793	-1885.81452	1
14126	H	64.41904	89.63338	63.94465	-986.68905	2101.57591	-715.41478	1
14127	C	66.63323	85.33530	63.48996	-647.47886	-715.55436	-225.69193	1
14128	O	66.19800	84.42780	64.14390	-482.57715	592.64948	198.77909	1

14129	N	66.91828	85.39845	62.19879	-279.77565	713.50686	1325.86870	1
14130	H	67.54504	86.09871	61.87911	-771.51105	-1259.00481	-424.76199	1
14131	C	67.17300	83.92780	61.67790	685.68798	321.67274	507.74959	1
14132	H	66.24200	83.39480	61.79890	1649.61620	2256.69318	1443.72038	1
14133	C	67.57000	83.97580	60.15290	605.11168	-412.29603	543.41774	1
14134	H	68.48300	84.59580	60.02690	2104.62655	2018.10975	-1181.52712	1
14135	C	67.61400	82.57980	59.52390	-543.91757	453.41528	574.47303	1
14136	H	66.79600	81.88480	59.80990	1862.33532	-1444.02710	-2084.39898	1
14137	H	68.52000	82.02080	59.84090	2864.49075	1300.75818	-30.77500	1
14138	H	67.66500	82.68580	58.41990	-2611.94440	-1738.28447	-233.10893	1
14139	C	66.50700	84.79580	59.46790	834.42392	349.32340	-114.72088	1
14140	H	66.63300	84.77480	58.36390	-2506.74778	-471.96867	-1841.65343	1
14141	H	66.60295	85.87860	59.83743	391.89101	516.01236	-2132.33554	1
14142	H	65.54000	84.29880	59.69790	-1698.05578	-2195.07427	-1482.05322	1
14143	C	68.20200	83.10680	62.39890	550.50155	589.32564	-425.55181	1
14144	O	68.02100	81.91380	62.76490	265.05037	-645.49038	-369.75357	1
14145	N	69.35700	83.66280	62.70190	611.51693	-452.93843	-365.46698	1
14146	H	69.64500	84.55180	62.35490	-1783.86180	-1016.25432	-2383.96528	1
14147	C	70.38900	83.01780	63.55090	-417.00848	393.99101	708.74961	1
14148	H	70.48900	81.98180	63.26390	-1071.58594	2667.34841	-1278.74246	1
14149	C	71.76000	83.63580	63.31290	-484.47360	707.47680	310.18206	1
14150	H	72.58800	82.97480	63.64590	-2638.63833	1671.58017	376.34261	1
14151	H	71.82400	84.63980	63.78390	-798.91887	3040.56766	122.07846	1
14152	C	72.03300	83.72280	61.79390	-215.29745	-521.99840	715.97184	1
14153	C	71.81600	82.59080	60.95990	279.85305	-717.87178	-487.64063	1
14154	H	71.47000	81.69580	61.45590	-2316.48263	1909.86806	940.49903	1
14155	C	72.08100	82.67680	59.54890	606.64568	99.14528	673.49999	1
14156	H	71.79200	81.91980	58.83390	-2128.87791	1667.81113	-1607.64148	1
14157	C	72.48800	83.89180	59.02390	195.93976	854.07363	-252.22381	1
14158	H	72.66000	83.92580	57.95890	-2538.06704	1495.79316	1104.10359	1
14159	C	72.42300	84.92880	61.19290	-50.29512	126.63266	-901.60167	1
14160	H	72.55756	85.81529	61.80934	511.98814	-3904.81753	450.05967	1
14161	C	72.64018	85.09469	59.80865	300.93074	-737.87690	334.27548	1
14162	H	72.92094	86.03221	59.32295	-974.94000	1867.87334	2476.95636	1
14163	C	70.05300	82.90880	64.99590	-703.64877	567.76549	118.20222	1
14164	O	70.29400	81.84380	65.59190	582.21902	-257.82227	-467.09306	1
14165	N	69.42700	83.89580	65.60790	-669.99197	-228.23948	-460.09759	1
14166	H	69.17200	84.72080	65.10890	-2598.22064	1215.83658	1291.98188	1
14167	C	68.97800	83.85380	67.00790	-783.83523	-179.54670	429.90268	1
14168	H	69.89000	83.70380	67.56490	346.22594	-2277.71589	-2142.51351	1
14169	C	68.17700	85.17171	67.40846	180.49574	-183.30667	-1170.58875	1
14170	H	67.22764	85.17190	66.79017	2484.04289	-1109.01840	3240.91712	1
14171	H	68.87797	86.04188	67.09398	1254.02814	-2507.01037	-120.57685	1
14172	C	67.94303	85.32891	68.95886	216.31558	-569.55285	-660.29215	1
14173	H	67.37700	84.47980	69.36990	-251.79211	455.35365	-3102.81808	1
14174	H	67.19733	86.23654	69.06552	-180.16972	581.53068	-285.70923	1
14175	C	69.32838	85.50546	69.65701	846.11513	-38.88936	-145.99056	1
14176	O	69.74393	86.67522	69.71577	881.52639	-665.14517	-593.87211	1
14177	N	70.01700	84.39780	70.10590	430.88271	-474.21138	-549.66895	1
14178	H	69.81800	83.47480	69.77790	1631.46249	1462.02418	-2258.10577	1
14179	H	70.95200	84.61280	70.38790	-1617.99244	-2635.09471	580.17461	1
14180	C	68.01400	82.64180	67.17590	-681.98160	-75.25730	-600.57343	1
14181	O	68.15500	81.79780	68.04290	503.60685	290.79634	534.27039	1
14182	N	67.09000	82.50080	66.23490	-542.00045	99.79091	-639.49165	1
14183	H	67.03700	83.21580	65.54290	-1827.24928	1527.47529	2055.77371	1
14184	C	66.19800	81.42780	66.04390	-649.22657	631.11082	107.95832	1
14185	H	65.61500	81.36480	66.95090	-749.82018	2991.41556	622.43786	1
14186	C	65.20800	81.57280	64.87290	376.31415	-425.96708	-713.01523	1
14187	H	64.70000	82.55680	64.95890	712.68056	-2278.81910	-2048.73038	1
14188	H	65.78400	81.60080	63.92390	-2781.34911	1454.07416	-219.07002	1
14189	C	64.14300	80.54880	64.85190	197.69820	-878.72599	142.15153	1
14190	C	64.10100	79.51580	63.85590	-289.94759	-542.79390	672.87159	1

14191	H	64.80100	79.56380	63.03490	2747.58171	331.57114	1496.35610	1
14192	C	63.15900	78.47080	63.93090	616.79588	321.75980	589.47814	1
14193	H	63.17600	77.65880	63.21990	2085.84444	1593.50673	-1734.42080	1
14194	C	62.29400	78.35380	65.04990	334.18835	-806.48764	263.33788	1
14195	H	61.65200	77.48780	65.10490	-1195.28903	-2707.66152	1066.80806	1
14196	C	63.23200	80.41480	65.92290	655.30633	-207.67647	599.07854	1
14197	H	63.26300	81.05080	66.79490	-1807.55544	938.41900	2397.98652	1
14198	C	62.34100	79.34080	66.02690	-637.91715	628.11748	-173.15066	1
14199	H	61.57100	79.40480	66.78190	-2428.13455	820.79013	1824.47044	1
14200	C	66.93500	80.04880	65.78090	195.05360	-792.53318	-406.56642	1
14201	O	66.63200	79.06580	66.49690	52.23850	680.28599	-397.62964	1
14202	N	67.94200	79.96780	64.95690	-147.37618	-825.15603	100.34977	1
14203	H	68.28900	80.79880	64.52890	641.78635	-2949.29133	887.70332	1
14204	C	68.76200	78.73780	64.76490	-283.59104	413.20314	761.76787	1
14205	H	68.18600	77.88280	64.44390	893.12959	-331.38519	-2998.45454	1
14206	C	69.92700	79.06480	63.73590	-20.02066	736.77696	-536.85183	1
14207	H	70.79800	79.64880	64.10390	720.16800	-286.26712	-3049.20242	1
14208	H	69.47600	79.59580	62.87090	-1766.34439	2477.45026	800.30865	1
14209	C	70.63800	77.74080	63.25190	-567.84164	-695.72988	-158.00889	1
14210	H	69.81100	77.09780	62.88090	1469.65111	2639.96115	-876.90192	1
14211	H	71.15600	77.18480	64.06190	1330.39681	2323.18840	1652.59379	1
14212	C	71.61500	77.98280	62.06390	-173.31241	676.02989	-586.85382	1
14213	O	71.30400	77.62580	60.88590	253.19284	748.00484	-3.06174	1
14214	N	72.76000	78.65180	62.30290	-756.73621	248.18430	280.04847	1
14215	H	73.02500	78.74080	63.26290	-76.03550	1762.26803	2605.15954	1
14216	H	73.53400	78.74680	61.67590	-1129.91214	2023.67923	-2127.49787	1
14217	C	69.42700	78.31480	66.03490	-551.28833	-311.69731	656.03123	1
14218	O	69.49300	77.10380	66.30090	607.35783	152.72270	481.06078	1
14219	N	69.91900	79.24580	66.90290	444.31337	-385.07350	-605.78570	1
14220	H	69.86900	80.20080	66.61990	2595.52861	35.76156	-1777.68910	1
14221	C	70.55000	78.86580	68.12590	-784.14317	-52.59372	462.38987	1
14222	H	71.32000	78.13480	67.92590	-462.13645	-2699.23387	1548.80362	1
14223	C	71.25000	80.09480	68.80590	197.12909	890.15955	14.39087	1
14224	H	71.58700	79.73080	69.79990	2746.32061	303.57606	-1504.58994	1
14225	H	70.61000	80.97980	69.01290	-3097.61543	-546.90067	-62.48631	1
14226	N	73.40700	81.20880	68.59690	-209.07347	622.14253	530.94185	1
14227	H	73.43300	81.28880	69.59390	-2040.68413	1011.31339	2170.50219	1
14228	C	72.35200	80.62980	68.01290	-248.12391	564.18458	-671.99799	1
14229	C	74.26900	81.55580	67.58590	-155.31937	-898.50238	-4.51232	1
14230	H	75.19500	82.08080	67.81790	973.62003	-220.44013	2983.57108	1
14231	N	73.76200	81.31280	66.40590	163.43278	-152.13122	814.13642	1
14232	C	72.56300	80.67780	66.66290	684.80954	300.46282	-521.73651	1
14233	H	72.02400	80.25780	65.82290	1199.36856	-2026.37391	-2086.51625	1
14234	C	69.64000	78.25780	69.17190	-747.16856	355.58843	383.07573	1
14235	O	70.02400	77.39280	69.98090	-534.25265	-579.67242	46.70353	1
14236	N	68.39300	78.68480	69.17490	45.48387	-842.94896	6.36779	1
14237	H	68.03400	79.38880	68.56790	-2083.58571	1357.88664	-1926.92519	1
14238	C	67.34400	78.10680	69.99190	-486.39842	359.06583	682.59747	1
14239	H	67.88300	77.80780	70.87890	1823.64178	-2248.54392	-1231.50603	1
14240	C	66.26800	79.14380	70.38190	354.39673	-755.01887	-368.51114	1
14241	H	65.65100	79.44880	69.50990	-1685.12818	2208.34413	1477.08682	1
14242	C	65.27500	78.49980	71.45990	818.16250	369.91638	158.81751	1
14243	H	65.85400	78.09680	72.31790	-704.60158	2358.52233	1959.37114	1
14244	H	64.71300	77.63880	71.03790	-1922.40656	1060.30325	-2253.51642	1
14245	H	64.49100	79.19980	71.82090	966.05373	2011.63690	2217.72032	1
14246	C	66.88300	80.46080	70.88990	578.45802	-638.70251	298.15505	1
14247	H	67.63100	80.93980	70.22190	1961.27994	-586.94183	-2388.95511	1
14248	H	67.49200	80.42380	71.81890	-2311.42056	1813.39268	1125.68567	1
14249	C	65.83800	81.51180	71.27090	-829.22184	-344.94732	-157.64989	1
14250	H	65.02200	81.53180	70.51890	1146.57994	789.58334	-2821.37180	1
14251	H	65.46700	81.24480	72.28390	429.82659	-2165.50649	-2241.44083	1
14252	H	66.38100	82.47880	71.20490	-2331.25248	-1872.54511	-978.29592	1

14253	C	66.76900	76.84280	69.45490	-340.18826	610.30084	-585.88040	1
14254	O	66.63400	75.81380	70.12590	101.89568	-622.84987	474.66044	1
14255	N	66.31500	76.98580	68.18590	158.99257	828.45462	32.50530	1
14256	H	66.41500	77.87280	67.74190	-2616.55087	-325.30913	-1716.40955	1
14257	C	65.74200	75.94280	67.37790	151.60799	-222.65958	-871.14220	1
14258	H	64.79300	75.72480	67.84490	332.72533	2444.91621	1951.89775	1
14259	C	65.55500	76.47180	65.99690	516.47904	744.65398	100.94974	1
14260	H	65.01800	77.43680	65.87590	-2309.33922	-1649.80974	1357.68420	1
14261	H	66.57200	76.68280	65.60290	-2378.86400	1325.20877	1575.77093	1
14262	C	64.89500	75.49180	64.95890	699.04891	-87.30804	578.92913	1
14263	H	65.50600	74.59380	64.72490	1876.96401	-2499.29325	358.83921	1
14264	H	64.58300	76.09980	64.08290	-1213.58057	2898.57565	153.97275	1
14265	S	63.30800	74.83580	65.62490	416.23263	-317.43383	192.86463	1
14266	C	62.41500	74.52080	64.05090	-723.11660	534.39399	151.57985	1
14267	H	61.57500	73.84080	64.30990	1894.43547	-1399.81738	-2085.62983	1
14268	H	63.09600	74.03980	63.31690	1019.44980	2208.15760	1995.74255	1
14269	H	62.01300	75.46580	63.62590	-1982.24411	1150.22911	2155.43673	1
14270	C	66.62700	74.71180	67.33690	574.44850	-552.29807	-443.20059	1
14271	O	66.22400	73.62780	67.63590	488.90100	-608.17075	121.37288	1
14272	N	67.94400	74.80680	67.04190	412.83426	217.61314	703.48041	1
14273	H	68.38100	75.69680	66.93390	-1566.75032	1034.45141	2524.56529	1
14274	C	68.78100	73.65580	66.86890	-596.84400	82.97288	684.35644	1
14275	H	68.16600	72.78480	66.69290	1497.15614	726.10748	2670.11566	1
14276	C	69.72500	73.87980	65.70990	-175.62620	-821.42401	-354.78026	1
14277	H	70.51200	74.64080	65.89490	2171.35181	2255.82464	-307.75434	1
14278	C	70.49500	72.60180	65.37190	378.51733	52.02063	-827.93085	1
14279	H	71.16400	72.77680	64.50290	-1830.41880	-1926.89381	1683.70826	1
14280	H	71.16100	72.19280	66.16290	-1694.63056	-1036.21179	-2439.81938	1
14281	H	69.76400	71.82480	65.06090	1340.02925	2669.43549	-988.26212	1
14282	C	69.01400	74.34080	64.41390	-814.01391	-209.93561	-353.21297	1
14283	H	68.75000	75.40280	64.60590	-2507.13629	1875.32597	309.26749	1
14284	H	69.68600	74.31480	63.52990	-1945.45291	-2290.22985	-931.81889	1
14285	H	68.06000	73.80680	64.21390	2327.78054	2116.14265	40.05353	1
14286	C	69.60800	73.28180	68.10590	732.54018	-357.93091	408.31525	1
14287	O	69.97600	72.13480	68.30190	1.35383	-550.82225	-565.88006	1
14288	N	69.88600	74.25980	68.99390	363.03646	-731.62391	213.54921	1
14289	H	69.62600	75.21180	68.84890	1755.34152	-2608.48845	-113.09448	1
14290	C	70.53000	73.95480	70.25190	897.70081	-103.05256	-122.32915	1
14291	H	70.92300	74.92080	70.53490	-36.69836	-2570.59466	-1813.53869	1
14292	H	71.34000	73.25280	70.12490	2707.14142	1502.01009	559.97968	1
14293	C	69.62700	73.38380	71.24690	-455.10011	563.46771	553.93053	1
14294	O	70.00600	72.62580	72.09890	-186.37563	-688.24524	339.42575	1
14295	N	68.35400	73.82580	71.22490	311.11183	604.43295	500.54223	1
14296	H	67.99000	74.44980	70.53890	1526.07374	630.11928	-2678.11031	1
14297	C	67.42000	73.44580	72.28490	488.89665	-662.84659	-391.23583	1
14298	H	67.91200	72.76780	72.96590	-202.70806	-176.52103	-3134.64129	1
14299	C	66.91300	74.68680	73.11490	284.28868	637.56471	586.63634	1
14300	H	66.12200	75.16780	72.50090	636.15078	1541.45354	-2667.85671	1
14301	H	67.73000	75.39380	73.37290	-1152.87383	-1009.69575	-2747.65767	1
14302	C	66.30000	74.35180	74.45690	529.35420	598.48763	-439.37193	1
14303	H	65.60900	73.48980	74.34190	-1404.50143	1893.60025	2083.23788	1
14304	C	67.30900	73.99080	75.58390	-356.46527	191.87426	-817.04821	1
14305	H	67.94500	74.88180	75.77790	-2886.42813	-572.73393	1112.98460	1
14306	H	67.87700	73.11080	75.21290	1554.72610	1907.30855	1960.41503	1
14307	H	66.84500	73.70680	76.55190	1700.32173	-1757.92658	1979.09737	1
14308	C	65.46100	75.57580	74.92890	-556.85359	-709.22100	135.53838	1
14309	H	66.10500	76.45080	75.16190	2764.59040	962.11966	1153.07932	1
14310	H	64.93300	75.42080	75.89390	-647.66229	-1903.03744	-2420.16700	1
14311	H	64.70300	75.83080	74.15790	-726.31647	962.86753	-2905.78333	1
14312	C	66.18200	72.68480	71.76890	-551.55292	145.25812	-711.43549	1
14313	O	65.92800	71.57280	72.17990	660.67273	-87.87243	423.57669	1
14314	N	65.43300	73.25880	70.81490	350.86310	-95.77548	-761.83622	1

14315	H	65.71600	74.14280	70.44990	-1155.90570	2419.27216	1645.97402	1
14316	C	64.18200	72.72380	70.30190	-367.08880	-590.07583	590.34509	1
14317	H	63.58800	72.69080	71.20390	-2345.06017	1344.25605	-1609.93625	1
14318	C	63.33000	73.64380	69.47090	-881.45777	-148.18660	-180.34394	1
14319	H	63.72500	73.82480	68.44790	-1263.21552	-2863.19262	-323.48226	1
14320	C	61.92300	73.14780	69.18390	-162.98024	889.47281	-117.16040	1
14321	H	61.36800	72.94880	70.12590	1868.77692	2273.08058	1113.10544	1
14322	H	61.30500	73.85280	68.58890	-2062.91018	1098.60995	-2106.10635	1
14323	H	61.96700	72.21880	68.57590	2163.49839	-1231.78059	-1923.59494	1
14324	C	63.22400	75.10980	70.05690	-710.87993	-201.85737	534.18567	1
14325	H	62.72800	74.93580	71.03590	-1722.85908	-2220.69218	-1413.68633	1
14326	H	64.20300	75.58080	70.29190	74.49284	-2991.69774	-970.78406	1
14327	C	62.38800	76.05980	69.16990	-901.93412	-89.79683	-99.51065	1
14328	H	62.69600	75.86280	68.12090	-2194.98692	-1319.68458	-1827.20860	1
14329	H	62.61200	77.12580	69.38790	-2958.87587	943.55482	502.97527	1
14330	H	61.29600	75.86780	69.23290	615.59011	228.60696	-3076.85130	1
14331	C	64.17900	71.32780	69.69790	615.77418	-500.64708	449.02746	1
14332	O	63.61300	70.39280	70.22690	672.86755	410.51495	-48.51765	1
14333	N	64.84000	71.21580	68.46890	30.93819	-690.30030	-484.97486	1
14334	H	65.25800	71.95580	67.94690	2834.41771	-1125.42655	773.12196	1
14335	C	64.86800	69.95580	67.69390	598.91025	-664.56113	176.39734	1
14336	H	63.81200	69.72680	67.68790	-2265.49285	-1205.97625	1819.72241	1
14337	C	65.36600	70.19380	66.22890	-475.69890	749.97196	206.64852	1
14338	H	66.39600	70.60980	66.18990	1947.96506	-2077.23152	1337.44816	1
14339	H	65.22500	69.21180	65.72890	-1103.00333	-1704.59296	2403.32535	1
14340	C	64.53200	71.18780	65.44590	645.79796	-525.54372	-371.75234	1
14341	H	64.74800	72.23680	65.73890	1034.52187	-432.58778	-2939.53373	1
14342	C	64.82900	71.16480	63.94490	-193.44510	495.40262	740.67958	1
14343	H	64.37600	72.06480	63.47790	1030.41163	-2830.14617	-909.25835	1
14344	H	64.51100	70.21780	63.45690	-1788.09069	1872.10513	-1787.78642	1
14345	H	65.92000	71.13280	63.73590	-2319.69691	430.01972	2081.42152	1
14346	C	63.01800	70.99680	65.50990	337.28319	463.18300	-709.33247	1
14347	H	62.67500	69.94880	65.36790	-2169.81831	-2099.82564	883.65550	1
14348	H	62.52000	71.27080	66.46390	1287.11327	-1973.07056	2085.31969	1
14349	H	62.58300	71.55980	64.65590	933.05301	2308.53467	-1923.09802	1
14350	C	65.59900	68.81180	68.33190	-487.30356	405.89265	-655.16212	1
14351	O	65.01500	67.77580	68.08990	51.76259	752.96699	-232.35441	1
14352	N	66.67700	68.82680	69.08290	716.34479	-416.55290	161.26411	1
14353	C	67.51000	69.99280	69.37990	-313.75432	-698.84754	494.59211	1
14354	H	67.00000	70.92280	69.70990	-1118.00607	2940.43275	46.30239	1
14355	H	68.07300	70.27080	68.46290	344.03567	2906.48788	-1154.20703	1
14356	C	67.20100	67.63480	69.73590	-534.45817	709.77158	205.01164	1
14357	H	67.07000	66.78880	69.07690	-857.55567	3023.80252	139.43755	1
14358	C	68.66500	68.04580	70.17490	481.33696	391.24665	668.35005	1
14359	H	69.12400	67.49880	71.02590	-2140.94963	-2003.45149	1140.50123	1
14360	H	69.38400	67.82280	69.35690	672.80993	2140.77173	2205.14159	1
14361	C	68.55100	69.51580	70.42490	-696.14943	-406.90384	-425.74198	1
14362	H	69.49600	70.06980	70.24090	-962.55716	2608.97393	1471.38199	1
14363	H	68.18300	69.79180	71.43690	-2261.40855	-1927.18248	-1034.51694	1
14364	C	66.39300	67.26680	71.00390	-453.74341	739.56402	280.38006	1
14365	O	66.32900	66.10480	71.31490	-137.54694	639.53244	442.38708	1
14366	N	65.84600	68.26680	71.68190	525.19233	644.56059	-146.24280	1
14367	H	65.99600	69.19580	71.35290	2330.43331	683.90243	-1999.89607	1
14368	C	64.95700	68.17180	72.79490	399.79504	-677.76227	460.70949	1
14369	H	64.63100	69.17880	73.00590	2056.58315	1120.06637	2100.98627	1
14370	H	65.55800	67.86280	73.63690	1733.48591	94.92812	-2623.78381	1
14371	C	63.76000	67.32980	72.57190	-10.08677	-839.03243	-356.89472	1
14372	O	63.42600	66.47880	73.44190	-437.01769	-217.15932	-620.87406	1
14373	N	63.06200	67.53680	71.42990	766.41190	160.47857	315.48648	1
14374	H	63.28600	68.31780	70.85290	-1861.68302	1369.43190	2134.71751	1
14375	C	61.89500	66.79280	71.11990	134.00087	-583.58071	687.69784	1
14376	H	61.24900	66.80980	71.98490	-1363.52244	-2722.36357	-792.31898	1

14377	C	61.08100	67.31480	69.93990	593.24576	-688.29568	-75.89158	1
14378	H	60.31700	66.55780	69.66190	1194.47358	2577.93466	-1351.18910	1
14379	C	60.20100	68.50380	70.43690	-62.19399	-708.20101	570.99408	1
14380	H	59.64400	68.05180	71.28490	1664.45034	1183.95113	2392.92520	1
14381	H	59.37700	68.71880	69.72290	-665.70437	3054.70418	-351.91805	1
14382	H	60.89200	69.32080	70.73390	1496.61065	-1903.13702	-2009.09239	1
14383	C	61.97000	67.64580	68.73790	-4.01097	820.47718	-397.80915	1
14384	H	62.59600	68.53580	68.96190	-5.14008	-236.63247	3137.22885	1
14385	H	62.67200	66.81080	68.52690	1511.82584	-448.24004	2722.44187	1
14386	C	61.18200	67.81180	67.43490	-828.62534	-319.95147	-206.06334	1
14387	H	61.83300	68.03080	66.56190	2986.70743	-737.51338	-658.69488	1
14388	H	60.42100	68.61980	67.48290	1471.44982	615.18607	2711.93800	1
14389	H	60.54100	66.91780	67.27590	1969.38797	-2313.68546	816.45382	1
14390	C	62.10100	65.27780	70.85890	542.50498	-411.58330	606.41449	1
14391	O	61.32600	64.41780	71.31790	-90.26999	-196.22098	-759.58929	1
14392	N	63.17400	64.90480	70.18990	-117.44128	375.04606	747.14141	1
14393	H	63.73500	65.66780	69.88090	734.43151	-2823.65248	-1177.20995	1
14394	C	63.66700	63.56780	70.06490	-589.92492	639.39638	-273.15172	1
14395	H	62.88200	62.91180	69.71890	1868.20173	2187.26408	-1274.33290	1
14396	C	64.85000	63.46980	69.11790	73.22357	-747.66018	516.81095	1
14397	H	65.76400	63.92480	69.55590	-60.91869	-1130.28062	-2935.46945	1
14398	C	65.11100	61.98380	68.79790	588.28790	-568.72396	-402.39460	1
14399	H	65.53400	61.39180	69.63790	2129.49122	1687.30096	1586.35080	1
14400	H	65.93800	61.98080	68.05590	869.28117	-2724.29525	1311.78956	1
14401	H	64.16200	61.56580	68.39990	-1383.60622	-1787.62488	-2188.20871	1
14402	C	64.66600	64.18280	67.82090	-511.99294	745.72906	114.90170	1
14403	H	64.71900	65.29080	67.87690	1588.00486	-188.69905	-2709.40205	1
14404	H	65.40800	63.84580	67.06590	1800.67259	-1935.62399	1705.62723	1
14405	H	63.66800	64.06080	67.34590	1347.81269	2032.19053	-1987.92073	1
14406	C	64.06000	63.02280	71.47490	-1.70514	752.11570	-515.52892	1
14407	O	63.68600	61.86980	71.71690	714.84410	-93.59885	-322.27999	1
14408	N	64.69800	63.81880	72.35490	551.30940	-398.39206	500.01400	1
14409	H	64.92200	64.75380	72.09190	1065.39191	2431.51348	-1688.46336	1
14410	C	64.99500	63.39580	73.70990	84.22080	855.54583	-303.97236	1
14411	H	65.58600	62.49180	73.72390	-1378.58275	-2174.01324	-1808.70182	1
14412	C	65.90700	64.41680	74.47290	-548.75752	-723.60389	81.93657	1
14413	H	65.40800	65.40280	74.35890	-798.90751	-3003.86307	486.60013	1
14414	C	65.96600	64.10380	75.97690	121.52595	468.18448	772.97202	1
14415	H	64.99500	64.04380	76.51390	1064.66948	1358.25911	-2630.55837	1
14416	H	66.52400	63.15380	76.11390	728.27879	-2508.23114	1754.02759	1
14417	H	66.62700	64.80880	76.52590	-2157.82906	216.12575	2279.31780	1
14418	C	67.28900	64.30380	73.77390	749.51981	-457.40855	-245.86273	1
14419	H	67.15200	64.24880	72.67190	-420.13663	-1908.78261	-2465.41282	1
14420	H	67.80800	63.36280	74.05590	1292.12572	-2513.34894	-1382.64763	1
14421	C	68.16400	65.49680	74.02690	-394.49375	463.21539	-679.15918	1
14422	H	67.70100	66.33980	73.47090	2086.51082	1736.69889	-1590.14961	1
14423	H	68.23500	65.67980	75.11990	2822.74157	-548.77616	1276.40157	1
14424	H	69.22100	65.29580	73.74790	1926.09764	-1485.74778	1995.22621	1
14425	C	63.73700	63.05580	74.48490	493.45836	-499.32038	-581.91839	1
14426	O	63.59500	61.94380	75.01890	-732.30512	90.81087	281.26470	1
14427	N	62.71100	63.97680	74.42690	-388.37517	-500.86328	-557.64953	1
14428	H	62.97700	64.85880	74.04390	1950.96197	-1152.01113	-2182.85226	1
14429	C	61.40000	63.89880	75.00690	-65.73122	687.61042	595.24979	1
14430	H	61.51400	63.67880	76.05790	-1951.21468	1538.10409	-1930.08375	1
14431	C	60.66100	65.21180	74.74190	522.64942	726.40915	-174.98094	1
14432	H	60.92700	65.60280	73.73690	-1874.72242	1772.08866	-1800.92861	1
14433	H	59.56300	65.07380	74.83190	-3107.24857	303.11924	-389.03888	1
14434	C	61.13800	66.33980	75.75290	-526.39631	-297.91956	682.35025	1
14435	H	62.24600	66.39680	75.69090	-1296.29539	1075.82747	-2657.14880	1
14436	C	60.60400	67.72780	75.32790	559.65290	571.52751	-437.71674	1
14437	H	60.92600	68.06380	74.31990	2176.88016	889.15141	2090.17434	1
14438	H	59.49500	67.79180	75.33190	-1717.87920	-2187.24171	-1470.74505	1

14439	H	60.93400	68.51280	76.04190	939.06574	2087.33093	-2158.57160	1
14440	C	60.79400	66.15080	77.20290	793.52293	-219.55549	-391.87721	1
14441	H	61.31900	65.24480	77.57390	-581.17914	1168.77396	-2862.59051	1
14442	H	60.95400	67.10180	77.75390	-2954.60589	506.49745	954.98199	1
14443	H	59.72800	65.90580	77.39990	1752.84334	232.71534	2602.23174	1
14444	C	60.68300	62.63780	74.55090	-422.82354	680.47202	435.46422	1
14445	O	60.15800	61.87580	75.38690	507.75188	597.42849	-94.31041	1
14446	N	60.66600	62.35580	73.27790	-572.47222	389.58514	482.87811	1
14447	H	61.20100	62.96480	72.69590	1749.94152	-2014.18665	-1667.02820	1
14448	C	60.10100	61.11180	72.65490	146.14881	299.24040	-848.85023	1
14449	H	59.04500	61.08180	72.87990	778.60536	-2130.16337	2180.45957	1
14450	C	60.12500	61.11180	71.07890	-81.54435	640.83186	643.53403	1
14451	H	59.92400	60.10280	70.65790	2240.83455	-2098.16604	688.90203	1
14452	H	61.15700	61.42380	70.81190	1734.81488	-2487.23910	-838.02460	1
14453	O	59.30200	62.05380	70.45490	-354.37435	-48.53850	704.05260	1
14454	H	58.40200	61.85880	70.72590	-972.02832	2985.12033	-206.01886	1
14455	C	60.70300	59.78680	73.11590	596.28258	-631.56435	277.53299	1
14456	O	59.91400	58.83680	73.29290	-337.54624	-10.70752	713.84530	1
14457	N	62.04400	59.67780	73.24190	215.16837	-355.06463	-735.05372	1
14458	H	62.55400	60.48180	72.94690	-1113.47260	-2283.51931	-1855.78678	1
14459	C	62.74300	58.45280	73.65390	-412.71609	-249.10353	773.99216	1
14460	H	62.41300	57.69680	72.95690	-618.05730	2898.96796	-1054.61660	1
14461	C	64.26900	58.73380	73.87290	-728.96113	259.56186	482.38398	1
14462	H	64.76100	57.78280	74.17290	901.55280	931.36218	-2866.70425	1
14463	H	64.35500	59.49580	74.67690	-1452.49062	-2621.83855	956.27393	1
14464	S	64.98900	59.21680	72.26490	-194.13488	-76.32355	517.39441	1
14465	H	64.69800	60.50780	72.31790	-681.37477	-1452.89683	2706.11261	1
14466	C	62.19100	57.92080	74.99590	116.85271	739.49730	-520.51915	1
14467	O	61.86400	56.75380	75.16990	182.68119	593.14954	488.29135	1
14468	N	62.14600	58.80680	76.01990	45.70287	804.95113	-250.27427	1
14469	H	62.48500	59.73680	75.89890	-674.89009	-2327.51731	-2006.34313	1
14470	C	61.69700	58.38880	77.38590	-740.98950	-479.25022	-229.57526	1
14471	H	62.07100	57.41880	77.67990	-2645.96527	1517.62944	770.64577	1
14472	C	62.30100	59.29480	78.44190	757.50892	468.49620	-195.30118	1
14473	H	61.96400	58.85080	79.40290	2406.12827	1321.26137	-1537.21872	1
14474	H	61.85500	60.29480	78.25690	2782.91557	1102.01246	969.11076	1
14475	C	63.83700	59.35180	78.28390	-803.14102	140.99230	408.08906	1
14476	C	64.38900	60.56680	77.83490	569.90361	535.86548	-468.51795	1
14477	H	63.80300	61.43580	77.57490	901.26748	2307.51083	1939.41664	1
14478	C	65.78200	60.60780	77.65190	-37.77197	-597.50180	-687.76150	1
14479	H	66.16600	61.51380	77.20790	-904.88168	1353.36004	2692.17978	1
14480	C	66.60500	59.53580	77.92290	-817.15962	-16.96333	-404.24424	1
14481	O	67.97300	59.58680	77.66090	-653.44068	-391.55089	208.15958	1
14482	H	68.15200	60.22280	76.96390	1760.09192	-2576.95817	-399.48619	1
14483	C	64.61200	58.27280	78.57190	-385.75690	437.13966	701.10737	1
14484	H	64.11800	57.43480	79.04090	2260.45440	-996.47659	1948.23164	1
14485	C	66.01500	58.33080	78.34490	-476.74657	-368.24947	684.51153	1
14486	H	66.62900	57.44280	78.37690	958.68698	-2912.64048	-704.03901	1
14487	C	60.22600	58.36380	77.44290	40.66128	834.47524	-365.30637	1
14488	O	59.63100	57.65280	78.25890	-322.55860	526.28303	-492.55391	1
14489	N	59.50100	59.13780	76.59090	188.73066	-563.22900	-599.85508	1
14490	H	59.91300	59.78880	75.95890	-2203.55087	1691.57533	1476.87599	1
14491	C	58.09000	58.99580	76.38390	-901.54697	-95.99147	97.20962	1
14492	H	57.66200	59.15280	77.36290	1913.20878	-2197.06582	1187.75425	1
14493	C	57.49900	60.00280	75.39790	-3.91098	-816.22786	406.45762	1
14494	H	57.89000	60.99280	75.71490	-1932.81911	-1896.28298	-1602.04474	1
14495	H	57.90100	59.81880	74.37790	730.76234	-3020.63486	489.87516	1
14496	S	55.72300	60.08580	75.22290	-8.62032	-298.44196	471.24165	1
14497	H	55.62900	59.09380	74.34990	-2337.76039	1913.19876	879.07513	1
14498	C	57.68600	57.57480	75.97290	-725.82512	212.06652	-509.56519	1
14499	O	56.79800	56.98380	76.56690	-675.41180	-371.42640	-171.72231	1
14500	N	58.36000	56.95880	75.04090	12.16073	-815.10765	-219.37167	1

14501	H	58.91300	57.53180	74.44090	-727.88212	2445.23033	1840.99497	1
14502	C	58.10400	55.59180	74.61790	-590.94656	130.60970	682.03685	1
14503	H	57.05600	55.50580	74.37190	1979.92371	-2441.04385	-139.40326	1
14504	C	58.88400	55.19280	73.32890	626.26332	-583.85032	-313.63045	1
14505	H	59.96700	55.39580	73.47690	-2093.11751	1786.25521	-1525.24674	1
14506	C	58.75700	53.70380	73.07890	-704.92997	108.48903	568.11519	1
14507	H	59.12800	53.48880	72.05390	2482.17114	1404.67173	-1328.13778	1
14508	H	59.29400	53.04680	73.79590	2783.72384	-1395.70830	-448.44861	1
14509	H	57.68400	53.41180	73.07590	2819.67443	1395.41107	22.14147	1
14510	C	58.35700	55.95380	72.10590	625.30349	-64.59327	-660.51060	1
14511	H	57.42400	55.51380	71.69390	1383.39231	2825.00579	-61.59749	1
14512	H	58.03500	56.99480	72.32590	2392.04041	2043.19427	41.54653	1
14513	C	59.39500	56.11680	70.97890	697.09019	-527.59108	-259.16004	1
14514	H	59.93700	55.16780	70.78090	1909.84300	-1424.44627	2054.67242	1
14515	H	59.03200	56.60880	70.05190	1920.85389	178.12630	2485.32042	1
14516	H	60.04100	56.97780	71.25290	2526.20734	1579.75436	1010.38550	1
14517	C	58.48800	54.59080	75.69290	-672.90234	35.56105	-614.31983	1
14518	O	57.74000	53.60180	75.90990	-478.48117	-400.52770	-484.00470	1
14519	N	59.64700	54.78980	76.37390	-594.65392	-518.80353	-299.83646	1
14520	H	59.99800	55.71780	76.27190	-2801.41960	-1160.56416	838.66875	1
14521	C	60.34200	53.84080	77.29690	-465.92880	-632.01678	-463.59049	1
14522	H	60.57700	52.90980	76.80290	2104.64880	-1398.78162	-1874.05700	1
14523	C	61.81500	54.30380	77.78890	563.73452	-478.79226	533.30326	1
14524	H	61.72400	55.38780	78.01790	-180.62567	2661.80876	-1667.44557	1
14525	C	62.20200	53.43880	79.01190	-735.72828	495.54516	211.16321	1
14526	H	62.13300	52.35980	78.75490	1744.68210	1919.39457	1780.51539	1
14527	H	63.25500	53.63080	79.30990	-2455.01550	-1863.10778	-632.41956	1
14528	H	61.54700	53.49980	79.90690	-3074.15489	510.41792	-432.74879	1
14529	C	62.82100	54.15980	76.66190	-535.57079	392.91337	-624.68714	1
14530	H	62.32800	54.42880	75.70290	2535.16225	-1816.52634	-414.01766	1
14531	H	63.23200	53.13380	76.55490	637.95677	-2996.20685	-716.92531	1
14532	C	64.08400	54.91880	76.90390	-180.83755	852.62476	267.91753	1
14533	H	63.83200	55.97580	77.13390	-2162.95064	-237.77774	-2272.29675	1
14534	H	64.72100	54.56480	77.74290	-681.95603	-2936.95997	-898.57017	1
14535	H	64.80100	54.81880	76.06190	-102.88974	-380.35460	-3121.37314	1
14536	C	59.39500	53.38480	78.45890	365.42209	-771.75666	319.85834	1
14537	O	59.23700	52.19880	78.85690	-130.96376	-582.10112	-517.33356	1
14538	N	58.74100	54.39080	79.02790	-580.04826	-497.83537	358.29632	1
14539	H	58.82900	55.33080	78.70690	-2465.17050	1949.98831	136.77065	1
14540	C	57.95400	54.24980	80.20890	552.93237	-538.66922	485.33727	1
14541	H	58.55600	53.66780	80.89190	-1936.24275	1681.77355	1822.31390	1
14542	C	57.67700	55.58980	80.88790	-544.96510	524.50920	-509.26825	1
14543	H	57.07200	55.33580	81.78590	2316.46170	-1887.20468	-985.23598	1
14544	C	58.98100	56.16480	81.44990	634.75023	581.47036	300.72474	1
14545	H	58.79600	57.04280	82.10490	2074.77167	-1603.44444	1738.53809	1
14546	H	59.55900	55.40180	82.01390	-3027.53279	730.20764	-446.17064	1
14547	H	59.56000	56.60080	80.60790	492.25962	-3013.89594	756.53021	1
14548	C	56.89100	56.57580	80.03690	-735.50513	-67.82815	-534.67985	1
14549	H	57.59600	57.08480	79.34490	-2011.17990	2111.92388	1180.32164	1
14550	H	56.23000	55.99780	79.35490	-1755.26170	1810.64938	1881.17820	1
14551	C	56.10400	57.58680	80.84990	614.68626	74.55363	669.36803	1
14552	H	55.43400	57.04080	81.54790	2510.66828	1886.50010	189.44233	1
14553	H	55.39900	58.12580	80.18290	-12.55402	61.42276	-3145.51997	1
14554	H	56.80600	58.30380	81.32690	2078.87938	-1735.19968	1601.73931	1
14555	C	56.78400	53.35880	80.02290	-743.53414	511.49723	-130.30185	1
14556	O	56.23600	52.76380	80.96890	588.39911	524.92125	43.25962	1
14557	N	56.27700	53.27880	78.79190	13.28607	588.62638	604.99153	1
14558	H	56.73500	53.86180	78.12490	946.06818	-1978.89572	2255.47178	1
14559	C	55.13000	52.49880	78.47790	-295.89285	791.67877	-342.26182	1
14560	H	54.47900	52.42980	79.33690	843.43458	1701.42202	2508.38742	1
14561	C	54.26500	53.22480	77.40490	754.02901	511.08116	-41.07688	1
14562	H	53.70300	54.02080	77.93790	-1909.60232	-2485.84722	268.71691	1

14563	H	53.51500	52.55080	76.93890	-2511.76953	-1578.68953	1047.36786	1
14564	O	55.06400	53.77880	76.36790	-400.51945	635.55216	-243.48482	1
14565	H	55.77900	53.17280	76.16290	126.75732	3123.91475	351.16297	1
14566	C	55.34500	51.08080	78.13790	729.63697	-446.46594	315.83076	1
14567	O	54.38400	50.33480	77.74290	442.93773	-651.90520	-49.52781	1
14568	N	56.56600	50.60580	78.30390	-107.75884	-765.91461	338.28262	1
14569	H	57.18900	51.23380	78.76590	-203.77245	1794.70073	-2575.99540	1
14570	C	56.93000	49.22180	78.07690	649.67172	-639.82059	2.69468	1
14571	H	56.17700	48.60980	78.54990	-1683.53299	-2008.38757	1740.78209	1
14572	C	56.90500	48.80080	76.58590	550.37529	503.16102	524.75426	1
14573	H	55.84500	48.89880	76.26890	-1913.41416	2467.82422	383.29633	1
14574	H	57.16400	47.73180	76.43290	1246.14911	2688.02245	1058.24095	1
14575	C	57.61500	49.74880	75.55590	-524.85807	656.88756	352.80837	1
14576	H	58.66700	49.92380	75.86590	53.68440	-3097.36282	-549.26111	1
14577	H	57.07500	50.71580	75.64090	813.94205	1730.01573	-2498.55361	1
14578	C	57.50000	49.15880	74.14190	-220.05618	494.47871	733.83724	1
14579	H	58.09000	49.79580	73.44890	-2571.25717	-1811.98947	59.64017	1
14580	H	58.01800	48.17680	74.12790	2258.20433	443.46897	-2145.24468	1
14581	C	56.08000	49.16180	73.63190	570.19697	-673.94438	228.30983	1
14582	H	55.39300	48.50380	74.20690	1472.61415	-1731.58635	-2175.14195	1
14583	H	55.70700	50.20880	73.64390	2314.10831	134.62230	-2127.20610	1
14584	N	56.00100	48.71280	72.26790	-364.77716	-342.77374	-679.79120	1
14585	H	56.26500	49.45680	71.59090	165.10505	-2618.56232	1736.11575	1
14586	H	55.01000	48.47780	72.05990	1485.64317	2105.19406	1805.33891	1
14587	H	56.61600	47.89280	72.09290	2555.77940	-661.07959	-1711.48814	1
14588	C	58.25800	48.62980	78.70690	530.68986	545.42282	502.32780	1
14589	O	58.67000	47.50480	78.41790	-483.71484	-550.91079	293.50382	1
14590	N	58.87400	49.39780	79.67090	-9.30974	-840.03168	83.26103	1
14591	H	58.55300	50.33080	79.81490	2297.01815	2051.55425	-642.69667	1
14592	C	60.05300	49.01480	80.43090	-738.17546	52.50969	532.72011	1
14593	H	60.85900	48.83280	79.73490	-210.22144	1446.03697	2786.21791	1
14594	C	60.48400	50.11080	81.40890	-591.45373	419.26880	-553.03451	1
14595	H	60.55300	51.07380	80.85790	-1981.72135	-900.86016	2271.44396	1
14596	H	59.62900	50.22680	82.10890	-1607.70201	-1667.68815	-2128.92854	1
14597	C	61.81200	49.86180	82.09690	-16.13933	55.14233	910.02739	1
14598	H	61.77700	48.88480	82.62590	487.95653	2621.51135	1669.67149	1
14599	C	62.94700	50.01980	81.06690	705.18292	-576.44655	-43.32926	1
14600	H	62.97300	51.01480	80.57190	-2305.40820	1828.95797	1112.75874	1
14601	H	62.94200	49.14980	80.37590	-378.26055	-366.92465	-3101.69494	1
14602	H	63.86500	49.83680	81.66490	2805.76968	1332.24762	-500.99800	1
14603	C	61.98100	50.95380	83.20990	-529.26154	-527.10529	-522.96582	1
14604	H	61.11500	50.89480	83.90290	-2600.06500	-10.89578	1771.37503	1
14605	H	62.95000	50.78680	83.72690	-2857.22398	-1163.83868	-616.42263	1
14606	H	62.00600	51.98380	82.79390	-1978.21852	-1094.01348	2188.15270	1
14607	C	59.83400	47.69080	81.19690	29.37427	590.26214	-694.39093	1
14608	O	60.73700	46.80980	81.21890	-395.33304	-155.10882	665.79296	1
14609	N	58.64700	47.46780	81.86090	190.50952	-793.34384	-216.75786	1
14610	H	57.93700	48.16280	81.93990	-2342.89876	-2093.71748	159.36980	1
14611	C	58.32400	46.20480	82.43990	-697.54255	580.86657	-86.48359	1
14612	H	59.16000	45.72380	82.92390	-135.59744	-1219.89506	2896.84235	1
14613	C	57.25300	46.40580	83.55490	439.01971	-366.94824	709.97302	1
14614	H	56.46500	47.09480	83.18390	-2983.55025	-793.80366	-605.41709	1
14615	H	56.84700	45.42880	83.89290	-1528.44556	2391.22976	-1357.97666	1
14616	O	57.79400	47.05480	84.72390	-58.33021	-271.59339	-739.23058	1
14617	H	58.33600	46.39680	85.16390	-3067.75475	-104.94495	689.99534	1
14618	C	57.74300	45.15880	81.47690	-760.62354	368.20265	-342.53415	1
14619	O	57.44700	44.02980	81.86390	658.98494	-55.19269	-431.64782	1
14620	N	57.64000	45.44880	80.18090	-27.63665	-200.09890	-819.67612	1
14621	H	57.87600	46.33480	79.79090	-2405.58554	1968.51410	486.14470	1
14622	C	57.07300	44.51080	79.22090	223.58277	529.74666	-707.69359	1
14623	H	56.64100	43.64980	79.70890	-2194.21227	2069.53962	894.79860	1
14624	C	55.93600	45.12680	78.34290	-518.88023	-145.33223	735.59014	1

14625	H	56.29600	45.99180	77.74590	2184.72905	100.66614	2261.64797	1
14626	H	55.54800	44.49680	77.51490	1248.43424	-602.57619	-2824.27692	1
14627	N	53.71900	46.31980	78.70290	-450.62011	535.76950	-471.76779	1
14628	H	53.67500	46.71180	77.78490	2145.22324	692.26068	-2194.77074	1
14629	C	54.76900	45.59380	79.19390	747.60014	320.33242	412.22830	1
14630	C	52.84700	46.50780	79.73890	-653.78111	361.98540	522.48238	1
14631	H	51.89400	47.02380	79.61890	821.71042	-3004.28058	-444.20312	1
14632	N	53.29900	45.96080	80.86590	-521.14493	-363.93868	555.54378	1
14633	C	54.52600	45.35480	80.48390	151.03952	173.87420	882.27310	1
14634	H	55.14700	44.83680	81.20490	-1933.72550	1915.08321	1578.41320	1
14635	C	58.04800	44.00880	78.19490	737.17950	260.16697	469.39380	1
14636	O	57.88200	42.94680	77.55890	260.74621	-502.24469	550.80751	1
14637	N	59.14200	44.76280	78.02990	-229.19614	-767.26064	-267.30605	1
14638	H	59.21600	45.65280	78.47390	2722.75767	-1531.41429	-373.61368	1
14639	C	60.37000	44.45780	77.32690	475.53858	-634.38824	450.40607	1
14640	H	60.06600	43.86780	76.47490	1926.73388	-1447.61399	-2022.45804	1
14641	C	61.19700	45.73880	76.87590	-753.09062	-29.10756	513.28186	1
14642	H	62.10800	45.47580	76.29590	-203.08343	-2886.69370	1234.49700	1
14643	H	61.43300	46.19080	77.86290	-2217.83936	860.91246	-2058.69972	1
14644	O	60.39300	46.65880	76.10090	299.48177	657.88616	317.99952	1
14645	H	59.93500	47.30180	76.64590	-931.22968	1921.92466	2310.24742	1
14646	C	61.25600	43.57680	78.15690	-178.70763	-160.85079	879.56899	1
14647	O	61.74400	44.02380	79.23190	668.96290	409.43745	92.06977	1
14648	O	61.55900	42.43480	77.70390	607.49542	-496.86289	-87.77135	1
14649	N	68.09800	39.69880	83.86190	571.61285	349.91433	513.31374	1
14650	H	68.31400	38.85080	84.42290	910.08563	2169.10908	2089.24296	1
14651	H	68.24600	39.59180	82.83790	1776.01328	-2241.62595	1311.15071	1
14652	H	67.12500	40.02180	84.03590	1021.37160	1012.12330	-2798.32677	1
14653	C	68.95200	40.75780	84.30590	777.55891	146.67247	453.14493	1
14654	H	68.94300	40.82480	85.38390	1946.09249	226.04804	2461.67677	1
14655	C	70.47100	40.56280	83.91090	-111.61165	613.31428	665.46182	1
14656	H	70.98000	41.53880	84.06090	2031.28577	2399.19909	-126.28571	1
14657	H	70.47900	40.45980	82.80490	230.72473	-2499.99811	-1896.04900	1
14658	C	71.15500	39.33080	84.51890	-126.72152	-755.37306	494.77692	1
14659	H	72.17500	39.10180	84.14190	2817.21167	-1316.06727	479.07368	1
14660	H	70.62200	38.43880	84.12690	2586.76849	178.09807	-1781.89115	1
14661	C	71.32300	39.38980	86.03290	463.17499	681.60177	-390.30625	1
14662	H	70.30800	39.45380	86.48090	140.17274	-556.15974	-3093.42273	1
14663	H	71.82700	40.34380	86.29990	-1194.98471	1307.19899	2600.28240	1
14664	C	71.99000	38.13380	86.56490	192.57395	-856.97157	244.87956	1
14665	H	71.54000	37.18180	86.20890	2223.30287	-2111.73266	704.08501	1
14666	H	73.02200	38.05280	86.16090	-2223.17803	-1828.22959	1270.15048	1
14667	N	72.01700	38.08680	88.06190	-231.46637	312.51116	749.28792	1
14668	H	72.40100	38.94980	88.49690	-1219.09390	2187.79300	-1904.10033	1
14669	H	71.06600	37.95380	88.46190	-1435.97863	-1999.74162	-1958.88362	1
14670	H	72.60700	37.30680	88.41590	2885.33725	1136.02598	-531.50744	1
14671	C	68.42100	42.10180	83.76190	-828.88752	-98.95561	366.88455	1
14672	O	67.82500	42.17680	82.71690	-522.37256	-577.22668	-132.52735	1
14673	N	68.61900	43.27580	84.43490	-646.96390	541.01008	-37.65773	1
14674	H	69.20800	43.27780	85.23890	2269.17026	2048.11863	744.51504	1
14675	C	67.99400	44.54780	83.99690	242.27881	241.13978	-845.34229	1
14676	H	68.34000	44.71780	82.98890	859.63306	-1423.90944	-2670.53162	1
14677	H	66.91700	44.46680	83.96490	-771.66451	-605.82432	-2989.27031	1
14678	C	68.37200	45.68480	84.92590	184.66813	-321.36860	833.10918	1
14679	O	68.20000	46.83880	84.64490	-682.82653	-368.19143	147.68288	1
14680	N	68.83800	45.43480	86.17690	-151.80695	593.35009	-581.00139	1
14681	H	69.14100	44.52880	86.46290	2037.25410	2010.44992	1306.10606	1
14682	C	69.04600	46.53980	87.06590	-543.62316	-345.00075	-645.67743	1
14683	H	68.12300	47.09580	87.14390	66.33524	-2802.41070	1428.39775	1
14684	C	69.42500	45.95680	88.48290	-272.01223	-709.62501	-503.87766	1
14685	H	69.61000	46.79780	89.18490	-409.90894	2764.32361	-1445.23903	1
14686	H	70.26400	45.23680	88.37490	2379.73334	927.90655	1836.86822	1

14687	N	68.12900	45.25980	90.58990	460.74564	311.05029	-635.32154	1
14688	H	68.44200	46.05880	91.10290	-330.13030	2963.30336	1004.02859	1
14689	C	68.28000	45.18480	89.23290	519.54692	329.33351	-673.09839	1
14690	C	67.11100	44.45380	90.92790	644.40650	-337.95750	549.52342	1
14691	H	66.88800	44.18780	91.96090	1809.78404	2565.69366	-200.30982	1
14692	N	66.50500	43.97780	89.88790	-540.84101	466.07973	-450.48082	1
14693	C	67.24500	44.40280	88.80090	233.82681	632.05969	614.22844	1
14694	H	67.06100	44.12980	87.76890	2200.32966	771.33471	-2112.30168	1
14695	C	70.13100	47.50080	86.71590	173.45819	439.65766	-779.78484	1
14696	O	69.95600	48.68880	86.84090	222.39656	-627.13672	425.28406	1
14697	N	71.22300	46.97380	86.14590	204.60913	810.01953	121.14355	1
14698	H	71.30800	45.98380	86.05590	1395.58742	-1035.56346	2622.62660	1
14699	C	72.34500	47.79380	85.73390	660.80815	628.31392	2.28335	1
14700	H	72.45100	48.61880	86.42290	-1545.53051	576.21836	-2679.09202	1
14701	C	73.65200	47.05680	85.70090	-425.79057	48.13732	804.88272	1
14702	H	73.55600	46.00080	85.36790	3039.25537	630.53926	-513.39387	1
14703	H	74.35000	47.50180	84.95990	-1972.72698	1038.17948	-2220.08060	1
14704	C	74.30700	47.04680	87.09390	480.53013	151.83766	759.92574	1
14705	H	74.48500	48.04780	87.54190	2370.68197	2029.45804	-399.24092	1
14706	H	75.34400	46.64680	87.06490	1467.22559	-1259.41518	2481.80352	1
14707	C	73.53900	46.29480	88.22990	58.71735	865.85843	279.80790	1
14708	O	73.14300	46.94180	89.21590	700.56881	-336.87543	-139.08814	1
14709	N	73.26100	44.98580	88.05190	-505.79474	159.24044	-656.87629	1
14710	H	73.59700	44.45680	87.27190	3144.97068	8.48997	-85.51932	1
14711	H	72.71800	44.56680	88.77890	2893.42752	214.46368	-1216.67940	1
14712	C	72.00600	48.49580	84.37690	-652.05618	177.10620	-612.29661	1
14713	O	72.38900	49.64980	84.14890	350.99120	170.81571	-686.47971	1
14714	N	71.16500	47.88080	83.49290	-302.53106	-766.33903	-184.04277	1
14715	H	70.90700	46.92780	83.63290	364.44118	-1764.43515	2579.18155	1
14716	C	70.59400	48.62080	82.36290	-862.50171	-289.28886	-62.07866	1
14717	H	71.41900	49.01280	81.78590	1036.01167	2208.48577	-1986.83081	1
14718	C	69.70100	47.63480	81.51590	-164.55527	-344.16843	-828.20327	1
14719	H	69.09700	47.05380	82.24590	658.45871	-2145.97582	2204.41515	1
14720	H	69.01800	48.11480	80.78390	2985.10277	-664.84523	738.49069	1
14721	C	70.56200	46.67680	80.62690	283.54917	211.53191	840.41961	1
14722	H	71.33500	46.24680	81.29890	-1916.84059	822.55660	-2355.28109	1
14723	H	71.11300	47.16180	79.79190	-944.70943	-446.17113	2967.60537	1
14724	C	69.74500	45.52780	80.02090	524.29088	-391.76342	634.89487	1
14725	H	69.31500	44.92580	80.84990	-1229.57383	1844.48205	2232.54572	1
14726	H	70.38800	44.89380	79.37490	1015.63131	-780.23833	-2873.66446	1
14727	C	68.59400	45.99380	79.11190	-663.46686	-12.73768	-625.38027	1
14728	H	67.85700	46.48980	79.77890	2253.08905	-497.15486	-2138.84385	1
14729	H	68.97400	46.63180	78.28490	916.62625	-2520.24030	1645.11743	1
14730	N	68.02900	44.78280	78.47990	-646.67135	411.61989	353.63473	1
14731	H	67.98800	44.08980	79.25490	456.55696	-1691.11499	2613.41005	1
14732	H	67.10500	44.86980	78.00990	1932.75723	1360.21106	2076.65635	1
14733	H	68.67200	44.54580	77.69790	417.66651	2948.47236	1015.03285	1
14734	C	69.71700	49.79980	82.79390	-617.67290	-324.69073	586.94729	1
14735	O	69.79800	50.86580	82.22390	540.16093	474.80293	-326.21401	1
14736	N	68.85600	49.66080	83.84290	594.48378	432.66991	-414.79883	1
14737	H	68.79800	48.77280	84.29290	-978.53363	2663.26302	-1359.31167	1
14738	C	68.00000	50.77580	84.28590	715.14807	-556.17579	103.35727	1
14739	H	67.57400	51.25780	83.41790	2428.98298	1120.09530	1656.39803	1
14740	C	66.81200	50.11480	85.12790	-332.12868	-304.81920	792.60759	1
14741	H	67.22400	49.50880	85.96190	-139.30877	1651.25559	-2674.35493	1
14742	H	66.27300	50.96480	85.59790	-1694.81756	919.65983	2485.96972	1
14743	C	65.87200	49.30880	84.17590	395.52658	651.74012	-500.24449	1
14744	H	66.45800	48.61780	83.53290	-1809.92321	376.01599	2545.78400	1
14745	H	65.40700	50.13980	83.60490	-2338.21175	-441.51441	-2058.16838	1
14746	C	64.58100	48.69080	84.76490	226.48407	674.72310	570.00413	1
14747	H	63.91200	48.26980	83.98490	-2066.60647	-2145.83371	-1011.31678	1
14748	H	64.00700	49.44380	85.34690	2912.66198	1184.58333	106.71804	1

14749	N	64.98200	47.51680	85.61290	-664.91099	244.64166	-459.03826	1
14750	H	64.97100	46.61780	85.17490	-2236.99295	368.58991	2181.33680	1
14751	C	64.91300	47.44980	86.91190	515.92537	620.47959	-424.59050	1
14752	N	65.22000	46.31280	87.50190	290.27672	-635.12157	-474.37570	1
14753	H	65.23700	45.48880	86.93590	-2931.03971	-12.51396	1143.27417	1
14754	H	64.79200	46.14780	88.39090	-219.68945	1131.84790	2927.26546	1
14755	N	64.55700	48.39180	87.74590	366.70747	732.70913	203.31074	1
14756	H	64.32200	49.30080	87.40390	1717.53574	-1465.36163	2191.12129	1
14757	H	64.48300	48.15980	88.71590	896.89385	606.79751	2953.91341	1
14758	C	68.76300	51.77380	85.17190	-285.50188	631.16787	-592.93069	1
14759	O	68.31700	52.89480	85.38790	455.07951	-469.12633	-443.22720	1
14760	N	69.99200	51.44480	85.66490	3.21938	-338.54617	773.33590	1
14761	H	70.22400	50.48180	85.78290	-2461.25588	946.01213	-1716.24788	1
14762	C	71.03900	52.33780	86.14090	-581.44329	507.81909	485.27773	1
14763	H	70.60600	52.99280	86.88290	-1990.57360	-1242.27221	-2095.85370	1
14764	C	72.06500	51.49980	86.96290	573.91930	-554.52735	441.09757	1
14765	H	72.56500	50.79680	86.26290	-1932.81945	2229.60763	-1091.46003	1
14766	H	71.46100	50.99980	87.75090	560.37078	3084.03253	-270.10028	1
14767	C	73.17300	52.34480	87.63990	60.06995	701.82141	-579.04172	1
14768	H	73.64300	52.97080	86.85090	1255.68737	-183.46375	2878.85681	1
14769	H	74.04000	51.75980	88.01390	319.95097	2014.62973	2395.22956	1
14770	C	72.66500	53.24480	88.79790	-478.15527	563.67583	533.93642	1
14771	H	72.29600	54.16380	88.29490	-1899.60117	-2176.04413	1246.82540	1
14772	H	71.81600	52.78380	89.34490	-611.93222	2480.08668	-1836.55526	1
14773	C	73.72900	53.65480	89.76990	779.41680	-154.22984	447.40765	1
14774	H	74.54200	54.24280	89.29390	-2182.45431	-1070.66177	1997.19874	1
14775	H	74.15700	52.71680	90.18490	-258.53165	184.47061	3130.07319	1
14776	N	73.08500	54.51480	90.80690	-312.61414	-447.45925	643.99139	1
14777	H	72.42900	53.95380	91.38690	1690.89145	-1863.86110	-1888.15628	1
14778	H	72.53100	55.23180	90.29690	245.16499	3099.80847	478.86093	1
14779	H	73.73600	55.06480	91.40390	2155.19886	-2109.17509	897.06441	1
14780	C	71.68500	53.15880	85.00390	623.75668	-425.37872	-511.30378	1
14781	O	71.94000	54.39380	85.13790	210.32796	-64.02608	758.47877	1
14782	N	72.06400	52.55680	83.85790	-512.68802	-561.07426	367.44925	1
14783	H	72.02800	51.56080	83.83890	-1340.09802	-2231.07034	-1767.67889	1
14784	C	72.45900	53.18580	82.59290	272.44450	717.63508	492.16348	1
14785	H	73.31700	53.82280	82.75190	-2566.36552	740.82608	-1662.27885	1
14786	C	72.73700	52.17980	81.49090	-525.34461	-458.00046	587.96226	1
14787	H	73.16400	52.69180	80.60190	-869.76759	-2305.19100	-1956.48282	1
14788	H	73.43100	51.39180	81.85490	1353.06864	498.04678	-2796.31559	1
14789	H	71.81100	51.66480	81.15690	-241.38724	2448.10649	-1961.30901	1
14790	C	71.42300	54.10280	82.09390	-689.97708	-585.91715	109.92600	1
14791	O	71.72400	55.20980	81.62890	-552.83839	-246.67264	507.09915	1
14792	N	70.15100	53.68580	82.18190	-342.29331	458.75259	-620.52691	1
14793	H	69.93300	52.74080	82.41190	-2053.05600	-911.11173	2202.96680	1
14794	C	69.05200	54.61880	81.81290	-661.84217	377.23300	501.10998	1
14795	H	69.27300	54.93580	80.80490	2243.27517	930.64832	-1999.95911	1
14796	C	67.72000	53.76380	81.88590	639.20273	-551.70776	344.22291	1
14797	H	67.86000	52.87180	81.23890	-2063.73426	-2288.81104	632.90689	1
14798	H	67.52600	53.54180	82.95690	-1559.68592	-2705.88566	379.19502	1
14799	C	66.42000	54.44080	81.37090	430.20625	-46.35091	-802.63639	1
14800	H	66.26400	55.30580	82.05090	-681.97645	-583.37952	3015.42744	1
14801	C	66.51600	54.88780	79.91790	-173.14037	-434.96732	782.48121	1
14802	H	67.34800	55.61980	79.84090	-803.72996	-2374.21637	-1901.40501	1
14803	H	66.83700	54.05780	79.25390	1898.90846	2069.68757	-1417.30952	1
14804	H	65.61300	55.35880	79.47290	-1667.41036	-79.12497	2666.77861	1
14805	C	65.08700	53.64980	81.60090	-731.35607	301.24535	-453.67448	1
14806	H	64.19400	54.26480	81.35690	-2511.54906	1572.20663	1057.59817	1
14807	H	65.13500	52.68680	81.04990	-595.74175	-3073.77495	-308.58642	1
14808	H	65.04700	53.31080	82.65790	-2822.71283	-1352.70024	317.36508	1
14809	C	68.94000	55.86580	82.65390	-70.47272	-828.70885	373.79973	1
14810	O	68.94800	56.97480	82.06590	-446.80757	137.32904	636.49899	1

14811	N	68.95500	55.70480	84.03490	279.57794	-554.94538	571.44036	1
14812	H	68.90000	54.78480	84.41390	1046.08587	-532.20686	2919.02149	1
14813	C	69.01700	56.76980	84.97390	-534.55167	-434.10288	597.71247	1
14814	H	68.18000	57.41880	84.76190	-1645.94003	-1799.36271	-1987.81324	1
14815	C	68.98700	56.10080	86.37390	385.92827	769.98546	-299.38731	1
14816	H	67.97000	55.65380	86.34790	1889.06635	1409.96097	2083.66615	1
14817	H	69.84200	55.41280	86.55090	-1619.21534	815.70040	2571.18664	1
14818	C	69.01600	57.12980	87.55390	-623.59984	585.04799	316.69085	1
14819	H	68.64300	58.10980	87.18590	2090.21703	-1164.78809	-2042.66681	1
14820	H	70.04000	57.51080	87.75690	2155.28233	1395.29939	-1818.27499	1
14821	C	68.28500	56.64680	88.80690	-56.65648	-649.82734	-637.15420	1
14822	H	67.27800	56.32580	88.46590	-516.46076	-2477.12087	-1869.58998	1
14823	H	68.78000	55.77180	89.27990	-2708.29037	-130.47564	1595.73357	1
14824	C	68.18300	57.76180	89.88990	-301.37460	-720.47852	470.67511	1
14825	H	67.70500	58.60680	89.34890	-1411.07974	-1846.54891	2120.69265	1
14826	H	69.18300	58.07080	90.26390	2505.33603	-21.34407	1902.90884	1
14827	N	67.28600	57.24180	90.94090	-427.52308	-725.09425	-64.30115	1
14828	H	67.23400	57.85680	91.77790	-2217.36352	404.32433	-2195.00503	1
14829	H	66.34800	56.94180	90.60490	2024.90662	1892.46171	-1488.81432	1
14830	H	67.76700	56.37380	91.25190	2451.35277	-664.42586	1856.78058	1
14831	C	70.26400	57.65280	84.87290	243.27956	-474.74816	-739.51352	1
14832	O	70.14300	58.87780	84.98790	-350.36558	642.74227	-296.23228	1
14833	N	71.49100	57.15780	84.71690	525.38516	-576.92895	322.17342	1
14834	H	71.63100	56.17080	84.69590	192.96560	-1746.91109	-2609.46204	1
14835	C	72.71900	57.94580	84.52690	-330.22362	621.77168	579.48541	1
14836	H	72.79500	58.56780	85.40690	-1952.93453	2422.54589	-464.26757	1
14837	C	74.01800	57.10780	84.51390	-88.98608	856.89754	298.76258	1
14838	H	74.13900	56.57280	83.54790	1097.55944	-2284.88143	-1863.57355	1
14839	O	74.08600	56.29880	85.65490	-367.30544	-694.24777	82.06081	1
14840	H	73.52300	55.52680	85.55590	2455.66144	-868.21927	-1764.69500	1
14841	C	75.19200	58.07780	84.76890	20.29836	-909.46653	-62.52683	1
14842	H	75.21200	58.81580	83.93790	3118.96169	66.95838	-407.21098	1
14843	H	76.17100	57.55180	84.75690	2081.85373	-2327.17554	-385.18214	1
14844	H	75.14700	58.74180	85.65790	1243.13381	322.57344	-2872.07085	1
14845	C	72.59200	58.81480	83.22690	-330.46249	261.44679	-808.63534	1
14846	O	73.01500	59.98280	83.18890	-340.56796	-20.52919	-712.19326	1
14847	N	72.00200	58.27580	82.17390	268.31858	-474.22387	-644.81715	1
14848	H	71.78800	57.30480	82.23390	1714.59334	745.53730	-2530.33002	1
14849	C	71.67800	58.96180	80.92490	197.77714	-849.81669	-264.85240	1
14850	H	72.62500	59.27280	80.50790	164.43913	870.78194	3018.76213	1
14851	C	71.09500	58.12480	79.80190	-407.85511	-507.48595	-638.40678	1
14852	H	70.05700	57.80880	80.03990	-2605.82938	1041.61792	1422.29096	1
14853	O	71.89200	56.91180	79.71290	480.89195	457.24105	428.13641	1
14854	H	71.56000	56.30780	80.38190	-2278.15747	2128.42482	-421.93905	1
14855	C	71.17200	58.81080	78.46790	509.30657	20.67635	756.06237	1
14856	H	72.19700	59.09080	78.14290	1932.07419	920.80895	2305.95456	1
14857	H	70.51100	59.70180	78.53390	-407.85607	3061.21716	600.69058	1
14858	H	70.87600	58.20880	77.58290	637.30372	-1572.87634	-2649.17538	1
14859	C	70.83300	60.20580	81.08790	-909.86007	-35.78903	-48.21613	1
14860	O	71.24500	61.35880	80.80990	298.18598	-476.17007	554.95443	1
14861	N	69.70300	59.95480	81.76090	-226.13355	-415.64329	699.12557	1
14862	H	69.43500	59.01180	81.94290	-1315.49295	1570.02918	2388.03537	1
14863	C	68.79200	60.93480	82.26090	-456.02518	37.45616	-788.72624	1
14864	H	68.27700	61.41580	81.44290	-286.12146	1164.47398	2908.66999	1
14865	C	67.64800	60.18880	82.90290	570.37181	-682.81244	-199.73525	1
14866	H	68.05500	59.43180	83.60690	-1276.19407	2174.53921	1881.73700	1
14867	C	66.77000	61.10180	83.78390	326.57539	660.06675	-537.69081	1
14868	H	65.86900	60.56480	84.14890	2409.09134	642.70293	1918.70740	1
14869	H	66.36600	61.97780	83.23390	-1844.74327	2366.54682	-945.83543	1
14870	H	67.30500	61.44380	84.69590	-2707.66627	1602.04970	-14.36530	1
14871	C	66.87700	59.43380	81.79990	-552.19502	-579.97955	-436.06809	1
14872	H	65.98800	58.91880	82.22390	1821.96405	-2564.38861	50.83576	1

14873	H	67.56900	58.76680	81.24290	2706.18772	-1097.80482	-1170.29860	1
14874	H	66.48400	60.21480	81.11490	1610.79832	-15.96195	-2702.46188	1
14875	C	69.33700	61.96280	83.14390	171.94929	749.49115	-490.04842	1
14876	O	69.12900	63.14880	82.91090	-217.41480	-646.23898	398.41338	1
14877	N	70.16800	61.60980	84.15190	639.72837	-179.72673	520.69012	1
14878	H	70.42600	60.68180	84.41090	574.47676	-1720.67927	2570.49908	1
14879	C	70.81100	62.52780	85.05990	765.64765	-88.77459	487.18964	1
14880	H	70.02500	63.10980	85.51790	-1690.19238	-1785.53545	-1962.99238	1
14881	C	71.57800	61.78180	86.15290	-646.68575	67.45467	639.29524	1
14882	H	72.12500	60.95180	85.65690	-2582.64648	1101.73039	-1419.27923	1
14883	C	72.63700	62.69880	86.91090	509.85807	454.90297	-603.78725	1
14884	H	73.14200	62.11380	87.70790	-1397.43705	-1333.21994	2483.52985	1
14885	H	72.14800	63.58180	87.37590	-35.65275	3117.99305	-418.41898	1
14886	H	73.44600	62.89480	86.17490	-1420.38108	-1983.24603	-1986.82636	1
14887	C	70.63500	61.17080	87.20590	553.34893	534.02336	489.97451	1
14888	H	69.64800	60.89180	86.77890	-1578.04832	140.24373	2718.14669	1
14889	H	70.45800	61.96580	87.96190	2868.32007	896.40040	931.36058	1
14890	C	71.26700	59.95680	87.91890	85.39618	-811.05417	-407.85981	1
14891	H	70.48700	59.54080	88.59190	-1870.51271	-1676.22946	-1894.64066	1
14892	H	71.59500	59.21580	87.15890	-1924.64270	-1979.66680	1508.27586	1
14893	H	72.13800	60.22880	88.55390	-2473.46250	-76.71059	1942.76220	1
14894	C	71.66200	63.52580	84.35490	438.07441	633.69871	-487.81940	1
14895	O	71.52800	64.71780	84.59990	-443.34025	-349.46283	552.22494	1
14896	N	72.44000	63.06280	83.35390	-624.40211	557.05801	-111.71691	1
14897	H	72.41000	62.08380	83.16990	386.38993	-135.32627	3119.39351	1
14898	C	73.23300	63.90780	82.52590	365.35043	-426.39720	718.43962	1
14899	H	73.88400	64.42880	83.21190	550.96647	1392.34146	2766.95635	1
14900	C	74.22100	63.07780	81.65290	-146.04760	808.90844	-394.70019	1
14901	H	73.76600	62.28180	81.02690	-2505.44589	-11.68796	1902.84800	1
14902	H	74.79000	62.50380	82.41590	2273.04631	-1218.22742	1802.05678	1
14903	C	75.19500	63.90380	80.72890	-542.81902	264.10424	683.40871	1
14904	H	74.55500	64.48980	80.03390	-767.21379	2580.81773	1627.57152	1
14905	C	76.09000	64.93880	81.32490	14.20169	-878.17541	-245.06582	1
14906	H	76.90300	64.44380	81.89790	1439.76558	-2322.83709	1558.75886	1
14907	H	75.62900	65.65480	82.03890	-739.09741	2217.17861	2106.20043	1
14908	H	76.67100	65.48180	80.54890	-1948.68896	-2390.62720	621.07902	1
14909	C	76.03300	62.90280	79.89590	-458.99115	-255.15187	745.43655	1
14910	H	76.48300	62.22980	80.65690	2600.30754	1525.48479	-899.73501	1
14911	H	76.84200	63.38880	79.30890	1497.07460	-1397.33276	2388.40010	1
14912	H	75.43400	62.30680	79.17490	2301.56355	-2144.06834	-63.26486	1
14913	C	72.43700	64.90980	81.66490	-222.19629	779.00499	418.60606	1
14914	O	72.81300	66.08780	81.57690	-433.56174	-600.34748	-274.28881	1
14915	N	71.36300	64.44380	80.99590	-324.41239	573.49571	527.76089	1
14916	H	71.19000	63.46780	81.10790	1198.28039	1442.96826	2525.90438	1
14917	C	70.42600	65.14580	80.24290	-623.76666	556.66821	363.98716	1
14918	H	71.03900	65.71780	79.56190	-2613.07726	-1465.26358	-960.75809	1
14919	C	69.50000	64.18580	79.47790	248.39544	-8.29385	877.31518	1
14920	H	69.27400	63.33580	80.15590	17.57965	1064.64299	-2960.48180	1
14921	C	68.14600	64.84580	79.02290	719.99373	-206.78992	-519.90188	1
14922	H	67.51200	65.16380	79.87790	860.76847	-3026.02063	22.42768	1
14923	H	67.58600	64.15180	78.35890	-522.75864	2584.60160	-1716.03735	1
14924	H	68.45800	65.75480	78.46590	-660.30959	-2856.39409	1141.59112	1
14925	C	70.28000	63.43880	78.39190	-471.10765	-680.19178	383.20717	1
14926	H	70.44600	64.25280	77.65390	-148.63059	2023.65396	-2404.36266	1
14927	H	71.27200	63.03780	78.69290	-1939.54892	2067.38678	-1364.65679	1
14928	C	69.41000	62.39680	77.58790	27.87344	617.60138	670.25563	1
14929	H	68.96100	61.73580	78.35990	-2867.19630	554.91047	-1170.25039	1
14930	H	68.57700	62.83380	76.99690	977.52840	-2604.20158	1469.96550	1
14931	H	70.16900	61.86880	76.97190	-1503.18671	-2078.04153	-1822.19629	1
14932	C	69.70600	66.19980	80.98090	615.56666	-32.45129	-671.91935	1
14933	O	69.55800	67.36380	80.51690	444.73037	316.86583	570.47189	1
14934	N	69.14000	65.92480	82.22190	-560.34921	575.99168	258.67863	1

14935	H	69.22700	64.99080	82.55990	-2543.67384	-1684.65722	-768.03624	1
14936	C	68.75000	66.92180	83.19690	-549.25090	-557.48047	467.96364	1
14937	H	67.89500	67.41080	82.75390	-1202.66214	2108.85369	2001.14120	1
14938	C	68.34200	66.10180	84.47590	406.38210	-489.19738	653.44511	1
14939	H	68.06800	66.67780	85.38590	743.46099	-750.85036	-2963.39598	1
14940	H	69.24300	65.50480	84.73090	-2010.00971	-2073.72596	-1248.09769	1
14941	C	67.11800	65.15880	84.29590	-81.02934	-73.17877	-905.27903	1
14942	H	67.27600	64.54180	83.38490	-1070.74360	-2563.83302	-1475.97244	1
14943	C	67.17400	64.17980	85.52090	463.14448	-513.33840	-594.50137	1
14944	H	66.20600	63.64480	85.41390	2399.23451	1929.74753	-646.50944	1
14945	H	67.27400	64.75380	86.46590	-2867.84577	1245.42519	-350.14706	1
14946	H	68.06800	63.52580	85.43190	1296.50617	-786.12915	-2756.68260	1
14947	C	65.84000	65.91780	84.21390	870.64524	268.71178	-34.95503	1
14948	H	65.86700	66.56680	83.31290	2138.08734	-2069.27399	-1022.21029	1
14949	H	64.97100	65.22780	84.18490	2231.15667	-824.78726	-2059.09983	1
14950	H	65.68500	66.60280	85.07490	-1727.56287	-1803.47867	-1913.43080	1
14951	C	69.78900	67.93480	83.58990	-666.59651	591.10016	-194.16668	1
14952	O	69.52000	69.15080	83.59590	-327.14884	-500.18694	516.15297	1
14953	N	71.02500	67.45980	83.92190	-668.40418	452.16205	-247.90648	1
14954	H	71.29900	66.50280	83.86090	1266.76997	2405.96981	1582.66527	1
14955	C	72.04000	68.25880	84.44690	15.43303	422.10510	808.10897	1
14956	H	71.72900	68.65180	85.40390	-1702.36420	688.91380	2554.52151	1
14957	C	73.35000	67.44380	84.73490	-744.59771	-367.26277	377.01897	1
14958	H	74.10400	68.14980	85.14490	2988.90615	-697.01464	-691.98039	1
14959	H	73.20500	66.70780	85.55390	-703.87624	-2780.78880	1292.28406	1
14960	H	73.77200	66.98480	83.81490	2028.40491	-2216.74908	932.64316	1
14961	C	72.37500	69.33780	83.44090	-762.43527	-335.32620	-371.07923	1
14962	O	72.35400	70.52480	83.71590	535.09965	467.64694	344.38631	1
14963	N	72.52600	68.93380	82.15690	567.82762	-253.64860	570.88218	1
14964	H	72.48400	67.96680	81.91890	-311.17023	2478.09920	-1913.22338	1
14965	C	72.88600	69.73780	81.06290	281.76155	528.84857	-687.29951	1
14966	H	73.82700	70.20980	81.30690	-2876.31137	100.50283	-1270.81010	1
14967	C	73.15900	68.74380	79.88290	38.65303	903.87174	-113.89831	1
14968	H	72.24600	68.13780	79.70290	2003.80494	-786.29881	-2294.49911	1
14969	H	74.00200	68.08380	80.18090	-1457.38086	2589.07619	-1034.86797	1
14970	C	73.42400	69.35880	78.57890	807.67268	-421.78101	-34.88021	1
14971	C	74.73300	69.62180	78.20490	-887.19590	-172.55521	120.66125	1
14972	H	75.61300	69.41980	78.79790	514.38192	-2657.95822	1602.77746	1
14973	C	74.94800	70.16980	76.88990	506.85242	-148.00777	743.40119	1
14974	H	75.94500	70.40780	76.54990	-2057.27705	-762.85986	-2254.74659	1
14975	C	73.86900	70.43680	76.05490	-115.11739	-903.73521	-38.23159	1
14976	H	74.11800	70.79380	75.06590	-810.10216	2960.38401	-691.43851	1
14977	C	72.34100	69.62080	77.69590	-637.40370	-2.52272	-652.04384	1
14978	H	71.31700	69.47980	78.01090	-913.71889	1686.08332	2494.08641	1
14979	C	72.56000	70.16080	76.43590	-547.91257	-660.70685	-307.74874	1
14980	H	71.70500	70.39580	75.81990	-2798.21263	423.81403	1374.26851	1
14981	C	71.85900	70.76280	80.73490	361.91530	-606.37613	-576.86767	1
14982	O	72.02600	71.98080	80.52490	251.12941	291.83528	689.48779	1
14983	N	70.56600	70.38080	80.67190	-574.94779	539.68619	-301.40694	1
14984	H	70.32800	69.41380	80.71090	1729.56689	2048.77939	-1646.00352	1
14985	C	69.44000	71.27380	80.50690	-831.09200	347.37310	-141.66520	1
14986	H	69.51600	71.89380	79.62590	-663.10323	-2419.00002	-1899.19963	1
14987	C	68.15900	70.43480	80.33790	507.21461	-180.16149	736.02051	1
14988	H	67.91400	69.83780	81.24290	-1462.49686	1425.98534	2392.88424	1
14989	H	68.37400	69.74180	79.49790	1822.66047	2229.26481	-1267.48312	1
14990	C	66.92100	71.17580	80.05790	-383.58289	-227.95308	-795.20599	1
14991	C	66.57200	71.44880	78.74590	-795.50275	442.43117	-53.67529	1
14992	H	67.31800	71.24980	77.98990	982.27208	1484.92119	2593.91150	1
14993	C	65.36200	72.05980	78.40290	-424.62679	560.01409	-580.97100	1
14994	H	65.06300	72.19480	77.37390	2881.47047	177.74285	1250.50455	1
14995	C	64.52500	72.43380	79.47390	287.06335	-522.43045	690.00874	1
14996	H	63.62600	73.01480	79.32790	-1612.45005	2071.34543	1734.28924	1

14997	C	66.02700	71.52980	81.08290	-416.92943	-447.70391	676.15239	1
14998	H	66.30100	71.35380	82.11290	-3035.20177	-817.83505	-130.08575	1
14999	C	64.89600	72.27080	80.79890	306.78485	561.44746	-649.70055	1
15000	H	64.14400	72.56780	81.51590	2267.31498	-343.02556	-2154.02936	1
15001	C	69.33500	72.26180	81.71990	787.55063	-102.23205	-448.06654	1
15002	O	69.08000	73.41680	81.52690	-372.56696	694.58838	48.66286	1
15003	N	69.63000	71.85980	82.96790	433.03109	-325.42850	647.49722	1
15004	H	69.70200	70.91080	83.26390	-1650.72846	-2672.16063	-181.32662	1
15005	C	69.74000	72.75980	84.02890	-875.54912	-117.10418	-226.16667	1
15006	H	68.80600	73.27580	84.19490	2218.07323	-1064.37813	1960.98867	1
15007	C	69.97200	71.99480	85.34890	-255.79290	521.70126	702.74376	1
15008	H	69.16700	71.24180	85.48590	1967.09899	1790.97782	-1679.62681	1
15009	H	70.95100	71.47480	85.41890	-258.16526	-3132.40923	-139.96202	1
15010	H	69.93600	72.73580	86.17590	-1650.24808	1788.44499	1994.08426	1
15011	C	70.81600	73.85580	83.78590	299.93807	614.64045	603.07982	1
15012	O	70.62400	75.02280	84.15090	-635.12172	-331.96871	-331.72942	1
15013	N	71.92800	73.46580	83.15890	219.79269	688.33212	-436.53449	1
15014	H	71.88900	72.59580	82.67490	-2318.58861	-1320.12745	-1667.22423	1
15015	C	73.00100	74.43080	82.80690	-56.28492	505.89737	-756.53874	1
15016	H	73.28100	74.87180	83.75190	560.35807	-260.08162	3084.89588	1
15017	C	74.19600	73.61780	82.23390	-178.32623	-426.60590	-785.91231	1
15018	H	74.96200	74.36980	81.94790	-90.42995	2301.01560	-2143.68278	1
15019	H	73.88900	73.19180	81.25490	-2496.61376	281.72810	-1893.61433	1
15020	S	74.87400	72.35080	83.38990	-391.10506	304.14548	-256.40390	1
15021	H	73.67600	71.91480	83.75190	2085.04461	-1803.58698	1515.87902	1
15022	C	72.62400	75.52980	81.86190	-616.08198	158.70291	653.22843	1
15023	O	72.81800	76.70480	82.13490	782.67298	-104.30276	13.08299	1
15024	N	71.91800	75.07780	80.72890	-223.12259	-529.41462	-618.55376	1
15025	H	71.92300	74.09580	80.55290	-2078.71397	-2344.42619	-284.32429	1
15026	C	71.54200	75.91280	79.63390	160.71277	284.92917	-851.13911	1
15027	H	72.31800	76.64380	79.46390	687.85511	2637.49308	1571.21349	1
15028	C	71.62200	74.98880	78.37290	-14.87462	-544.45953	-731.29581	1
15029	H	71.04500	75.42080	77.52690	546.99020	792.51684	2995.15359	1
15030	H	71.17500	73.99780	78.60090	1747.68890	-1667.58371	-2015.68209	1
15031	C	73.02200	74.78780	77.81290	67.32814	600.59950	682.78706	1
15032	C	73.70700	73.56580	77.87990	108.14474	662.31673	-617.32671	1
15033	H	73.23900	72.61380	78.08190	2252.51218	599.02628	2113.19251	1
15034	N	74.94100	73.72080	77.23790	664.40130	-435.37845	-285.81253	1
15035	H	75.57100	73.04880	76.91690	-2958.82831	-154.63791	-1058.13439	1
15036	C	75.03800	74.99780	76.86390	318.30645	-448.54322	727.28329	1
15037	C	73.88500	75.72880	77.20590	101.30690	-666.07712	-614.43403	1
15038	C	73.84600	77.15180	77.05090	602.07279	-458.97011	508.23793	1
15039	H	72.96800	77.73480	77.28890	-102.26161	3138.63819	191.62225	1
15040	C	74.99200	77.74080	76.45190	-384.88471	-657.20590	-501.39323	1
15041	H	74.97600	78.77380	76.13690	2077.72398	2362.45752	-9.15197	1
15042	C	76.13500	75.64780	76.26290	273.95214	365.00384	-789.41334	1
15043	H	77.00800	75.08280	75.96990	-1844.42720	-2080.93541	-1471.74127	1
15044	C	76.07400	77.02980	76.04390	265.68115	714.65104	500.13841	1
15045	H	76.95300	77.55880	75.70590	-2227.71763	1240.99214	-1842.67167	1
15046	C	70.21200	76.64580	79.76090	-791.09693	346.49207	292.50624	1
15047	O	70.11700	77.79280	79.22390	-397.74122	-250.32718	634.63805	1
15048	N	69.22300	76.15280	80.47990	-738.81374	392.55939	112.79924	1
15049	H	69.32500	75.27080	80.93290	-2383.06337	1963.14052	604.41252	1
15050	C	67.91700	76.79680	80.50690	-228.98232	-612.60296	635.40201	1
15051	H	67.50100	76.72480	79.51290	-2652.48398	586.45764	1587.01682	1
15052	C	67.04200	75.89380	81.32190	253.12686	-868.38801	-115.23913	1
15053	H	67.50300	75.63980	82.29990	1794.50829	-2443.81903	-840.06832	1
15054	H	67.00500	74.91080	80.80590	2392.61939	1490.38827	1397.26214	1
15055	C	65.64000	76.49380	81.61290	-712.02831	-496.01506	280.06384	1
15056	H	65.63400	77.50380	82.07590	-2855.05416	-392.98280	1261.92571	1
15057	C	64.73900	76.55180	80.32490	-185.66717	-392.15166	801.99488	1
15058	H	64.91700	75.65380	79.69490	2031.57726	-631.98670	2317.65245	1

15059	H	63.67100	76.57880	80.62790	-3050.89579	-760.90833	-106.20553	1
15060	H	64.89500	77.50380	79.77390	1268.44632	2145.45816	1919.96860	1
15061	C	64.90600	75.60280	82.61490	217.91727	481.57359	-743.00063	1
15062	H	65.60700	75.23780	83.39590	-1776.92534	1897.96495	1771.57885	1
15063	H	64.05500	76.15680	83.06690	1742.36489	-1253.92117	-2300.01577	1
15064	H	64.60100	74.61180	82.21590	1329.07292	-1922.97514	2105.69656	1
15065	C	67.88300	78.25880	80.97990	-721.79164	-420.42846	-365.66070	1
15066	O	67.19700	79.02380	80.29190	491.88635	473.02935	397.38934	1
15067	N	68.52100	78.78280	82.02490	-50.66107	833.81815	-121.87301	1
15068	C	69.31500	77.97980	82.97190	-774.94738	288.15534	384.54396	1
15069	H	68.96900	76.92580	83.03290	-430.51626	2323.24255	-2077.36036	1
15070	H	70.36000	78.03480	82.59890	-123.70575	-1711.17270	2637.19759	1
15071	C	68.47200	80.19080	82.39590	123.65519	-846.88794	-314.54923	1
15072	H	67.44000	80.42380	82.61490	-718.05829	-2317.42853	-2003.03358	1
15073	C	69.25900	80.17180	83.75390	-400.17499	590.16441	-568.34580	1
15074	H	68.88300	80.87580	84.52690	2876.13069	1213.09254	393.07118	1
15075	H	70.32300	80.40280	83.53390	1018.20321	2831.75888	-917.94886	1
15076	C	69.11600	78.74880	84.28590	826.15565	200.65177	329.63118	1
15077	H	69.94800	78.54280	84.99390	2720.23055	1575.50067	-127.94379	1
15078	H	68.10900	78.61380	84.73490	1975.53506	-1680.30383	1781.02962	1
15079	C	69.05500	81.12380	81.23090	627.27813	121.76532	650.49701	1
15080	O	68.57200	82.24780	81.04590	358.18926	669.48263	217.07301	1
15081	N	70.09900	80.67380	80.54090	-757.99160	-237.76688	285.63601	1
15082	H	70.39500	79.77580	80.85690	1831.42459	-1978.30896	-1621.85199	1
15083	C	70.60700	81.42980	79.40390	-215.14607	876.68391	128.79633	1
15084	H	70.77000	82.44380	79.73990	-1946.65767	-2362.23219	727.05515	1
15085	C	71.94100	80.76680	78.92290	439.12220	-738.99675	-304.14882	1
15086	H	71.86800	79.65880	78.87490	1433.13192	865.53009	-2663.68481	1
15087	H	72.71000	80.96280	79.70090	2497.91656	-1128.30750	1544.52622	1
15088	C	72.44600	81.21980	77.54890	551.45682	363.65370	-628.57169	1
15089	C	73.03200	82.49780	77.40790	126.03326	887.00283	-169.68381	1
15090	H	73.19700	83.12680	78.26990	2997.77976	-929.91023	-216.35544	1
15091	C	73.38000	82.91680	76.12890	-268.62169	687.00284	536.02284	1
15092	H	73.80300	83.90780	76.04790	286.85084	3044.91548	737.85674	1
15093	C	73.21100	82.08580	74.99290	-484.43244	-749.27995	188.03130	1
15094	O	73.66500	82.54480	73.75290	658.54087	-314.36535	-301.87013	1
15095	H	74.19700	83.33680	73.85990	-741.21548	2282.44509	2034.51966	1
15096	C	72.14500	80.45680	76.39290	-380.39147	-828.65090	-9.54060	1
15097	H	71.53000	79.57280	76.46990	-237.42891	-3112.42521	-393.27223	1
15098	C	72.59800	80.86680	75.14790	360.82114	-783.09724	-296.67797	1
15099	H	72.46700	80.20280	74.30690	2569.56100	-1632.10586	-794.86662	1
15100	C	69.60500	81.53480	78.26890	-278.55029	-734.90649	462.35613	1
15101	O	69.34000	82.63880	77.79490	698.00129	-336.44272	152.40644	1
15102	N	68.89900	80.39980	77.87590	717.85149	441.77882	46.82945	1
15103	H	69.15900	79.51980	78.26490	-1642.63553	-2014.54850	-1772.44720	1
15104	C	67.79400	80.35980	76.99690	794.35812	-98.70473	-436.69619	1
15105	H	68.02800	80.90180	76.09190	-809.75792	-1680.34789	-2533.56455	1
15106	C	67.37900	78.88380	76.66290	784.30748	152.04994	-439.53793	1
15107	H	67.35800	78.20080	77.53890	2473.25549	1467.80879	1275.44927	1
15108	H	66.31400	78.74980	76.37590	1805.91656	-974.83447	-2384.65707	1
15109	C	68.31100	78.32080	75.65290	-698.59298	500.17537	-305.35791	1
15110	C	68.11000	78.68280	74.28590	540.67500	540.67818	-496.77827	1
15111	H	67.23800	79.29980	74.12290	1016.32147	2082.23211	2128.29188	1
15112	C	68.99100	78.15880	73.25190	212.00214	-690.14627	556.95980	1
15113	H	68.92600	78.57780	72.25790	-1771.57840	-172.91884	2594.19260	1
15114	C	69.92600	77.15880	73.58790	-488.10877	111.40820	762.09517	1
15115	O	70.77300	76.70680	72.57590	624.88106	256.11046	-409.33888	1
15116	H	70.57700	77.24380	71.80390	-2369.74769	-1734.43725	1128.82661	1
15117	C	69.24800	77.30080	75.92290	399.94764	-446.97378	686.80953	1
15118	H	69.32500	76.81380	76.88390	2438.68726	1984.75587	-108.51194	1
15119	C	70.03300	76.73280	74.90990	274.87732	481.77146	-723.73318	1
15120	H	70.81500	76.02580	75.14390	1698.21567	2136.86009	1564.64652	1

15121	C	66.60900	81.16880	77.39390	-503.59349	535.04360	539.97494	1
15122	O	66.03000	81.91280	76.59390	-555.71653	-31.06093	-560.21566	1
15123	N	66.26200	81.14380	78.69490	-423.91051	460.76442	-566.27583	1
15124	H	66.72900	80.59280	79.38290	231.56496	-420.20322	-3109.34610	1
15125	C	65.22400	82.07880	79.20490	673.00490	-614.10019	-37.36801	1
15126	H	64.38800	81.88480	78.54990	-2063.42445	-1517.23627	-1827.15623	1
15127	C	64.68300	81.72780	80.60790	-832.15514	-43.89968	-370.19135	1
15128	H	65.60700	81.77480	81.22190	-1925.12662	1278.53341	2134.82225	1
15129	C	63.60600	82.80080	81.01090	505.36527	-397.43725	646.60697	1
15130	H	62.70300	82.86080	80.36690	-2007.05635	1127.90983	2144.24123	1
15131	H	63.25600	82.57980	82.04190	-2206.49127	-827.25388	2084.53196	1
15132	H	64.00900	83.83280	81.09290	-2810.47507	-735.62911	-1207.60337	1
15133	C	64.11400	80.29080	80.63890	612.56915	-593.56585	322.31913	1
15134	H	63.25500	80.13980	79.95190	2849.58568	596.58090	-1192.55142	1
15135	H	64.84000	79.61680	80.13490	-1849.77837	-2543.24136	-92.03029	1
15136	C	63.65900	79.83980	81.99690	532.32684	449.11009	-588.53994	1
15137	H	64.50200	79.89380	82.71890	2476.88810	-656.72205	-1825.36783	1
15138	H	63.43900	78.75180	81.95090	2383.43696	-183.50493	2045.42916	1
15139	H	62.80200	80.44580	82.35890	-734.01996	2926.88786	890.37542	1
15140	C	65.58000	83.61280	79.03390	-662.43462	-189.91493	597.12955	1
15141	O	64.77400	84.26080	78.37690	-448.56273	-99.99674	642.19884	1
15142	N	66.82900	84.06580	79.36490	-665.14497	222.68035	-469.75304	1
15143	H	67.45400	83.43180	79.81190	-2950.53399	-175.34435	1077.88206	1
15144	C	67.30383	85.37166	79.00321	-70.28142	653.88680	-269.41389	1
15145	H	66.76273	86.09454	79.63529	-2143.42259	1.89083	1965.59452	1
15146	H	68.39850	85.39292	79.41026	27.86315	-2851.45878	841.36129	1
15147	C	67.17405	85.77957	77.45987	-177.94703	-99.09072	287.17896	1
15148	O	66.81087	86.87901	77.18224	-482.22246	578.01194	720.98514	1
15149	N	67.89100	84.89680	76.61290	356.73523	-663.28731	381.39508	1
15150	H	68.32900	84.14080	77.09390	888.15468	2662.37180	1421.68347	1
15151	C	67.82524	85.10631	75.17263	506.91651	454.88670	204.47504	1
15152	H	68.20599	86.15258	74.95940	1866.42450	418.79333	123.18792	1
15153	C	68.53600	83.92580	74.53290	-676.89647	-545.29416	-275.52940	1
15154	H	68.10500	82.98380	74.93690	-1566.49989	1817.76903	-2034.70393	1
15155	C	68.34900	83.93880	73.05490	-859.83284	287.47088	97.46273	1
15156	H	67.38300	83.53880	72.67890	559.45597	-3034.42126	614.42889	1
15157	H	68.68700	84.91880	72.65490	-2379.23533	1914.79470	755.66312	1
15158	H	69.02400	83.17980	72.60690	2573.12642	-623.55059	-1699.53856	1
15159	C	70.05800	83.94780	74.75490	-859.47197	15.31935	304.17799	1
15160	H	70.56200	83.01280	74.42890	-557.06634	2791.46622	1340.00734	1
15161	H	70.17300	83.76380	75.84390	1858.38971	1313.36782	-2172.48219	1
15162	C	70.72899	85.31468	74.33884	382.15411	-205.37208	-616.18146	1
15163	H	70.14094	86.09695	74.81557	1338.79562	-895.23147	1034.17896	1
15164	H	71.74469	85.44374	74.76151	-1230.30921	-2208.92273	-885.58789	1
15165	H	70.75153	85.50756	73.27866	-1331.13081	-1992.30762	1829.43167	1
15166	C	66.26897	85.22469	74.66566	-231.61022	-13.16659	59.68676	1
15167	O	66.07171	86.07418	73.77530	567.96435	-10.10846	-357.06394	1
15168	N	65.47600	84.30180	75.09290	-415.11655	435.25446	-592.37158	1
15169	H	65.70400	83.60980	75.77290	-77.01283	-2431.77744	1994.68136	1
15170	C	64.05600	84.33580	74.67990	-310.60242	222.51014	-827.92897	1
15171	H	64.10600	84.16680	73.61490	-2580.20351	-1213.99403	-1329.28347	1
15172	C	63.18100	83.19080	75.19690	304.73127	-482.89879	710.91393	1
15173	H	62.22600	83.07180	74.64190	2747.40308	654.17390	1386.38344	1
15174	H	63.77500	82.27180	75.00590	524.28411	-1982.39564	-2386.09722	1
15175	O	62.80900	83.14980	76.55590	289.23783	159.36988	717.33531	1
15176	H	63.47300	83.61580	77.06990	2995.73456	32.18442	-960.60649	1
15177	C	63.32316	85.73722	75.10167	-451.70506	598.13246	-489.41847	1
15178	O	62.39570	86.08161	74.34486	-1.13636	-267.43065	-234.90064	1
15179	N	63.79069	86.38467	76.13713	-62.38843	-81.57369	855.78473	1
15180	H	64.51948	85.97386	76.65445	647.01429	1592.66552	-909.66416	1
15181	C	63.42492	87.70011	76.43223	376.88077	-398.30170	-147.66734	1
15182	H	62.35410	87.64803	76.13683	199.59375	1469.14172	3151.54694	1

15183	C	63.94576	87.95331	77.97285	226.52320	1824.87398	721.07949	1
15184	H	64.61269	87.11249	78.34924	-870.22335	-2485.20361	-1739.20406	1
15185	C	65.02598	89.10684	78.17954	274.70409	37.23329	-327.24181	1
15186	H	65.99987	88.91381	77.65083	-1037.35946	939.45709	-3126.03971	1
15187	H	65.28578	89.31312	79.28109	-922.27808	-3671.46271	-824.96466	1
15188	H	64.55965	90.06420	77.75983	522.86165	1644.51195	-1897.09334	1
15189	C	62.76613	88.20671	78.93606	197.99332	308.95583	207.86632	1
15190	H	61.78247	88.35910	78.46295	1440.60956	1283.49414	831.03810	1
15191	H	63.12047	88.97116	79.62045	-160.39045	-1123.57756	-1097.39004	1
15192	C	62.73504	86.85039	79.69990	153.86989	-344.80607	417.17489	1
15193	H	63.70480	86.34664	79.69268	-3550.95509	-1258.35936	-718.17780	1
15194	H	62.40582	86.92622	80.76631	-1564.58707	5116.84186	900.55802	1
15195	H	62.04047	86.16155	79.14593	56.10803	494.64655	-2895.01910	1
15196	C	64.23291	88.70222	75.40989	-790.19378	475.98117	-236.60188	1
15197	O	63.81908	89.81273	75.19776	-555.12160	-49.72273	-431.17487	1
15198	N	65.39731	88.20280	74.99301	892.52587	132.44543	-39.38178	1
15199	H	65.72201	87.32529	75.39087	-1196.83438	995.53673	1486.52419	1
15200	C	66.15048	88.72623	73.85193	-123.61859	234.70199	-756.33164	1
15201	H	66.20803	89.79415	74.20384	2732.59001	-2396.24257	-840.62635	1
15202	C	67.61236	88.11399	73.73548	523.64981	572.19577	932.40377	1
15203	H	67.73647	87.31746	72.92226	-168.85797	565.08145	-1757.86138	1
15204	H	67.79477	87.52232	74.64482	-341.12011	-2108.72751	2100.32358	1
15205	C	68.74333	89.22708	73.55406	-203.36941	-177.54824	36.54590	1
15206	O	69.87312	88.77760	73.95449	700.75900	928.05014	-12.01109	1
15207	O	68.48226	90.42603	73.32495	812.33904	-211.98573	181.29939	1
15208	C	65.18777	88.58645	72.57295	229.31073	-876.60888	-244.75422	1
15209	O	65.30030	89.45579	71.65655	301.56682	-66.65163	264.00047	1
15210	N	64.50231	87.45900	72.54980	-122.79536	164.36436	116.43581	1
15211	H	64.52175	86.80618	73.39020	-1244.57844	722.86462	1507.97518	1
15212	C	63.96189	87.03817	71.30324	-140.21598	244.77644	549.22460	1
15213	H	64.56463	87.32305	70.51375	585.18662	-3290.37265	-26.65414	1
15214	C	63.71535	85.48150	71.45673	375.76732	655.41396	72.32220	1
15215	H	62.91859	85.45195	72.22507	-1265.84220	2854.86769	1959.05570	1
15216	H	63.15554	85.24151	70.52508	448.42476	-357.94650	1582.37696	1
15217	O	64.86565	84.66944	71.69913	-67.15522	940.95992	633.30689	1
15218	H	65.27264	85.17579	72.48313	-2105.35522	-2421.38806	1499.67618	1
15219	C	62.48725	87.83214	71.04823	0.67966	-674.98743	582.94846	1
15220	O	62.30217	88.35339	69.98113	375.59391	-295.31093	-659.79508	1
15221	N	61.85239	87.89036	72.21792	79.37033	-546.97609	-556.71858	1
15222	H	62.25032	87.38953	73.00220	-3388.12526	1242.75630	-3129.71737	1
15223	C	60.80495	88.86185	72.42694	177.53649	-12.99871	-69.38844	1
15224	H	60.08442	88.79312	71.58891	-778.45983	403.48158	-3106.72230	1
15225	C	60.18730	88.58602	73.87045	390.84176	-186.36632	545.85527	1
15226	H	59.22436	89.16554	74.11419	-364.74975	390.18261	-3784.25915	1
15227	H	61.02135	88.77451	74.61514	1135.03391	283.30534	-25.00369	1
15228	C	59.75254	87.11705	73.95743	1163.74495	-847.87624	-895.97677	1
15229	C	59.42539	86.24229	72.86990	275.67872	615.23972	702.80102	1
15230	H	59.24527	86.71426	71.89717	-1202.84870	414.30915	-2933.23390	1
15231	C	59.30100	84.85880	73.12290	25.30453	-618.46486	669.56098	1
15232	H	59.12100	84.20580	72.28090	1154.23989	2424.67675	1639.17636	1
15233	C	59.18800	84.30980	74.35190	550.80277	-533.65806	493.23056	1
15234	H	59.20900	83.23180	74.40590	-120.72906	-1414.18726	-2807.79720	1
15235	C	59.67731	86.50799	75.26283	-230.44236	473.33810	-483.25512	1
15236	H	59.98884	87.12939	76.08295	-1997.33202	-1305.34595	991.38052	1
15237	C	59.35132	85.16467	75.47891	3.98898	-141.79039	67.57385	1
15238	H	59.40800	84.60080	76.43090	499.78648	3074.09538	445.39565	1
15239	C	61.34685	90.37344	72.17042	-238.64635	859.21006	168.24069	1
15240	O	60.43496	91.14557	72.02575	-624.61482	291.34737	329.11633	1
15241	N	62.65928	90.56553	72.02635	705.54738	-147.60829	-278.80955	1
15242	H	63.43113	89.88263	72.12892	914.77078	-169.01913	2072.49917	1
15243	C	63.05873	91.84285	71.63178	-25.65066	361.64814	-121.25434	1
15244	H	62.10892	92.41060	71.42431	-2633.97799	-605.09869	705.94310	1

15245	C	63.86616	92.57961	72.86237	375.85575	852.94311	-275.62944	1
15246	H	63.26944	92.26376	73.79115	-656.57782	-424.93800	2216.13817	1
15247	C	65.34337	92.16384	73.03165	-24.90791	-679.12779	-1370.19484	1
15248	H	65.47540	91.03416	73.17544	747.46000	-4176.03822	3035.10883	1
15249	H	65.91704	92.40008	72.09801	-494.53273	-589.06885	-2004.50890	1
15250	H	65.84919	92.66959	73.83999	-357.53892	1515.60522	641.82761	1
15251	C	63.80586	94.10435	72.55279	467.00744	868.88641	-590.65371	1
15252	H	62.79826	94.29129	72.21787	3150.90270	-1256.64606	-280.71553	1
15253	H	64.44909	94.43357	71.73825	2099.69441	-159.35703	388.80555	1
15254	C	64.10861	94.88583	73.89320	40.11293	1130.58150	-124.78529	1
15255	H	63.92074	95.98854	73.60965	603.99964	472.67334	-921.94340	1
15256	H	65.15283	94.76681	74.29328	-2190.94268	406.40601	1778.45025	1
15257	H	63.41062	94.67084	74.72931	2672.86980	1272.47727	377.97710	1
15258	C	63.95040	91.95579	70.25713	661.62440	-501.87121	437.21482	1
15259	O	64.05993	93.05081	69.76618	-591.64845	112.72252	-70.11802	1
15260	N	64.32047	90.76093	69.80071	-823.58159	395.62994	191.79443	1
15261	H	64.29722	89.84594	70.31753	2067.11021	-1149.88138	79.33277	1
15262	C	65.19816	90.80900	68.63250	-366.38592	-198.12727	355.38782	1
15263	H	65.54105	91.85214	68.71081	-595.98143	-2839.09654	1883.46004	1
15264	C	66.24033	89.64868	68.85400	-202.28332	-76.37071	1186.09177	1
15265	H	65.66283	88.67098	68.92420	111.33232	-793.79812	-246.97487	1
15266	H	66.68667	89.62149	69.85209	-1015.86743	-2322.85366	-1459.99076	1
15267	C	67.29528	89.47441	67.74846	-755.05347	541.38732	52.07694	1
15268	H	66.79811	89.77975	66.80855	-3823.38804	2675.65750	-594.86661	1
15269	C	68.43410	90.39341	68.10839	-323.69565	-418.26698	57.19173	1
15270	H	68.18612	91.46548	68.29788	-1800.39179	-1222.75952	840.74901	1
15271	H	69.18771	90.40731	67.28083	1866.88697	2216.40017	562.27767	1
15272	H	68.95354	89.92079	69.03659	-160.80476	-1316.49285	-2353.85430	1
15273	C	67.72305	88.04835	67.61220	-661.63843	-57.21965	-71.85084	1
15274	H	68.11625	87.84120	66.59322	1208.62024	-433.65484	3868.74897	1
15275	H	68.43018	87.73949	68.41012	2727.32140	4638.09790	-712.57171	1
15276	H	66.78529	87.34406	67.44049	-839.94078	1613.35276	2126.73745	1
15277	C	64.37722	90.62744	67.26514	27.85055	-482.33210	-533.62167	1
15278	O	64.91399	90.84532	66.18527	-593.22098	-220.45777	642.19315	1
15279	N	63.20927	90.00006	67.50829	501.07332	-738.86222	218.78855	1
15280	H	62.93054	90.07505	68.49669	-966.25916	1244.99225	-1481.74108	1
15281	C	62.26479	89.95469	66.48097	-365.13832	120.93913	-90.04256	1
15282	H	62.69978	89.89054	65.45059	4477.68727	-1270.25121	565.69744	1
15283	C	61.28502	88.73467	66.89336	1040.19826	-132.71503	691.51368	1
15284	H	60.24999	88.84218	66.39924	2129.72781	525.68794	2668.64361	1
15285	H	60.98812	88.71674	68.02238	3039.06931	-1157.50798	620.67918	1
15286	C	61.85720	87.38654	66.56242	-710.92708	-123.53180	242.68256	1
15287	H	62.75936	87.46388	65.89027	-1161.10410	2391.26515	-11.35938	1
15288	C	62.58487	86.76078	67.74843	-628.19777	-42.02890	267.02491	1
15289	H	61.89455	86.50020	68.68310	-282.88494	-2494.92561	-295.16411	1
15290	H	63.34366	87.37208	68.11540	-154.22725	2862.12016	797.36263	1
15291	H	63.03073	85.81644	67.39869	-983.15304	-927.72257	-1929.11452	1
15292	C	60.82074	86.56613	65.83436	-258.32108	1215.37276	302.77209	1
15293	H	60.46891	87.17021	64.89731	-2091.02823	25.91826	-263.16297	1
15294	H	61.13167	85.58558	65.42589	-1572.77739	-2454.28727	-1365.20732	1
15295	H	59.95596	86.39228	66.53420	1279.22321	455.59740	3227.59962	1
15296	C	61.41408	91.30640	66.61029	596.38786	-264.64670	-73.19584	1
15297	O	60.90624	91.73205	65.56772	534.71317	172.00504	493.66023	1
15298	N	61.22677	91.80521	67.84363	-478.61880	569.46527	-628.08186	1
15299	H	61.53785	91.11926	68.56715	2948.33544	476.75104	-656.87760	1
15300	C	61.32232	93.24482	68.06557	273.76093	132.87554	-241.45478	1
15301	H	61.59793	93.15774	69.13233	1025.35031	3636.75605	-1133.90836	1
15302	C	62.56318	93.95023	67.44846	-658.87353	-279.45482	-591.10951	1
15303	H	63.47146	93.26538	67.55789	-1955.99575	675.47766	711.18197	1
15304	H	62.38583	93.88188	66.31898	2916.52340	-849.97296	191.86112	1
15305	C	62.77511	95.46787	67.89510	112.07615	-36.70493	-178.97503	1
15306	H	63.23088	95.49104	68.89932	274.80740	2872.72713	1312.31242	1

15307	H	61.76375	95.84725	68.07459	-53.26057	439.97854	2753.25417	1
15308	C	63.52762	96.22252	66.75794	1.13687	-216.71453	130.15449	1
15309	O	63.66718	95.61882	65.46346	-69.88385	-193.85233	-82.41457	1
15310	O	63.75858	97.41084	66.88612	-301.77889	-18.53751	-2.11122	1
15311	C	59.88086	94.00042	67.89934	175.32035	-528.85409	134.58230	1
15312	O	59.76774	95.08119	67.38451	-299.65172	410.27045	621.56817	1
15313	N	58.96708	93.17488	68.41892	359.65107	174.06538	-614.02362	1
15314	H	59.15768	92.16753	68.64457	4608.68962	3088.74624	1994.71346	1
15315	C	57.71188	93.76006	68.87766	-298.83205	-216.70503	-526.91485	1
15316	H	57.54110	94.07522	67.86661	-1812.64228	-1512.43966	1182.23862	1
15317	C	56.64025	92.81421	69.40514	-367.06225	-73.50671	-372.96862	1
15318	H	56.52339	92.01247	68.66552	-1320.61529	435.77471	-1216.33295	1
15319	C	57.21871	92.08179	70.61271	-343.90261	182.16994	-97.90838	1
15320	H	56.71335	92.44584	71.50743	3412.38877	-2317.37919	-3937.18902	1
15321	H	57.14702	90.92627	70.55602	1540.87822	-528.00187	-1191.24637	1
15322	H	58.30507	92.30220	70.76117	-1568.97390	-3015.20614	1600.27795	1
15323	C	55.26683	93.38978	69.60287	-778.46744	-753.27612	5.89143	1
15324	H	55.39174	94.29093	70.28960	636.20786	-2255.95566	-3264.70434	1
15325	H	54.63393	92.72992	70.21339	-2535.79966	1702.85929	3341.66670	1
15326	C	54.53643	93.75495	68.21021	221.91748	383.10351	16.83158	1
15327	H	55.23539	94.10410	67.39009	-2060.63221	-692.02556	-2864.30455	1
15328	H	53.99932	92.89418	67.78023	261.24360	-1583.87238	-249.02756	1
15329	H	53.88591	94.68319	68.28506	-275.26764	-1236.54666	-214.94532	1
15330	C	57.93087	95.04374	69.92775	-295.92174	128.91337	300.09960	1
15331	O	57.12646	95.96117	70.01805	680.43985	-457.34205	394.50820	1
15332	N	59.03288	94.87998	70.66403	132.95087	-628.15882	111.44540	1
15333	H	59.68174	94.09278	70.43292	-2771.60961	10.51548	783.31148	1
15334	C	59.62274	95.91629	71.48509	346.92577	788.44306	-234.91651	1
15335	H	59.00102	96.86906	71.52048	-1615.86306	918.22583	2188.33614	1
15336	C	59.59717	95.17694	72.88150	-301.06248	1228.40664	506.14066	1
15337	H	59.63068	94.05579	72.73508	-749.94915	654.75412	-126.37179	1
15338	C	60.88469	95.49250	73.75858	329.68144	-479.73481	-327.07799	1
15339	H	60.91403	94.85079	74.72708	982.14344	-2375.86059	2152.88227	1
15340	H	61.79763	95.36242	73.15300	2087.21394	-1289.29766	-451.06201	1
15341	H	60.84723	96.55255	74.10987	-151.01890	330.51056	-1625.02011	1
15342	C	58.34915	95.50385	73.83276	-248.17862	654.96176	42.85189	1
15343	H	58.42737	96.51685	74.18129	1724.54469	-45.13287	-210.13091	1
15344	H	58.29534	94.91437	74.77298	431.18468	-888.54494	-1249.21589	1
15345	C	57.06412	95.33779	72.94120	126.08300	164.92758	-445.59721	1
15346	H	56.10856	95.36357	73.62175	2494.50901	-256.96643	-852.71034	1
15347	H	57.14778	94.55238	72.21396	-1232.36920	3460.60142	-478.01380	1
15348	H	57.00236	96.23405	72.28154	365.85214	1340.19782	886.06838	1
15349	C	61.20595	96.01601	71.14244	-422.84889	986.31496	453.26068	1
15350	O	61.68460	95.07361	70.54986	877.25652	675.11725	-452.80990	1
15351	N	61.84973	97.18017	71.48417	111.66443	690.50359	-535.24613	1
15352	H	61.41690	98.00604	71.95491	51.78135	-817.25006	509.61375	1
15353	C	62.88787	97.52216	70.57572	-82.37810	256.73206	-702.52370	1
15354	H	63.20009	96.63667	69.94415	-2028.41715	-915.26411	1292.42899	1
15355	C	62.43371	98.69360	69.57576	788.87135	-162.11755	-485.37720	1
15356	H	62.70807	98.41966	68.56512	2137.72358	-1674.81349	1712.03709	1
15357	H	63.05973	99.61841	69.77082	210.83515	-23.59414	426.94421	1
15358	C	60.88219	98.90602	69.56939	1073.27194	105.97282	101.97519	1
15359	H	60.44815	99.03042	70.65236	-342.52858	1588.14003	1646.58543	1
15360	H	60.83431	99.91573	69.11525	74.94663	4189.98803	-2018.87996	1
15361	C	60.18541	97.85828	68.68224	589.42160	747.18244	159.45214	1
15362	H	60.11276	96.88607	69.24068	-1740.09050	-1365.08980	-291.55162	1
15363	H	60.70179	97.63154	67.75084	4469.67010	-1819.24605	3974.74500	1
15364	C	58.65535	98.24570	68.23313	-69.70563	-931.14745	342.05409	1
15365	H	58.40549	99.25807	67.91678	-1512.41571	550.51447	-1820.15740	1
15366	H	57.93893	97.99336	69.04303	3261.74180	-719.84923	495.49005	1
15367	N	58.28228	97.33485	67.21713	-67.27505	-337.49159	907.72510	1
15368	H	63.54047	96.41625	64.89881	974.65567	-560.80854	2076.94504	1

15369	H	58.57114	96.33375	67.19924	1034.68716	2725.88463	-955.33925	1
15370	H	58.24577	97.59314	66.18801	-1224.47904	-2549.03456	462.09735	1
15371	C	64.12220	98.16853	71.41264	538.98420	-238.84647	304.08219	1
15372	O	63.87959	99.00140	72.25464	694.26807	280.97715	-835.21038	1
15373	N	65.31063	97.68184	70.91238	-472.62619	518.38884	-110.47612	1
15374	H	65.17778	96.88068	70.32241	-684.19042	124.05293	864.47296	1
15375	C	66.48621	98.13135	71.61939	-857.25945	800.71491	445.63752	1
15376	H	66.37034	99.23084	71.88941	1721.75091	-723.40104	-492.40349	1
15377	C	66.52660	97.24360	72.90917	-625.04921	53.19170	236.88241	1
15378	H	66.34260	96.17431	72.74717	1089.97899	727.56789	2562.70932	1
15379	H	65.69975	97.39090	73.65084	-1811.25203	-1783.47251	2348.29452	1
15380	C	67.88845	97.47828	73.66334	1019.06647	144.09228	703.29654	1
15381	H	67.99023	96.64330	74.46357	1379.54199	1589.42127	-3096.57772	1
15382	H	68.64856	97.22344	72.95533	-1148.56000	5582.93993	-2381.68739	1
15383	C	67.92480	98.90160	74.33749	-9.84721	-374.39953	-141.55595	1
15384	O	67.64063	99.91838	73.67491	237.60735	-149.42159	16.34471	1
15385	N	68.37644	98.91406	75.60484	-41.26508	-807.40664	42.31012	1
15386	H	68.85928	98.19006	76.15338	-2606.97207	129.76568	-1172.27639	1
15387	H	68.41488	99.75715	76.14257	1780.82199	1875.05752	-202.19682	1
15388	C	67.78386	97.82221	70.69373	307.65652	894.93700	357.11379	1
15389	O	67.73929	96.89094	69.84355	1161.33625	-409.59464	186.05514	1
15390	N	68.81373	98.59069	70.85508	-349.49201	42.45555	-162.14971	1
15391	H	68.82085	99.33351	71.53302	-1999.15512	1423.64886	772.66714	1
15392	C	70.04459	98.03337	70.27912	71.98624	-152.02902	-240.90748	1
15393	H	70.62457	98.92657	69.98213	3434.88264	-2976.56080	-1919.31044	1
15394	H	69.57341	97.47753	69.47108	2066.25641	2428.04606	746.54205	1
15395	C	70.81625	97.14218	71.39419	-443.17061	638.35511	-289.19229	1
15396	O	70.97286	97.51172	72.56401	648.45567	221.00175	34.71793	1
15397	N	71.45732	96.17727	70.80951	-104.01693	342.46081	322.69345	1
15398	H	71.34910	96.06112	69.69844	758.25654	-2043.12597	797.14640	1
15399	C	71.89260	95.02769	71.55838	142.23614	860.34588	-36.63600	1
15400	H	70.89482	94.93419	72.11226	-1024.83579	-1017.14694	-1376.84879	1
15401	C	72.34951	93.75333	70.78050	441.61198	-336.24322	-741.48467	1
15402	H	72.59018	92.86829	71.44475	2566.58759	-1583.50201	1990.94996	1
15403	H	73.28132	93.93026	70.17649	-1911.06308	1229.47372	3095.89674	1
15404	S	70.95325	93.10530	69.58216	341.93313	46.24010	-430.08840	1
15405	C	73.22717	95.34903	72.38959	707.59087	209.31745	-790.46242	1
15406	O	73.54533	94.76351	73.39025	592.90518	180.04316	815.87865	1
15407	N	73.90360	96.39314	71.80307	-30.08313	-324.45835	262.67012	1
15408	H	73.34953	96.83757	71.10276	36.48052	-2148.13149	-918.25266	1
15409	C	75.06640	96.78571	72.46487	410.01736	187.56319	412.77389	1
15410	H	75.77327	95.98293	72.78177	1593.23479	773.94555	-2058.87944	1
15411	C	75.75458	97.70646	71.37197	95.24971	-418.19210	52.83758	1
15412	H	75.57407	97.17538	70.37757	-590.53656	134.95210	-1781.52678	1
15413	H	76.89201	97.83271	71.55410	-11.64402	3869.12641	619.62049	1
15414	C	75.16684	99.14635	71.38260	805.97920	-320.98034	675.55786	1
15415	H	74.07667	99.13885	71.40010	1282.24890	-100.48360	-1751.15115	1
15416	H	75.39611	99.62236	72.32374	-1798.33324	-593.59858	523.76456	1
15417	C	75.90616	99.94119	70.03709	148.81597	392.46245	-717.51615	1
15418	O	75.77513	99.48423	68.91049	46.42234	-1441.03484	689.33541	1
15419	O	76.41678	100.98534	70.40038	-142.50271	-256.16414	-763.69726	1
15420	C	74.71617	97.81466	73.73854	-795.82149	-905.92391	192.59001	1
15421	O	75.54253	98.12169	74.58362	-19.01240	-326.90793	421.38874	1
15422	N	73.42158	98.15921	73.69890	-1060.54108	-74.46064	-456.40544	1
15423	H	72.70886	97.91196	72.97308	1415.10278	312.45932	-1094.51410	1
15424	C	73.04230	98.89968	74.85030	479.37258	-334.83227	-160.27547	1
15425	H	73.97505	99.56707	75.00624	329.55702	-2084.04936	-2258.63834	1
15426	C	71.77972	99.91911	74.63700	-200.76243	-291.81264	-488.12614	1
15427	H	70.71534	99.56037	74.69601	-2258.36684	-2182.59662	2142.39567	1
15428	H	72.05263	100.67614	75.42464	1286.87863	709.88699	-693.07166	1
15429	C	71.99488	100.63836	73.35059	366.78018	457.78836	-416.99713	1
15430	C	73.20005	101.36339	73.12364	-1033.27431	9.95270	667.17618	1

15431	H	73.88615	101.40385	73.96090	503.80715	1726.16748	176.80990	1
15432	C	73.36298	102.02873	71.87077	-1350.62058	-7.09289	-448.07585	1
15433	H	74.30449	102.58292	71.61037	-112.17583	5320.13921	-616.75997	1
15434	C	72.28126	102.02448	70.95406	444.88526	379.21438	-981.63358	1
15435	H	72.36909	102.61909	70.05269	-3049.60975	1385.30690	1965.97114	1
15436	C	70.94803	100.57165	72.37745	-479.72436	-675.07777	-32.71266	1
15437	H	70.02350	100.01793	72.63039	1629.97845	1081.56632	2674.89099	1
15438	C	71.15554	101.14016	71.13038	98.63996	-211.37749	725.53480	1
15439	H	70.31371	101.02910	70.41405	1152.54949	2213.82894	1405.37302	1
15440	C	72.51756	97.79243	75.89214	288.61758	-336.67092	-110.26151	1
15441	O	72.14018	98.26737	76.95288	15.20443	-588.51129	192.75300	1
15442	N	72.62116	96.52043	75.55122	28.00707	9.27077	610.71436	1
15443	H	72.99830	96.21722	74.66391	-2591.29510	-4.70720	-2453.64138	1
15444	C	71.77595	95.56772	76.13987	325.72275	-318.44772	-502.96299	1
15445	H	71.42742	96.15734	76.99179	-1107.86168	819.89816	-29.68886	1
15446	C	70.66514	95.16599	75.01601	438.64282	-441.76148	-343.06871	1
15447	H	70.41796	96.04999	74.35914	-836.89287	2196.66127	206.44397	1
15448	H	71.23191	94.50707	74.29338	-320.13793	-125.80367	2652.75914	1
15449	C	69.48625	94.39071	75.56999	587.73722	-630.63877	250.69947	1
15450	H	69.07949	94.82355	76.54315	3067.88335	2739.97183	256.43657	1
15451	H	69.92662	93.42942	75.91344	-2664.64783	-2330.53883	-181.93698	1
15452	C	68.32447	94.25436	74.46670	-310.86474	-1436.52870	1075.20495	1
15453	O	67.16918	94.01099	74.84099	-241.25164	-181.96078	-725.79434	1
15454	O	68.65280	94.33573	73.25473	-363.26399	-323.78586	286.84978	1
15455	C	72.51919	94.22428	76.59117	-46.67506	83.13648	-496.88817	1
15456	O	71.83548	93.20857	76.93112	-400.07145	265.68782	339.27191	1
15457	N	73.81432	94.35244	76.73131	-785.40742	-332.36567	-221.08491	1
15458	H	74.13296	95.24449	76.31063	24.90560	1436.46760	237.25869	1
15459	C	74.41881	93.91911	77.98700	-483.19430	365.34481	-678.85197	1
15460	H	74.21407	92.78199	78.04010	573.54537	-852.38796	521.79853	1
15461	C	75.89705	94.45862	77.88066	-535.48451	-766.41771	-213.91985	1
15462	H	75.95825	95.46640	78.45152	-2628.26284	-1537.69032	2132.85945	1
15463	H	76.23672	94.69395	76.81331	2046.32473	-3233.88565	-903.63245	1
15464	C	76.93397	93.34510	78.40022	87.46022	-192.18277	-4.21027	1
15465	O	77.08146	92.84261	79.52372	669.26361	176.91222	-409.30700	1
15466	N	77.86957	93.22828	77.40358	-390.16257	-198.55351	-645.36319	1
15467	H	77.64992	93.70268	76.49708	31.19499	334.24307	464.19481	1
15468	H	78.69401	92.56530	77.45342	-1406.65031	-97.08844	485.70252	1
15469	C	73.66287	94.64984	79.20304	952.28137	-625.85422	-53.76170	1
15470	O	73.94854	95.80330	79.48742	676.49025	441.47979	1328.62036	1
15471	N	72.67825	93.89389	79.76477	-491.09310	-115.70681	277.17306	1
15472	H	72.50502	93.03689	79.27537	3628.28025	-873.02065	1405.23133	1
15473	C	71.43098	94.51538	80.29346	662.20126	17.80075	-789.17671	1
15474	H	71.76899	94.86323	81.25036	1655.26361	-749.88702	-2417.11686	1
15475	C	70.97910	95.58523	79.30806	485.91317	821.44660	-954.07657	1
15476	H	71.19521	95.41124	78.27925	-962.10380	1405.77537	1676.73582	1
15477	O	71.62200	97.27799	79.42839	-522.81621	204.63789	159.84971	1
15478	H	71.67733	97.60329	78.46833	-2876.34173	918.28115	-1940.84092	1
15479	C	69.49297	95.89105	79.51075	-209.44910	-1045.58611	-1160.05803	1
15480	H	68.82790	94.93697	79.44662	903.93985	266.35122	-117.29187	1
15481	H	69.09083	96.67634	78.82658	2874.43560	-2818.24107	-3925.78016	1
15482	H	69.55505	96.28865	80.51756	1975.78958	-777.04284	565.51177	1
15483	C	70.26511	93.33255	80.28337	128.25373	408.98889	240.74032	1
15484	O	69.71709	92.97391	81.34142	125.75227	-280.82765	743.40739	1
15485	N	69.97497	92.86619	79.09093	147.37929	748.01452	-87.73618	1
15486	H	70.50157	93.19185	78.29735	3074.07278	-4415.95923	-385.16386	1
15487	C	69.72138	91.41460	79.20513	511.15677	818.33187	254.87897	1
15488	H	69.16639	91.34985	80.19563	-1586.61013	-1728.17014	1204.92493	1
15489	C	68.80686	90.79811	78.08637	883.44928	-456.39808	48.87870	1
15490	H	68.57617	89.73284	78.30443	-4030.21480	439.58977	129.77550	1
15491	C	67.54245	91.74750	77.96191	-138.78842	-511.66017	-782.50069	1
15492	H	66.87957	91.27570	77.21427	-165.57477	1051.07717	1663.14385	1

15493	H	66.99655	91.99979	78.90680	1227.44983	-872.31288	703.48101	1
15494	H	67.84274	92.73727	77.46909	358.89959	-370.37664	833.61184	1
15495	C	69.42393	90.96004	76.62253	-989.67265	-1099.20002	0.06158	1
15496	H	68.69872	90.88314	75.78211	1842.72040	-4200.09196	-3839.70569	1
15497	H	69.93563	91.96595	76.51795	358.03605	2169.75440	326.77910	1
15498	H	70.19433	90.14944	76.40231	-1757.50618	468.96815	2549.62427	1
15499	C	71.09130	90.64682	79.41768	205.57678	-1742.37217	10.52134	1
15500	O	71.05952	89.74497	80.22926	182.30213	382.45544	160.18202	1
15501	N	72.09024	91.03166	78.59819	953.40633	588.64825	-803.22576	1
15502	H	71.88006	91.81124	77.91693	-178.02738	-1289.43638	2620.45857	1
15503	C	73.14113	90.09720	78.26001	744.37733	855.73895	-62.02468	1
15504	H	72.65236	89.14744	78.60646	-2321.35182	1651.45561	442.27964	1
15505	C	73.50623	90.03526	76.74699	70.16202	-559.46439	523.84935	1
15506	H	74.33944	90.70622	76.66497	-3237.61389	299.04436	-812.27963	1
15507	H	72.71343	90.50822	76.15851	-699.07459	1411.88185	-278.53277	1
15508	N	73.28496	87.86853	75.30593	131.49927	-36.27223	1042.72985	1
15509	C	73.83426	88.51989	76.31041	-27.97684	-465.59310	345.58950	1
15510	C	73.88370	86.64616	75.22914	-133.82088	-605.64960	12.14326	1
15511	H	73.65677	85.87499	74.45190	2869.35617	-1639.12256	1090.81859	1
15512	N	74.80384	86.59978	76.23972	75.67363	306.99463	1163.74050	1
15513	H	75.26757	85.72144	76.25347	-806.98475	1128.35480	-1641.90659	1
15514	C	74.86527	87.73400	76.90346	-360.61261	263.94586	133.02705	1
15515	H	75.44616	87.78432	77.83007	-3057.03891	-1194.99483	2209.73524	1
15516	C	74.45054	90.29692	79.23698	-1139.15288	813.49952	-33.86564	1
15517	O	75.55719	89.75463	79.07633	-264.50849	-102.29409	-843.63678	1
15518	N	74.21803	91.07636	80.31521	140.29345	485.91382	427.99532	1
15519	H	73.25462	91.40085	80.35794	-2092.12670	-222.02906	-1447.51944	1
15520	C	75.17598	91.02981	81.37680	1113.69752	-123.95809	-302.13598	1
15521	H	76.07528	90.89079	80.72734	-5295.31814	179.47402	1310.14425	1
15522	C	75.24408	92.38842	82.20319	-349.94803	708.31592	-175.71460	1
15523	H	75.67402	93.20979	81.57151	-294.14481	-1432.11709	1975.24961	1
15524	H	75.95383	92.38022	83.03023	1015.77461	16.34705	-5091.40279	1
15525	C	73.78883	92.70096	82.69215	375.73091	447.04760	603.04924	1
15526	H	73.35114	92.72322	81.62460	130.40576	392.93234	-2802.24575	1
15527	H	73.36892	91.89918	83.30476	685.87675	-98.38377	-68.83296	1
15528	C	73.74208	94.13251	83.32841	-395.75349	1011.02633	633.21987	1
15529	H	72.64712	94.41384	83.49491	-1615.31670	-823.57302	2132.43916	1
15530	H	74.21821	94.76898	82.59541	105.84074	1408.12863	1253.90275	1
15531	C	74.52563	94.31709	84.71443	504.54733	712.71906	-49.36950	1
15532	H	73.84458	94.58103	85.63395	-1088.95458	717.40954	3668.80119	1
15533	H	75.16224	93.41648	84.83780	2626.98682	-3745.32306	812.99757	1
15534	N	75.41007	95.42735	84.55408	192.59368	43.90097	-386.28417	1
15535	H	72.52936	96.88547	79.63656	-747.32698	-330.12402	3071.55512	1
15536	H	76.01970	95.62414	85.40739	-904.13883	818.94024	-1503.07648	1
15537	H	76.22032	95.19746	83.92744	-677.77374	-50.24416	491.66952	1
15538	C	74.66549	89.80062	82.31318	-330.20137	-120.75942	-591.74798	1
15539	O	75.46300	89.10341	82.89739	-555.54145	256.96947	45.86379	1
15540	N	73.33657	89.77545	82.47345	-499.35729	-473.91291	84.45842	1
15541	H	72.79873	90.50638	82.03155	-1139.09309	-216.34677	-1345.36846	1
15542	C	72.74545	88.66228	83.13968	183.98902	289.67978	309.79566	1
15543	H	73.50394	88.61680	83.92862	4150.68562	1140.12866	904.50854	1
15544	C	71.22499	88.96786	83.58377	-499.69978	441.48389	589.53177	1
15545	H	70.80910	88.20180	84.23862	-358.56401	2463.61323	4880.96225	1
15546	H	70.46728	89.02764	82.73561	-1168.71899	1447.22434	-1576.12848	1
15547	C	71.18518	90.29282	84.38344	-28.08646	-979.58235	-207.20371	1
15548	C	70.60672	91.50832	84.00865	17.84122	32.11432	-177.24076	1
15549	H	70.02495	91.78846	83.03945	2189.04383	-4575.93442	2263.88397	1
15550	N	70.62813	92.38050	85.02849	-86.32567	-333.10864	-268.83012	1
15551	H	70.29983	93.37907	84.82086	1472.70520	236.40699	-1671.79578	1
15552	C	71.35997	91.89873	86.06738	-367.06463	-137.74899	600.54473	1
15553	C	71.83769	90.51440	85.66819	-791.20573	-215.84613	-298.94153	1
15554	C	72.60626	89.77051	86.57316	-479.62369	79.95039	-696.03308	1

15555	H	72.84644	88.72186	86.33694	642.84026	-420.25939	3427.88371	1
15556	C	73.01826	90.41075	87.75979	81.05152	292.84959	-38.08770	1
15557	H	73.69898	89.80935	88.37488	-1144.23309	-2516.71564	-288.61441	1
15558	C	71.72602	92.52494	87.30931	191.31698	287.60276	-205.11888	1
15559	H	71.38543	93.60343	87.59820	-285.72871	-3027.29088	427.72210	1
15560	C	72.57855	91.70810	88.13963	108.97761	252.79790	-79.04524	1
15561	H	72.96552	92.18311	89.00329	-781.53630	-863.71709	-1179.90392	1
15562	C	72.67888	87.37567	82.20243	-442.32561	-320.68088	-930.52699	1
15563	O	72.90024	86.26157	82.68277	707.22721	967.60083	937.62896	1
15564	N	72.49154	87.63205	80.93160	913.01846	935.94865	253.91302	1
15565	H	72.34548	88.63876	80.54270	-767.79865	156.21668	-2806.18729	1
15566	C	72.74286	86.52956	79.96406	1038.85215	18.67060	646.08187	1
15567	H	72.27758	85.67643	80.47760	1137.31101	-2737.90269	3303.43254	1
15568	C	72.11776	86.70672	78.59794	714.20786	-268.74128	724.96724	1
15569	H	72.68430	87.54356	78.09370	2232.15199	3378.88818	-1875.91434	1
15570	C	72.29386	85.47299	77.74513	-527.98696	-180.71922	-905.04803	1
15571	H	71.74025	85.59064	76.74755	1191.19636	404.63554	728.34542	1
15572	H	71.89646	84.53354	78.21798	-1452.68503	3569.74989	-452.47094	1
15573	H	73.34468	85.25638	77.58038	-3600.40007	2923.76153	-426.56976	1
15574	C	70.65438	87.13154	78.63622	82.00521	168.63429	76.30563	1
15575	H	70.39825	87.86200	79.44066	491.77374	-1025.78140	1146.12243	1
15576	H	70.04355	86.24483	78.92603	-1394.98356	-298.88991	-1235.82530	1
15577	C	70.34330	87.67595	77.16772	243.05005	335.11986	331.54714	1
15578	H	71.07104	88.42899	76.73997	1327.98141	-2124.28949	-124.86026	1
15579	H	70.41189	86.64819	76.68806	-783.55257	3027.41414	1354.95861	1
15580	H	69.31839	87.99138	77.01593	804.10061	-2497.75860	-1628.65138	1
15581	C	74.36720	86.23900	79.98313	891.28816	303.67135	-120.05988	1
15582	O	74.66972	85.07914	79.70519	-110.48328	942.59596	649.77164	1
15583	N	75.20601	87.24756	80.19133	233.09732	163.48002	-234.61991	1
15584	H	74.78570	88.14337	80.30331	-1836.11314	-620.86259	710.89020	1
15585	C	76.58125	86.86845	80.23329	358.95844	78.44348	99.54568	1
15586	H	76.72653	86.33752	79.22344	913.31419	-1725.44803	-1533.99996	1
15587	C	77.41105	88.14334	80.44453	247.41546	629.88082	174.69311	1
15588	H	77.72054	88.65134	79.46571	-47.53409	1287.74224	3886.72751	1
15589	H	76.72918	88.81520	81.12405	1796.09967	-847.51292	-2955.58182	1
15590	O	78.76534	88.37718	81.19986	568.40770	-229.79357	1170.17199	1
15591	H	78.83230	89.33454	81.01625	-2158.14266	249.66648	-1398.29383	1
15592	C	76.92810	85.84871	81.48949	-436.02499	-1025.49826	179.28256	1
15593	O	77.48561	84.77179	81.29859	-426.87432	-181.34428	-471.56886	1
15594	N	76.37821	86.30745	82.59408	-342.31835	481.46371	629.05358	1
15595	H	75.90054	87.23154	82.55774	317.36629	-677.42084	1394.44991	1
15596	C	76.62063	85.59652	83.84616	510.28627	-210.02817	-566.99057	1
15597	H	77.59401	85.02575	83.80178	2264.94724	1281.27831	2043.94047	1
15598	C	76.43653	86.54058	85.10842	-1204.94122	-47.24500	-449.16635	1
15599	H	75.53136	87.03673	84.85320	-206.25794	2604.99502	-1353.58016	1
15600	C	76.20044	85.53477	86.33535	164.78554	-417.46522	159.39995	1
15601	H	75.77646	86.02576	87.26069	2196.99945	214.76143	-2287.21351	1
15602	H	75.51400	84.69780	86.20590	-1205.53578	-2376.94491	1671.83810	1
15603	H	77.16032	85.07737	86.68961	89.63678	-773.99362	2560.17281	1
15604	C	77.69032	87.42927	85.36946	598.68747	597.52510	-410.48287	1
15605	H	77.42619	88.17961	86.20242	2407.91974	1344.61488	1046.81711	1
15606	H	78.53138	86.87429	85.74241	385.81563	-1815.97393	-1014.23725	1
15607	C	78.06236	88.16270	84.01841	47.54144	-218.95488	-514.16101	1
15608	H	78.57524	89.09424	84.24209	463.01657	-1087.78049	1733.02907	1
15609	H	77.06779	88.45572	83.51278	-2759.98968	2101.89193	432.08612	1
15610	H	78.89896	87.64117	83.39693	1227.49870	455.79922	-1657.26106	1
15611	C	75.78700	84.21280	83.67290	785.59210	-41.69588	-461.03959	1
15612	O	76.22800	83.19180	84.17690	-760.26374	-47.55351	208.24251	1
15613	N	74.61500	84.11980	83.04490	568.63411	-188.08241	-594.93911	1
15614	H	74.13500	84.95480	82.78790	-339.13717	2869.24803	-1245.24213	1
15615	C	73.91400	82.81280	82.88690	-714.12081	390.46939	411.11572	1
15616	H	74.00400	82.22380	83.78790	627.52040	2153.46706	-2206.13327	1

15617	C	72.40500	82.98880	82.63790	728.78165	-305.49799	-454.97175	1
15618	H	71.80800	82.06780	82.46190	-1939.59620	-1719.67361	1782.95134	1
15619	O	72.05500	83.93480	81.60190	-711.95499	-76.44498	333.02175	1
15620	H	72.41500	84.72780	82.00590	2028.88158	-1577.80108	-1814.49979	1
15621	C	71.88900	83.50080	83.95390	610.30246	-359.87625	573.99564	1
15622	H	72.21200	84.53380	84.20790	2197.15808	-1938.77183	-1145.37609	1
15623	H	72.03100	82.81280	84.81390	1808.91683	84.80891	-2572.71327	1
15624	H	70.78500	83.62080	83.92590	-1622.85904	-2138.11175	-1641.04629	1
15625	C	74.57400	81.90580	81.81590	620.58496	-666.18084	50.28313	1
15626	O	74.51000	80.70880	81.83790	-641.08760	129.02499	442.70360	1
15627	N	75.20800	82.54480	80.80190	479.05021	677.55215	155.26194	1
15628	H	75.17800	83.52780	80.63590	-837.16039	-1004.73959	2861.44842	1
15629	C	76.14000	81.91880	79.89590	163.53308	867.18234	229.57076	1
15630	H	75.54400	81.19980	79.35290	2581.68508	1356.24594	-1180.56144	1
15631	C	76.52300	82.92480	78.72290	281.23824	729.14528	-469.79061	1
15632	H	75.62500	83.11680	78.09690	2071.08828	-1560.73574	-1781.27019	1
15633	H	76.66500	83.94280	79.14390	2175.09361	-2265.87376	-181.68689	1
15634	C	77.84600	82.66780	77.99590	-611.28743	136.94309	662.58982	1
15635	H	77.88700	81.63180	77.59590	-1864.58453	2010.47920	-1542.57063	1
15636	H	78.72200	82.60580	78.67690	3008.43310	-858.42995	332.64770	1
15637	C	78.18500	83.71880	76.95690	-100.08441	-888.55719	178.60636	1
15638	O	77.71100	83.55580	75.80090	695.97028	2.01554	373.16019	1
15639	O	78.82900	84.76080	77.27790	526.81165	293.53919	509.83473	1
15640	C	77.35300	81.31380	80.52590	123.66998	725.30763	538.59594	1
15641	O	77.70100	80.15980	80.26390	-47.60118	737.08425	-279.40682	1
15642	N	77.95800	82.09480	81.38790	501.09383	643.90192	-216.72006	1
15643	H	77.75900	83.05180	81.58290	-1879.33957	-2215.99323	-1206.51688	1
15644	C	79.11300	81.64780	82.15290	-452.63025	499.63369	-613.95687	1
15645	H	79.84000	81.34180	81.41590	786.17076	-2556.41567	-1656.77418	1
15646	C	79.73600	82.80780	82.92590	554.46504	-703.14981	172.04613	1
15647	H	79.00500	83.27380	83.62090	2004.73176	-30.22616	2424.53360	1
15648	H	80.07200	83.58180	82.20390	1772.73343	-1970.85715	1694.51011	1
15649	H	80.64900	82.46280	83.45690	2.80618	2331.74634	-2112.14993	1
15650	C	78.82700	80.48580	83.13890	-364.78748	-599.64303	-582.07331	1
15651	O	79.55900	79.51980	83.22390	155.80951	287.15421	718.95277	1
15652	N	77.64800	80.51980	83.78290	449.33258	348.72806	623.82791	1
15653	H	77.05800	81.29980	83.58990	1784.10871	2072.15124	-1556.07570	1
15654	C	77.12500	79.38880	84.44290	-295.09981	-726.39276	465.53266	1
15655	H	77.86300	79.04080	85.15090	-2727.53363	-1206.29691	-1001.81550	1
15656	C	75.91800	79.80180	85.39390	-757.97348	-220.69563	-456.31201	1
15657	H	75.08100	80.21480	84.79090	1548.95543	-1156.06598	2482.43323	1
15658	H	75.49200	78.90680	85.89490	1945.07207	1925.55312	-1551.50444	1
15659	C	76.28200	80.82580	86.48490	-429.60876	81.85717	800.11669	1
15660	H	76.98000	81.55880	86.02790	3043.05091	527.76234	-599.61179	1
15661	C	74.98200	81.56780	86.85190	-739.86855	-312.57104	-431.67682	1
15662	H	75.18900	82.57080	87.28190	-2660.18509	-1222.97732	-1151.50683	1
15663	H	74.37200	80.96780	87.56090	447.33926	-2204.42072	2199.69159	1
15664	H	74.21300	81.76580	86.07590	-2694.53847	-1171.12975	-1125.23053	1
15665	C	77.11200	80.14080	87.64290	469.81814	-361.58067	-692.80686	1
15666	H	78.19900	80.15580	87.41590	-732.39479	-2433.87245	-1854.20845	1
15667	H	76.72400	79.10680	87.76490	765.36022	-721.81661	-2965.03469	1
15668	H	77.02300	80.76480	88.55790	-1923.97086	-2479.18462	224.06694	1
15669	C	76.81200	78.16480	83.60190	-22.31535	583.42087	700.40925	1
15670	O	76.88800	77.02780	84.09590	685.45654	-368.42810	-134.30301	1
15671	N	76.40900	78.34580	82.33290	119.54106	-327.95053	-768.65511	1
15672	H	76.25200	79.28280	82.02990	-478.66696	1307.72408	-2821.16322	1
15673	C	76.00000	77.24280	81.44990	226.40760	-710.74026	524.44150	1
15674	H	75.30300	76.60780	81.97590	-1972.63729	1232.05443	2118.71901	1
15675	C	75.34000	77.71080	80.16190	-746.49746	356.20258	-383.81280	1
15676	H	74.36600	78.17280	80.43090	-560.59934	2524.15006	-1792.37861	1
15677	H	76.02600	78.35680	79.57290	2904.65159	-1130.66475	427.57756	1
15678	H	75.07000	76.89780	79.45490	-1751.90925	-2497.87211	767.90308	1

15679	C	77.21500	76.45580	81.18090	254.29364	646.04355	591.11207	1
15680	O	77.05800	75.22780	81.01690	85.78053	472.65664	626.78914	1
15681	N	78.42600	76.99280	81.18490	358.51261	-73.79128	760.72061	1
15682	H	78.51000	77.98480	81.24190	2131.35755	-951.09259	2109.73081	1
15683	C	79.72500	76.37280	80.94990	790.95648	-213.49684	400.32231	1
15684	H	79.67100	75.84580	80.00890	-2579.11328	-1694.61832	-612.10266	1
15685	C	80.84500	77.40480	80.87490	-626.90113	612.71879	-251.04114	1
15686	H	81.81300	76.89780	80.67290	1830.89959	-2197.76584	-1309.90773	1
15687	H	80.83100	77.90280	81.86790	-790.79718	1507.55025	2645.78122	1
15688	C	80.72800	78.48680	79.85590	479.70328	135.08583	-763.60172	1
15689	C	79.79900	78.45180	78.78390	-183.74456	-156.55681	-879.30592	1
15690	H	79.19800	77.57480	78.59390	1926.01378	2015.95197	1457.61271	1
15691	C	79.71500	79.51180	77.92990	-489.63198	-675.39204	368.18083	1
15692	H	78.93100	79.51880	77.18690	-2290.19744	314.94731	2134.01736	1
15693	C	80.60300	80.61280	78.00890	-880.95828	130.84427	195.55891	1
15694	H	80.63700	81.41480	77.28690	-1401.23023	-534.01084	-2765.79328	1
15695	C	81.56500	79.61080	80.03390	-30.08665	719.81308	558.94089	1
15696	H	82.29100	79.66680	80.83190	-3115.34577	373.38735	231.14680	1
15697	C	81.49000	80.62980	79.09190	-431.76577	-325.69810	-734.13219	1
15698	H	82.21500	81.42980	79.14390	989.86037	1265.28560	-2705.07949	1
15699	C	80.06500	75.30780	81.89290	31.90069	-619.47539	-668.34391	1
15700	O	80.91900	74.45080	81.59690	674.12057	393.73415	119.00462	1
15701	N	79.44000	75.24380	83.07190	604.30545	-486.62010	-332.69820	1
15702	H	78.65900	75.82680	83.28190	105.38128	2691.56887	1625.60081	1
15703	C	79.63100	74.13880	83.98890	-66.99465	63.58043	907.14952	1
15704	H	80.68900	74.07380	84.19190	2817.10129	-1089.75806	880.11018	1
15705	C	78.87000	74.41180	85.37190	-411.44980	-610.69340	-537.78586	1
15706	H	78.83600	73.47280	85.96590	-1799.52483	-1148.24537	-2311.16187	1
15707	H	77.82200	74.75780	85.24390	738.91547	2930.71442	873.58066	1
15708	C	79.70500	75.33080	86.30090	16.30274	410.88287	813.85533	1
15709	C	79.44800	76.73280	86.29990	328.68061	-573.89021	-627.75002	1
15710	H	78.60500	77.12880	85.75290	2073.69103	1839.07786	1488.56453	1
15711	C	80.18400	77.60480	87.17890	-239.16738	833.38714	-282.33993	1
15712	H	79.91800	78.64980	87.23690	-69.32709	882.12279	-3019.15209	1
15713	C	81.22300	77.03480	87.99790	-586.87850	17.73531	-697.64610	1
15714	H	81.76900	77.73080	88.61790	22.20190	-2098.03390	2344.35216	1
15715	C	80.73400	74.83380	87.05290	-299.66440	445.90339	-736.76483	1
15716	H	80.89600	73.77180	87.15890	-2127.09584	-1154.87293	-2009.96469	1
15717	C	81.50200	75.61880	87.92690	-213.40335	885.98350	30.71242	1
15718	H	82.33500	75.21480	88.48390	-441.49341	2000.91161	-2387.39660	1
15719	C	79.16300	72.79280	83.47990	-512.18341	551.44290	-514.81054	1
15720	O	79.55200	71.72080	84.04290	546.98955	-434.99900	-367.70305	1
15721	N	78.30700	72.68380	82.44790	-838.63012	80.80121	53.31956	1
15722	H	77.94400	73.50180	82.00890	1039.05760	-615.25822	2905.17518	1
15723	C	78.01100	71.39980	81.79690	-309.55387	391.59378	-763.07386	1
15724	H	77.51000	70.87580	82.59890	1354.97506	1384.02390	-2479.26333	1
15725	C	77.14300	71.47680	80.57290	-596.12525	-477.18205	498.38036	1
15726	H	76.78100	70.46380	80.29490	-985.45094	-236.74442	-2978.43327	1
15727	H	76.21100	71.97380	80.91690	-387.48183	-1088.87301	2926.16466	1
15728	N	77.72300	73.44280	79.04490	341.93191	-771.55333	-21.45493	1
15729	H	77.43600	74.19280	79.63990	-1938.80414	-1989.10208	-1477.40910	1
15730	C	77.73900	72.10080	79.28290	344.02764	657.14981	530.33019	1
15731	C	78.21500	73.63280	77.79190	-501.13935	-650.85986	-395.84316	1
15732	H	78.09200	74.62580	77.35890	2928.43007	-608.88172	975.59552	1
15733	N	78.44100	72.46680	77.21390	490.42239	-384.41680	-569.54534	1
15734	C	78.16100	71.51680	78.14890	-688.54299	-588.20201	106.66745	1
15735	H	78.36500	70.47680	77.92590	1216.27355	1923.67520	-2172.18291	1
15736	C	79.20000	70.61280	81.39290	735.05954	475.77954	254.50403	1
15737	O	79.29400	69.44680	81.75690	-83.43832	41.34332	-784.19131	1
15738	N	80.23700	71.24080	80.70990	572.91786	430.53569	-446.17982	1
15739	H	80.12400	72.15080	80.31990	-1145.03920	-2406.47985	-1672.11428	1
15740	C	81.53600	70.68980	80.37790	262.62537	-782.51813	-387.48458	1

15741	H	81.30400	69.88380	79.69790	319.28447	-2656.90068	-1654.43720	1
15742	C	82.43700	71.71380	79.66390	595.61793	253.45936	-642.22165	1
15743	H	82.58700	72.59480	80.32390	637.66042	936.40154	2935.09243	1
15744	H	83.49300	71.39880	79.52090	1359.47320	-2172.67367	-1824.70490	1
15745	S	81.70000	72.38080	78.16590	99.41861	-448.52625	316.46604	1
15746	H	80.97600	71.33580	77.79290	1224.90468	-1566.27297	2438.15991	1
15747	C	82.28600	70.13480	81.59390	-536.82951	549.70559	491.00799	1
15748	O	82.97200	69.12480	81.49390	-432.37493	390.92855	532.77952	1
15749	N	82.03700	70.65580	82.81090	10.04037	-152.43001	830.26295	1
15750	H	81.50900	71.49380	82.92690	-1332.28925	1918.42969	2107.80908	1
15751	C	82.76200	70.16280	84.01490	-508.81131	510.36718	-558.64783	1
15752	H	83.68700	69.72280	83.67190	2442.91795	1691.13637	-1034.61871	1
15753	C	82.99500	71.37380	84.95390	747.48769	-516.64910	76.07140	1
15754	H	83.61300	70.98680	85.79290	-2661.14238	1489.24911	773.74709	1
15755	H	82.07200	71.89880	85.27890	-560.36490	-2073.15394	-2299.18467	1
15756	S	83.97900	72.63280	84.11290	-393.35366	170.28612	357.05201	1
15757	H	85.18200	72.12980	84.34390	-934.84142	706.51112	-2919.78420	1
15758	C	81.93800	69.10780	84.71990	-663.17384	500.13723	376.18375	1
15759	O	82.51800	68.29280	85.42290	-489.82023	-377.73486	-490.93762	1
15760	N	80.65300	69.10580	84.45990	620.55471	-132.67695	556.75935	1
15761	H	80.19800	69.73580	83.83490	-2555.32480	-1828.15402	-162.46305	1
15762	C	79.68700	68.14480	85.04490	-411.87352	253.31633	-773.07312	1
15763	H	80.05800	67.92580	86.03490	-1436.50210	-2775.98866	-358.57345	1
15764	C	78.28300	68.75380	85.06290	-345.68825	763.58357	359.01361	1
15765	H	77.45500	68.03180	85.23190	2182.10346	2181.03833	616.21628	1
15766	H	78.09100	69.16680	84.04990	1968.74098	-958.03083	-2259.30567	1
15767	C	78.00400	69.82480	86.20890	21.66441	198.75540	889.65046	1
15768	H	78.90500	70.47180	86.14290	-1124.67544	653.13390	-2864.74213	1
15769	C	76.81100	70.73680	85.85990	-442.51807	603.47208	521.00884	1
15770	H	76.67900	71.41480	86.72990	-1424.58125	2302.51876	-1602.24900	1
15771	H	77.14500	71.31780	84.97290	-1675.25388	735.45172	-2559.46507	1
15772	H	75.93600	70.06580	85.72890	2457.59394	1188.55643	1563.90277	1
15773	C	77.83700	69.07980	87.51390	259.07306	560.55749	670.90048	1
15774	H	76.86500	68.54180	87.53190	2630.65550	885.60610	1481.07384	1
15775	H	77.89600	69.81380	88.34590	1042.12469	-1661.88916	-2459.74120	1
15776	H	78.56200	68.26680	87.73190	100.03453	2293.77046	2151.00823	1
15777	C	79.65200	66.80780	84.29190	-497.04322	-497.78045	580.18417	1
15778	O	79.37600	65.74280	84.89590	483.03343	-539.98788	-314.19584	1
15779	N	79.98800	66.80280	82.99990	630.53445	-66.55911	557.37642	1
15780	H	80.13000	67.65680	82.50490	1403.00927	-2147.30901	-1821.77255	1
15781	C	80.27200	65.57980	82.21990	348.30010	-448.08950	-713.69030	1
15782	H	79.38000	64.97580	82.30090	1653.53871	1518.54351	-2204.10108	1
15783	C	80.25600	65.98080	80.69390	-330.36906	570.92528	629.56462	1
15784	H	80.91000	66.86380	80.53090	2649.74001	-536.50494	1609.11980	1
15785	H	79.24200	66.28180	80.35290	28.02504	-800.85526	-3042.37928	1
15786	C	80.67100	64.84780	79.76590	95.16582	863.10047	278.30207	1
15787	O	80.29900	63.70080	79.96890	494.90230	508.91229	345.98732	1
15788	N	81.33000	65.20580	78.66090	438.82548	-590.04873	-414.66491	1
15789	H	81.30100	66.17680	78.42390	-88.44591	2770.89819	-1487.45648	1
15790	H	81.92300	64.53680	78.21290	-1620.76387	-664.79494	2613.31177	1
15791	C	81.38000	64.62380	82.85090	827.58549	-12.68046	382.61268	1
15792	O	81.10700	63.45380	83.05790	-128.54851	778.97455	-17.35391	1
15793	N	82.53700	65.11480	83.31390	-336.41963	-722.01654	279.61803	1
15794	C	83.22100	66.26080	82.69590	545.21241	-111.42309	722.34294	1
15795	H	82.94100	67.16080	83.28390	1549.02701	-2008.63643	1861.21499	1
15796	H	82.92800	66.49280	81.64990	909.45614	-1204.18131	-2760.62730	1
15797	C	83.43800	64.25680	84.07790	-238.07708	-339.70476	-812.01661	1
15798	H	83.55400	63.29780	83.59490	2126.73239	-1230.34476	1965.06675	1
15799	C	84.69700	65.12580	84.13990	-794.25120	-125.86467	429.85360	1
15800	H	85.61200	64.50480	84.24490	2282.02598	693.88454	2051.61105	1
15801	H	84.61000	65.77680	85.03590	-1598.53836	-1253.88925	2402.22045	1
15802	C	84.69800	65.91280	82.85790	-745.90164	-524.29326	-14.08283	1

15803	H	85.34200	66.81680	82.82290	1915.70789	-1911.19203	-1604.87836	1
15804	H	85.02000	65.31480	81.97890	2196.43781	-1270.72493	1859.87777	1
15805	C	82.95000	63.89680	85.48290	699.85510	-16.64032	-584.27471	1
15806	O	83.29800	62.85680	86.07890	430.43769	-589.05475	-302.26665	1
15807	N	82.18500	64.85480	86.18890	647.91516	-462.28353	281.37551	1
15808	H	82.04200	65.79680	85.89690	-1847.35312	-2155.36681	-1356.43157	1
15809	C	81.67900	64.58180	87.53990	887.62622	204.82628	40.21058	1
15810	H	82.46700	64.31080	88.22590	1310.86746	1453.57780	-2463.12085	1
15811	C	80.99100	65.83580	88.13590	-474.95018	757.05842	-180.93058	1
15812	H	80.39700	66.35780	87.35590	2521.47463	1877.07192	130.35679	1
15813	C	80.07500	65.51980	89.33090	-484.17800	742.03202	215.43246	1
15814	H	79.23600	64.80180	89.20790	-1420.43333	-679.00593	2723.88442	1
15815	H	79.60200	66.50280	89.53890	-348.43063	1610.18341	-2680.32306	1
15816	H	80.59200	65.06380	90.20190	-2652.82464	1246.87961	1142.82060	1
15817	C	82.10400	66.82480	88.54790	342.79674	752.15329	384.97640	1
15818	H	82.94700	66.77280	87.82690	1060.16392	253.18339	2951.30088	1
15819	H	82.54800	66.39380	89.46990	211.16541	-1465.18218	2776.12618	1
15820	C	81.75600	68.27980	88.67090	768.55745	474.63903	-124.45175	1
15821	H	81.18400	68.37880	89.61690	-1083.06842	-2623.20134	1357.94100	1
15822	H	82.69900	68.86180	88.75190	-1627.98157	-1946.31068	1860.04758	1
15823	H	81.16100	68.59880	87.78890	-1718.41937	-506.04212	2586.34539	1
15824	C	80.71800	63.40580	87.53890	685.09411	526.56062	291.25758	1
15825	O	80.75900	62.52280	88.33690	-297.37391	285.74901	-673.45637	1
15826	N	79.82600	63.35580	86.53090	-564.81906	398.55425	-484.56808	1
15827	H	79.63700	64.12880	85.92890	1420.45157	-2166.26829	-1785.44820	1
15828	C	78.94800	62.20480	86.22690	3.46571	435.45703	-801.13430	1
15829	H	78.49300	61.75780	87.09790	1788.16026	-1479.33231	2124.21398	1
15830	C	77.77100	62.67180	85.34990	-247.32046	-653.19514	-586.19084	1
15831	H	78.14500	63.09380	84.39290	-1169.14294	2061.70156	2068.98953	1
15832	H	77.13300	61.79380	85.11490	2696.87489	115.39037	1616.09935	1
15833	C	76.80000	63.71180	86.07290	-89.35583	-902.76136	92.13284	1
15834	H	77.33300	64.63980	86.37290	241.23475	258.76471	-3126.19143	1
15835	C	75.74100	64.25280	85.11390	508.89365	-686.87176	-317.30970	1
15836	H	76.09600	64.59780	84.11990	1290.22365	-2286.51655	-1733.60642	1
15837	H	74.99800	63.47780	84.82990	-1470.30461	176.98919	-2775.80717	1
15838	H	75.09800	65.00780	85.61490	2434.08427	-1731.40928	987.76611	1
15839	C	76.08600	63.16980	87.28090	-698.92658	-473.00164	-345.28551	1
15840	H	75.75700	62.14180	87.01690	-444.39435	-2545.30035	1795.04485	1
15841	H	76.70900	63.27280	88.19590	1112.26189	2060.49673	2101.29792	1
15842	H	75.17000	63.75080	87.51990	-1081.19711	-1744.84542	2384.27211	1
15843	C	79.71000	61.03980	85.48290	407.63862	567.41295	-585.93883	1
15844	O	79.10700	60.24680	84.78490	-160.11677	548.56613	545.03674	1
15845	N	81.05000	60.89580	85.67690	535.16889	-564.79892	-327.51905	1
15846	H	81.56300	61.63580	86.10390	1084.70637	-1558.34142	2508.62718	1
15847	C	81.67900	59.58380	85.48290	568.02070	-235.90330	673.16649	1
15848	H	80.94000	58.86180	85.16790	-1777.96583	935.53677	2421.12261	1
15849	C	82.84300	59.77880	84.44790	539.89634	-555.84947	480.61868	1
15850	H	83.72900	59.14880	84.67490	1893.32725	1319.30710	2138.44966	1
15851	H	83.19000	60.83380	84.42090	1060.88305	2829.74290	874.81911	1
15852	C	82.46800	59.21580	83.06090	638.82962	-68.15783	-647.07204	1
15853	C	82.09700	57.87180	82.98090	-614.41689	664.29035	-112.52206	1
15854	H	82.06500	57.29180	83.89090	-1039.31101	257.72386	-2958.31663	1
15855	C	81.76000	57.32380	81.74990	-200.07316	-400.13889	794.55057	1
15856	H	81.57400	56.26280	81.67190	1132.54480	2819.76813	-815.15411	1
15857	C	81.73300	58.12080	80.62590	794.88340	-446.15328	-23.63556	1
15858	O	81.35100	57.56780	79.39290	474.27188	613.47937	-149.45392	1
15859	H	80.98200	56.68280	79.44890	-2193.12138	-319.55392	-2233.00921	1
15860	C	82.57200	59.98580	81.93490	662.44523	-600.59580	-178.61133	1
15861	H	82.88300	61.01080	82.07090	2145.09316	-1742.62567	-1503.34871	1
15862	C	82.18800	59.43480	80.71690	-585.85399	-486.28005	-501.75474	1
15863	H	82.27300	60.00980	79.80690	-2931.97802	-993.46169	561.03920	1
15864	C	82.20300	59.06980	86.83590	541.32979	112.43807	725.10050	1

15865	O	82.67700	57.91880	86.94890	332.09874	31.53896	715.78136	1
15866	N	82.03300	59.88880	87.89690	-705.35059	-270.74143	-376.63232	1
15867	H	81.63800	60.79980	87.80690	-2286.10306	230.95421	2149.09730	1
15868	C	82.49000	59.51680	89.18790	-428.60429	-658.60830	-462.58456	1
15869	H	83.47100	59.07480	89.09290	-656.54819	-2944.77325	891.89752	1
15870	C	82.64400	60.75380	90.06890	594.76028	562.03824	-402.27382	1
15871	H	83.36700	60.50080	90.87390	1955.73995	-1226.39319	2137.58443	1
15872	H	81.69200	61.08180	90.53790	2705.22946	-863.29827	1354.50209	1
15873	H	83.13700	61.58380	89.51890	-2831.04941	-1372.20502	-20.94952	1
15874	C	81.62000	58.45680	89.91790	690.61544	503.73551	317.41432	1
15875	O	80.36400	58.52880	89.88090	473.31981	534.42028	-337.62487	1
15876	N	82.22900	57.62180	90.79390	-74.95390	-710.43364	449.82023	1
15877	H	83.21700	57.48780	90.80390	-2531.29487	1335.52380	1306.57900	1
15878	C	81.49200	56.95580	91.86190	-485.07052	583.70129	505.42101	1
15879	H	82.21900	56.51580	92.52890	415.96401	-2019.59418	-2376.22379	1
15880	C	80.59000	57.87080	92.75390	-491.30625	-658.90044	394.86630	1
15881	H	79.86600	58.38380	92.08590	1816.04908	1152.37066	2296.13454	1
15882	H	80.09300	57.24080	93.52290	2201.76944	-1700.96961	-1468.72051	1
15883	C	81.46100	58.86380	93.52190	-583.73211	606.76237	-350.06750	1
15884	C	82.52500	58.47380	94.32090	-97.74378	-758.65384	496.32802	1
15885	H	82.86400	57.44780	94.30990	2840.28852	-959.12381	954.49927	1
15886	C	83.30600	59.40880	95.01490	402.20585	465.13548	673.29818	1
15887	H	84.13400	59.10480	95.63690	2263.76029	-1687.84156	-1387.37393	1
15888	C	82.96400	60.78380	94.84590	562.69367	510.87950	503.81442	1
15889	H	83.47000	61.57380	95.38290	2290.66345	1104.58151	1852.29232	1
15890	C	81.16500	60.24680	93.35090	630.27321	595.89160	281.28258	1
15891	H	80.29800	60.48480	92.75290	-1224.04756	2160.53694	-1931.84211	1
15892	C	81.88600	61.18680	94.02290	-516.25570	734.96358	157.35180	1
15893	H	81.69100	62.24580	93.93990	-141.20022	-1686.02368	2652.47297	1
15894	C	80.76400	55.70980	91.43490	-500.67091	191.22002	-737.70899	1
15895	O	79.70800	55.31080	91.95290	-20.76668	609.16259	502.11245	1
15896	N	81.30300	54.90280	90.49790	-613.53821	139.25076	-562.89642	1
15897	H	82.18100	55.22180	90.14890	-1239.73952	2117.27393	1969.37129	1
15898	C	80.71900	53.68480	89.94390	612.00407	597.23992	-316.55411	1
15899	H	79.65100	53.83680	89.97990	2833.75944	-1174.44528	-699.07934	1
15900	C	81.27100	53.31280	88.53290	-560.37603	454.47798	-557.56567	1
15901	H	80.83700	52.33080	88.24890	1578.57404	-2692.15327	398.29759	1
15902	H	82.36400	53.11580	88.57390	1257.69372	-2241.60671	-1814.28556	1
15903	C	80.98500	54.38180	87.51690	-841.99760	349.42617	19.80891	1
15904	H	81.51500	55.32680	87.76390	2395.44139	-729.31323	-1904.78056	1
15905	C	81.53700	54.10480	86.08490	671.95339	-472.07004	396.33259	1
15906	H	81.59600	55.10380	85.60390	-965.80976	2726.10573	1238.46084	1
15907	H	82.55700	53.69280	86.23790	-2210.97216	-2224.80784	-245.06818	1
15908	H	81.03200	53.33780	85.45890	-1644.81482	-2509.38904	946.45502	1
15909	C	79.54200	54.65580	87.23390	-438.41855	552.71613	-577.70672	1
15910	H	79.04100	54.79480	88.21590	-1489.29346	-1960.43075	-1958.81150	1
15911	H	79.34300	55.38180	86.41690	-2620.30005	1269.85404	1191.52198	1
15912	H	79.14800	53.69780	86.83090	-875.74175	-2192.85269	2079.11032	1
15913	C	80.97300	52.63780	90.95190	-295.42717	226.19485	832.47203	1
15914	O	82.06500	52.10580	91.11790	-627.35600	133.17096	460.77888	1
15915	N	79.89800	52.16980	91.66690	699.98022	-390.63673	264.76956	1
15916	H	78.97800	52.45280	91.40590	-682.54242	2389.00221	-1930.03381	1
15917	C	80.08900	51.23780	92.72590	-238.89617	603.03427	640.88165	1
15918	H	79.15000	50.75680	92.95390	2214.23644	-2229.66527	-154.84179	1
15919	H	80.83200	50.52280	92.40490	-1666.71564	2604.77001	-579.18770	1
15920	C	80.71500	51.67880	93.95290	774.96208	-244.92028	-413.39912	1
15921	O	81.35700	50.96780	94.71090	241.13544	-647.48386	382.42068	1
15922	N	80.54900	52.96080	94.25390	210.37923	-723.05530	381.58078	1
15923	H	80.17900	53.60180	93.58590	2801.91022	231.30967	1412.09814	1
15924	C	81.11800	53.58680	95.39990	-687.52660	598.73800	16.46173	1
15925	H	82.06300	53.10980	95.61590	-2114.34932	-2272.06003	515.26344	1
15926	C	81.44900	55.05980	95.20090	14.46586	-473.49130	779.13268	1

15927	H	82.12800	55.25980	94.34390	-3143.66611	68.32620	104.50435	1
15928	H	80.47800	55.52680	94.93090	1235.10165	-2883.76761	237.98003	1
15929	H	81.73900	55.58780	96.13490	-2909.47399	-1185.33090	-167.86302	1
15930	C	80.21700	53.42580	96.59890	723.55233	-554.90228	-2.54632	1
15931	O	79.01700	53.23880	96.46890	631.29480	-307.86580	360.98858	1
15932	N	80.81200	53.47280	97.79790	-256.05364	543.33727	593.20607	1
15933	H	81.79700	53.59180	97.89590	-556.24216	1897.09413	2447.41798	1
15934	C	80.10400	53.53380	99.00590	-86.72511	664.13658	618.75064	1
15935	H	79.05200	53.39680	98.80390	-475.19793	2330.06184	-2059.90897	1
15936	C	80.72100	52.50880	100.05290	230.36682	-429.05876	-770.90253	1
15937	H	81.81400	52.47280	99.85790	1869.39229	-1429.11700	-2088.35420	1
15938	H	80.40300	52.62580	101.11090	2229.68911	-1199.15006	1867.82008	1
15939	C	80.28200	51.06780	99.72490	737.32720	385.05736	373.53773	1
15940	H	80.89900	50.69980	98.87790	-910.52263	-2102.76751	-2155.81621	1
15941	H	80.52600	50.40280	100.58090	1206.09344	-2445.06171	1570.10765	1
15942	C	78.78400	50.94080	99.35690	-220.94944	-409.60827	-784.12589	1
15943	H	78.65100	51.25080	98.29890	592.24843	643.37699	-3022.17373	1
15944	H	78.23800	51.66280	100.00090	-865.79467	1998.83832	2270.08175	1
15945	C	78.18400	49.58980	99.52590	655.94020	477.55902	-416.08993	1
15946	H	78.30600	49.19080	100.55490	2211.02539	2206.23220	-377.00458	1
15947	H	78.65300	48.87980	98.81090	2548.99670	-723.66099	1696.21839	1
15948	N	76.74200	49.65680	99.25790	416.26646	494.79098	542.74894	1
15949	H	76.66100	49.91580	98.25390	-1361.29987	743.28023	2737.26568	1
15950	H	76.41300	50.36980	99.93990	2244.37531	-1615.88694	1499.97171	1
15951	H	76.27200	48.73580	99.36890	-544.92497	471.79777	3062.46467	1
15952	C	80.22600	54.95980	99.62690	-378.19203	-96.29545	-824.10495	1
15953	O	81.26600	55.62880	99.55690	-515.08317	-299.62246	-518.21129	1
15954	N	79.06500	55.53180	100.15290	70.80141	-566.95695	-621.46542	1
15955	H	78.24600	54.96680	100.20890	2164.26931	2075.14709	952.85317	1
15956	C	78.96600	56.92180	100.51590	-589.40826	-553.58529	-421.41694	1
15957	H	79.79100	57.47180	100.08790	-1675.87924	-833.15247	-2528.93495	1
15958	C	77.72400	57.53680	99.83390	623.27081	199.74475	-634.89096	1
15959	H	76.80700	57.08980	100.27490	1411.86485	-2624.29912	-1008.91922	1
15960	H	77.67100	58.59880	100.15690	-2148.84816	713.62940	-2184.35595	1
15961	C	77.84300	57.42380	98.31090	-242.60111	-876.89297	60.45187	1
15962	C	78.61700	58.35580	97.58790	105.34580	-787.70608	447.07090	1
15963	H	79.29400	59.02580	98.09690	-525.39720	2291.80635	-2090.40849	1
15964	C	78.64100	58.25080	96.16690	851.10042	-138.40312	-296.51924	1
15965	H	79.20400	58.96380	95.58290	-2920.42460	1090.93755	423.32218	1
15966	C	77.93600	57.23580	95.50590	-630.03242	-493.47572	437.02616	1
15967	H	78.04600	57.12480	94.43790	1998.86955	251.13034	-2416.54305	1
15968	C	77.15700	56.45480	97.64590	577.85381	-618.90545	338.36670	1
15969	H	76.68800	55.65580	98.20190	-267.36934	-1292.25015	2856.01635	1
15970	C	77.20800	56.31680	96.28190	561.30100	446.83096	-562.79151	1
15971	H	76.74300	55.47580	95.78890	-2001.23461	2387.81635	437.74347	1
15972	C	78.97800	57.25380	102.00090	-768.63764	349.27438	344.46275	1
15973	O	79.06900	58.41480	102.47090	125.32698	449.02694	637.41289	1
15974	N	78.95100	56.16180	102.83090	540.14932	-557.66368	-331.54521	1
15975	H	78.58300	55.30280	102.48390	-2360.81145	1736.90962	-1143.65227	1
15976	C	78.88800	56.33080	104.26790	675.31176	-597.84226	-134.12552	1
15977	H	78.72600	57.37580	104.48790	2697.96271	376.01024	1574.11554	1
15978	C	77.73800	55.52780	104.91990	583.94266	-608.02770	-347.51156	1
15979	H	77.73700	55.67180	106.02190	-2152.12641	2287.11714	188.87393	1
15980	H	78.02200	54.47280	104.71790	854.06480	-2371.74791	-1882.44824	1
15981	C	76.39500	56.07880	104.37490	-387.71609	-456.11444	-687.81310	1
15982	H	76.33400	56.03080	103.26590	2421.74602	-1977.78675	-348.90118	1
15983	H	76.43600	57.17880	104.52490	2443.08952	841.08750	1795.02413	1
15984	C	75.12500	55.41780	105.00790	97.14733	-453.00127	-785.36823	1
15985	H	74.21200	55.89580	104.59090	-829.78562	-2235.84412	-2051.99492	1
15986	H	75.24900	55.59280	106.09790	-2546.31834	-786.16770	-1672.25282	1
15987	C	75.05000	53.89580	104.84890	-167.98973	-550.29803	-707.39136	1
15988	H	75.91600	53.36880	105.30390	2465.04029	-386.94185	-1916.26684	1

15989	H	74.88900	53.64780	103.77790	-1773.59602	2596.47137	104.49781	1
15990	N	73.87300	53.41980	105.56690	-551.26435	350.18367	-534.93112	1
15991	H	74.07600	53.58480	106.57290	2814.68176	-460.90583	-1327.91516	1
15992	H	73.01100	53.99980	105.60990	-241.20627	2579.86855	-1784.46744	1
15993	H	73.73800	52.42180	105.30890	1431.47478	1835.82938	2116.32622	1
15994	C	80.16700	55.94380	104.98190	-566.28741	-635.08442	327.77637	1
15995	O	80.39300	56.21780	106.18890	-474.92593	-350.84747	-524.38406	1
15996	N	81.09000	55.32780	104.18990	-623.65888	50.73588	566.69900	1
15997	H	80.83000	54.95680	103.30190	-1478.77195	1668.88869	2219.52028	1
15998	C	82.53200	55.16980	104.40690	222.09073	827.13953	312.99667	1
15999	H	82.59600	54.28380	105.02190	-3144.52774	-72.28619	70.32920	1
16000	C	83.29300	54.91580	103.09090	63.11093	744.29227	-522.96944	1
16001	H	82.81500	54.08480	102.53090	-1224.14638	-2204.00011	1882.04021	1
16002	O	84.67700	54.54080	103.24590	-725.06844	-109.93823	-292.94466	1
16003	H	84.78500	53.96080	104.00290	-304.29553	-2261.69628	-2165.72399	1
16004	C	83.23200	56.06680	102.10790	-556.50453	-374.31243	617.77335	1
16005	H	83.45200	55.63380	101.10790	-1792.42401	-2551.05235	421.39563	1
16006	H	83.82700	56.93980	102.45090	-1821.08005	-628.06650	2487.45375	1
16007	H	82.23100	56.54280	102.03790	1180.34726	2425.35769	-1619.45875	1
16008	C	83.20700	56.25880	105.24790	-485.58654	578.43675	-510.94779	1
16009	O	83.00500	57.44880	105.00190	547.13124	-567.29965	-49.45441	1
16010	N	83.99000	55.88980	106.24490	529.58547	240.29309	-611.94015	1
16011	H	84.16600	54.94980	106.52790	88.04386	-84.20542	3143.78497	1
16012	C	84.73700	56.88680	106.99290	821.10572	-384.26135	-97.87550	1
16013	H	84.96900	57.66880	106.28490	-2004.76628	1616.49215	-1807.23311	1
16014	C	83.91500	57.42980	108.20490	901.59265	121.77557	-61.25690	1
16015	H	84.21500	58.48080	108.40390	58.48733	-2968.54791	1040.44643	1
16016	H	82.85200	57.49980	107.89190	1198.21386	1397.51495	2551.36468	1
16017	O	83.89700	56.69080	109.40790	-31.33697	777.03860	137.31799	1
16018	H	83.44200	57.18580	110.09290	1292.49466	1810.80216	2224.56272	1
16019	C	86.04500	56.31880	107.48390	910.25559	-53.67074	2.28316	1
16020	O	86.23700	55.11080	107.49890	224.73168	386.38818	-651.02003	1
16021	N	86.96200	57.19680	107.92490	592.41732	-115.38395	-590.25465	1
16022	H	86.55800	58.10780	107.88190	-196.95547	-3017.49164	868.43480	1
16023	C	88.24100	56.92680	108.44490	-44.60705	39.58217	-909.88706	1
16024	H	88.79900	56.31480	107.75190	-2313.53670	-391.48440	2095.83257	1
16025	C	88.99900	58.27680	108.62790	528.28372	275.33553	-690.33156	1
16026	H	88.48300	58.99280	109.30190	1616.71985	2514.68091	980.21583	1
16027	H	90.03800	57.98680	108.89590	2278.22391	-1515.91739	-1552.39059	1
16028	H	89.10200	58.71980	107.61390	-2193.15855	-1988.53404	1064.90103	1
16029	C	88.23700	56.08880	109.70490	636.87901	275.86417	591.38404	1
16030	O	89.01500	55.11480	109.84290	668.78163	-409.00382	95.25881	1
16031	N	87.28400	56.41280	110.61790	542.61366	463.04814	-451.47439	1
16032	H	86.91200	57.33580	110.56290	2022.12249	-1412.01961	1953.31705	1
16033	C	86.97200	55.47480	111.74990	-589.19915	-411.36289	-561.31626	1
16034	H	87.90700	55.26180	112.24790	2295.20594	491.90314	-2094.82391	1
16035	C	85.97400	56.15380	112.70390	-440.56961	335.32811	724.50292	1
16036	H	85.55200	55.42080	113.42490	-2658.59194	-436.23655	1624.75006	1
16037	H	85.16200	56.58080	112.07790	1386.42037	-1331.91514	2490.39492	1
16038	C	86.51500	57.41880	113.51390	-524.96174	589.96805	455.85510	1
16039	H	85.63700	57.75580	114.10590	-403.58530	-2866.71174	-1231.79094	1
16040	H	86.86800	58.20880	112.81690	3080.02555	295.04673	569.75107	1
16041	C	87.65700	56.97980	114.46190	-379.69386	543.51629	-625.99810	1
16042	O	87.51800	56.06080	115.23690	-568.76345	-231.43650	-496.56068	1
16043	N	88.78900	57.67580	114.32290	105.92758	837.51450	-4.59422	1
16044	H	88.76800	58.52780	113.79990	-1547.03354	-1699.33908	2148.75782	1
16045	H	89.56800	57.40480	114.88790	25.26782	-2350.18093	-2091.46775	1
16046	C	86.38100	54.13380	111.32290	180.00555	27.32998	-893.47752	1
16047	O	86.84900	53.05580	111.69790	-204.81051	-507.76855	569.07907	1
16048	N	85.41700	54.13580	110.31590	-576.83895	-497.44063	-363.98067	1
16049	H	85.05700	54.93680	109.84490	1266.94635	-2491.28727	1444.49330	1
16050	C	84.85500	52.81180	109.85490	416.52979	487.10829	-648.59807	1

16051	H	84.53200	52.34680	110.77490	299.29514	-727.32019	-3046.25245	1
16052	C	83.70500	53.01180	108.93090	-15.29436	-675.26288	-612.56601	1
16053	H	84.01300	53.65080	108.07590	1428.91896	-2800.76377	-110.17758	1
16054	H	83.34100	52.09480	108.41990	2239.82015	-1322.46097	-1769.89517	1
16055	N	82.20500	53.38680	110.95190	-135.16195	-113.48893	-825.54455	1
16056	H	82.76300	52.85980	111.59290	2109.15876	335.39947	-2310.23435	1
16057	C	82.52300	53.64980	109.61990	-546.29797	-362.55731	633.68899	1
16058	C	81.11100	54.09780	111.23090	-452.77879	119.68693	782.37932	1
16059	H	80.61100	53.96480	112.18990	515.65026	-1085.65638	-2907.52150	1
16060	N	80.67200	54.79180	110.20390	-672.10464	-496.37782	120.65113	1
16061	C	81.57800	54.50080	109.14890	-415.10380	170.73927	793.71780	1
16062	H	81.39700	54.85780	108.14190	-2409.73621	-1633.57327	1192.82690	1
16063	C	85.90800	51.89980	109.19590	-57.11934	500.76370	759.88427	1
16064	O	85.88900	50.70180	109.38790	747.08667	-254.89254	-22.77120	1
16065	N	86.82900	52.50780	108.42890	434.81749	-696.92036	194.69990	1
16066	H	86.68300	53.45680	108.15990	2062.99251	-2373.89735	-83.06334	1
16067	C	88.02200	51.87180	107.84890	682.44651	538.86219	-274.49097	1
16068	H	87.57200	51.13580	107.19990	-1843.79418	-2538.43053	234.56273	1
16069	C	88.70700	52.92580	106.97790	-743.15574	-519.11314	98.44841	1
16070	H	89.07900	53.71380	107.66690	1482.52963	-2243.39052	-1633.25781	1
16071	H	88.02500	53.45380	106.27890	1598.24750	-2654.66864	544.57836	1
16072	H	89.64100	52.60980	106.46590	-670.78534	1167.49753	2843.45262	1
16073	C	88.99100	51.29980	108.85590	656.08552	-500.36518	-388.12045	1
16074	O	89.45100	50.19180	108.67390	-267.34786	-76.77617	-739.09253	1
16075	N	89.27600	51.98380	109.97890	-430.61950	-549.47687	474.67284	1
16076	H	88.76800	52.80380	110.22890	-911.04899	-2824.16187	1045.14387	1
16077	C	90.10100	51.42580	111.06990	-685.54544	552.14713	237.93275	1
16078	H	91.01100	51.07180	110.60790	-937.79610	2652.29756	-1408.57459	1
16079	C	90.26000	52.46080	112.19890	-150.36184	-552.95767	-709.28142	1
16080	H	90.54900	51.99480	113.16490	-2813.47406	1355.73689	380.22020	1
16081	H	89.29800	53.00080	112.32690	-1967.51298	1885.96383	1571.70587	1
16082	C	91.46800	53.42280	111.91590	547.78928	-534.48686	495.68306	1
16083	H	91.24700	53.92980	110.95190	945.15212	-928.87648	2853.43690	1
16084	C	91.52600	54.66780	112.80790	-324.36065	-543.92493	656.03875	1
16085	H	91.94300	54.47580	113.81990	-1370.29770	-1637.02729	-2310.98510	1
16086	H	92.19500	55.45480	112.39790	-1482.15837	2656.29835	-803.43753	1
16087	H	90.49100	55.02780	112.99190	-1680.46250	1661.10919	-2077.25499	1
16088	C	92.83900	52.70780	111.87190	-401.11306	622.08389	-532.51380	1
16089	H	92.94400	52.02380	111.00290	-152.06164	-2008.65723	2416.69188	1
16090	H	93.60500	53.51180	111.82990	2247.42890	2158.53128	433.62692	1
16091	H	93.04000	52.07480	112.76290	1888.77528	1844.73379	-1711.05564	1
16092	C	89.46100	50.19980	111.71690	-554.61851	177.36824	701.70494	1
16093	O	90.15700	49.23380	112.03990	-668.38767	417.15757	-53.52294	1
16094	N	88.19500	50.21680	112.07190	504.38531	-570.37054	364.61650	1
16095	H	87.72300	51.07580	111.88590	-1725.82391	1957.80252	-1756.91984	1
16096	C	87.47100	49.11180	112.69890	394.57747	402.03212	717.02845	1
16097	H	88.04300	48.79080	113.55590	-2404.20558	-1920.06895	656.77771	1
16098	C	86.10000	49.48680	113.13590	601.96840	-204.01925	-653.80516	1
16099	H	85.43700	48.61080	113.30090	-2440.18554	-196.75757	-1976.10911	1
16100	O	85.50100	50.38680	112.30590	203.56133	657.91341	386.44529	1
16101	H	85.67800	50.08280	111.41290	-2043.42410	390.47843	-2360.12092	1
16102	C	86.15600	50.20880	114.52090	-427.06329	239.43245	-769.24642	1
16103	H	85.14000	50.56980	114.78890	-2914.04759	63.16303	-1184.29867	1
16104	H	86.84200	51.06980	114.37390	-874.83740	-2997.72464	382.79595	1
16105	H	86.58700	49.54880	115.30390	-2521.49096	-1567.58855	-1040.66119	1
16106	C	87.33200	47.86380	111.81290	737.98452	-530.38323	74.32013	1
16107	O	87.28100	47.98280	110.59890	396.32778	-502.71341	462.41837	1
16108	N	87.22900	46.69980	112.39890	-249.40738	613.04579	-524.06403	1
16109	H	87.31500	46.64780	113.38990	1722.25761	-1493.91079	-2168.01418	1
16110	C	87.00800	45.43480	111.73590	786.20236	-460.38551	37.17575	1
16111	H	87.60700	45.49580	110.83890	767.49152	2902.13019	-941.71299	1
16112	C	87.63800	44.22280	112.49690	-387.94917	-654.79188	502.18925	1

16113	H	87.57500	43.32580	111.84390	-1412.57714	-1579.46339	-2325.54240	1
16114	H	88.73700	44.38180	112.50190	-2510.80954	-1313.94657	1366.60385	1
16115	O	87.05400	43.98480	113.80390	453.46026	474.88097	438.73578	1
16116	H	87.22400	44.78680	114.30390	-843.74822	-2911.98385	-840.63382	1
16117	C	85.56100	45.12680	111.38790	-851.26790	-304.48452	-118.67241	1
16118	O	84.61300	45.60580	112.09190	45.16908	705.48613	-351.96066	1
16119	O	85.32200	44.42480	110.35290	-400.57190	247.81106	633.84467	1
16120	H	78.81643	97.81752	70.47917	-999.51011	-1799.44688	34.70880	1
16121	N	79.00165	98.81334	70.30291	337.16018	-408.64395	326.15397	1
16122	H	78.17767	99.23284	69.91062	651.27822	-1981.11924	3655.34230	1
16123	C	80.21607	99.15755	69.65814	-23.80751	382.25219	81.15436	1
16124	H	80.99903	98.51346	70.23415	-922.71476	-1953.95251	-824.40764	1
16125	C	80.06015	98.81547	68.09730	-863.79145	640.91630	-868.40744	1
16126	H	79.91511	97.70714	68.00250	517.17908	-1337.29804	-613.52376	1
16127	H	79.13055	99.24670	67.70343	-1483.08750	-3339.35046	1699.72515	1
16128	C	81.26809	99.14127	67.24452	247.47063	394.38337	-479.20139	1
16129	H	81.44003	100.24567	67.12204	-1255.02474	-1414.78800	-4137.43763	1
16130	C	82.56952	98.52018	67.70410	442.04183	141.82847	-580.36623	1
16131	H	82.66535	98.88469	68.77755	402.62583	699.56120	-653.04030	1
16132	H	82.59802	97.38192	67.79985	-1139.92931	-755.52689	-1015.78187	1
16133	H	83.43677	98.81884	67.11406	2569.24061	2319.36480	-914.21328	1
16134	C	80.87975	98.72210	65.83409	669.17669	319.89136	-470.11043	1
16135	H	80.64229	97.61961	65.82229	-1482.17975	4195.27418	-2765.59314	1
16136	H	79.99241	99.26787	65.42286	4580.60282	-3701.15156	2745.61682	1
16137	H	81.71708	98.91770	65.17688	1349.68885	-1682.52879	-131.96712	1
16138	C	80.58365	100.72955	69.85347	446.79515	930.46142	263.20462	1
16139	O	81.17885	101.41174	68.98192	50.78799	-191.59852	89.09510	1
16140	N	80.14298	101.27718	70.95075	-223.50937	929.00465	-636.16441	1
16141	H	79.57317	100.72903	71.55932	-625.63369	3105.21123	-3631.15209	1
16142	C	80.78666	102.51057	71.36576	548.79937	-553.10755	-1381.60845	1
16143	H	80.13700	102.98935	72.05469	1212.72743	1746.08307	2085.04076	1
16144	C	82.13014	102.13405	72.04989	14.01703	292.53845	-174.00082	1
16145	H	82.84393	101.75532	71.20770	-852.37603	1783.84516	-929.91186	1
16146	O	82.38835	100.98285	73.08587	-54.62125	88.78276	-202.33989	1
16147	H	81.46150	100.75954	73.26198	-2353.08810	1054.61044	-1058.41922	1
16148	C	82.57972	103.36515	72.83639	-1262.96121	-143.60963	-174.30725	1
16149	H	81.89587	103.58321	73.68326	2431.31280	1118.05497	-136.55100	1
16150	H	83.64538	103.20654	73.27351	856.70041	-175.03162	548.01490	1
16151	H	82.66831	104.29292	72.15255	-1046.93994	1128.36850	-1414.59087	1
16152	C	80.99493	103.20178	69.78402	474.00983	-573.78425	749.54240	1
16153	O	82.06194	103.81877	69.54296	-88.39270	-206.52259	223.15221	1
16154	N	79.77454	103.66257	69.38360	629.72097	-376.63546	221.63443	1
16155	C	79.63049	104.16432	68.08083	566.46921	256.75562	-1.74071	1
16156	H	80.26918	103.50532	67.51102	360.75307	794.98255	-788.78320	1
16157	C	78.06588	104.05402	67.73818	264.00246	-356.71166	-314.67800	1
16158	H	77.79897	104.72085	66.89304	-873.92536	52.21787	-999.81848	1
16159	H	77.72999	103.06776	67.43130	-552.63295	-207.31977	-2706.58297	1
16160	C	77.46578	104.44484	69.11679	608.88859	259.15133	-306.54949	1
16161	H	77.52019	105.51509	69.39763	1171.48463	2152.54114	2144.64581	1
16162	H	76.37773	104.17094	69.13944	-665.46811	-1229.12994	4001.12650	1
16163	C	78.47649	103.51709	70.01940	-119.84923	616.81481	-524.33483	1
16164	H	78.48150	103.93264	71.11042	-3010.09312	474.61934	274.51003	1
16165	H	78.12640	102.42338	69.96373	-1676.65395	-1785.89799	1579.71180	1
16166	C	80.04571	105.74885	67.79942	188.34318	-285.27973	-376.09263	1
16167	O	79.81823	106.30934	66.72047	-643.10040	-532.19785	-280.92653	1
16168	N	80.73247	106.28584	68.76836	-109.01711	302.92440	582.37394	1
16169	H	80.98189	105.64576	69.49409	-1025.71307	1061.37789	-1386.00753	1
16170	C	81.40612	107.52797	68.61722	398.95572	602.40439	-597.74884	1
16171	H	80.78877	108.18230	67.97375	-488.09382	624.06608	1034.70554	1
16172	C	81.76437	108.03988	70.11599	662.13331	-10.57934	406.39412	1
16173	H	82.53004	108.84277	69.85237	-1343.78004	-839.94613	-3986.31806	1
16174	O	82.00178	107.07819	71.06907	68.78403	100.06306	-190.82817	1

16175	H	83.00832	106.99593	71.00948	1198.31506	1880.91982	232.21280	1
16176	C	80.64696	109.09548	70.48774	-705.85551	-845.65510	-125.30275	1
16177	H	80.28449	109.65151	69.60178	836.30205	-1055.18077	-874.35338	1
16178	H	79.87565	108.49438	70.95657	-2466.23678	-1642.16647	-152.89917	1
16179	H	80.93873	109.76771	71.36219	3042.16155	5494.83857	1888.85851	1
16180	C	82.81560	107.10475	67.93640	108.50921	94.97476	497.37001	1
16181	O	83.27248	107.71689	67.00827	-160.30986	-448.73739	268.91925	1
16182	N	83.41224	106.05884	68.54460	-1124.24637	527.24885	890.26837	1
16183	H	82.87556	105.52703	69.29297	2315.44495	-2228.88997	46.66726	1
16184	C	84.84242	106.15956	68.80933	-341.27313	-1186.01685	1066.65845	1
16185	H	85.20615	107.22837	68.58377	424.04812	-2334.13306	-1937.46184	1
16186	C	85.25840	105.72400	70.23621	-622.05590	-405.19453	-1067.08740	1
16187	H	84.79752	104.67924	70.45932	690.66851	-1607.79321	2399.21104	1
16188	H	86.34837	105.66528	70.36979	-395.73179	518.89289	1479.19117	1
16189	O	84.56093	106.48557	71.47586	410.50586	-41.39748	527.05891	1
16190	H	84.90752	105.83231	72.13281	-1317.52630	2371.36568	-2502.36310	1
16191	C	85.58203	105.07756	67.83067	422.42181	14.65291	877.15748	1
16192	O	86.78372	105.20760	67.64635	-26.21095	533.79122	136.24525	1
16193	N	84.78811	104.05632	67.51595	-180.90212	-572.92373	-243.81801	1
16194	H	83.81631	104.15170	67.76719	-1885.20836	-168.12144	221.11407	1
16195	C	85.48811	102.80095	67.40481	757.23803	-106.62520	858.92752	1
16196	H	86.48622	103.13296	66.97376	-1519.29301	-2830.11975	-2743.54905	1
16197	C	85.69168	101.92674	68.77008	308.24735	138.93284	-760.32464	1
16198	H	86.14414	100.94316	68.56368	-1371.70731	-1619.37520	-1386.13113	1
16199	C	86.71008	102.72395	69.68951	-411.14673	189.43161	653.98101	1
16200	H	87.50483	103.11549	69.09358	2855.31881	-1723.21245	2634.00219	1
16201	H	86.08267	103.42096	70.33152	-247.25693	-599.14370	-967.72374	1
16202	H	87.14340	102.04998	70.45469	-673.71846	1677.93500	-908.28469	1
16203	C	84.47415	101.60543	69.64274	-780.29660	186.35261	-134.57120	1
16204	H	84.14843	102.59708	70.06077	-825.65007	2222.92867	-3764.45538	1
16205	H	83.55295	101.18921	69.06557	-2651.72099	-959.98354	-2082.57130	1
16206	H	84.82867	100.83362	70.38190	2383.79157	-836.73957	608.00349	1
16207	C	84.68232	101.96129	66.30334	-220.88813	79.19548	-690.35477	1
16208	O	83.57370	101.43756	66.55028	3.72257	-149.92582	637.94252	1
16209	N	85.50532	101.72135	65.30565	634.97259	762.18039	-140.35528	1
16210	H	86.39714	102.17521	65.01167	517.33697	1014.96359	-349.52107	1
16211	C	84.72395	101.55564	64.05609	457.94100	144.17723	-279.16583	1
16212	H	83.68489	101.20204	64.44771	1659.67928	-2651.78719	-1588.51139	1
16213	C	84.57997	102.95504	63.36832	483.26095	-290.66437	902.63652	1
16214	H	85.57175	103.56767	63.10241	-1569.31262	-3514.63335	1930.98547	1
16215	H	83.98316	102.86769	62.42360	2999.77165	-2208.74436	119.56005	1
16216	C	83.70815	103.90147	64.29458	-375.22137	-687.75099	-285.16713	1
16217	H	82.62118	103.52786	64.34194	-1302.36419	76.99594	1201.93953	1
16218	H	84.19000	103.90453	65.29293	1488.30005	-185.23096	-676.31672	1
16219	C	83.66838	105.34608	63.63999	210.71889	-632.80866	-1327.07244	1
16220	O	83.70620	105.61043	62.44510	166.83632	725.23499	-186.39730	1
16221	N	83.55617	106.32063	64.63135	-164.51462	-462.66613	-310.25881	1
16222	H	83.96658	106.05628	65.54106	-3337.04781	1565.68847	3694.12840	1
16223	H	83.95341	107.23258	64.45939	-2973.79203	-1842.24137	1213.75636	1
16224	C	85.66592	100.48155	63.19900	-348.33389	-0.93382	304.62169	1
16225	O	86.62368	100.85428	62.56292	-70.97983	428.43012	368.35427	1
16226	N	85.17010	99.23140	63.36153	-71.02740	-649.93505	408.37313	1
16227	C	85.42960	98.16014	62.47172	399.68426	931.46363	71.30137	1
16228	H	86.36759	98.28926	61.91032	-964.57354	-542.50956	1078.41402	1
16229	C	85.34478	96.93048	63.46426	-944.30658	-909.35079	-756.16123	1
16230	H	85.02690	95.98226	63.00973	-3048.23267	895.19565	166.19871	1
16231	H	86.30305	96.85875	64.07664	3700.65644	530.81647	-1805.99885	1
16232	C	84.23244	97.35124	64.49167	-271.53482	503.59047	816.49637	1
16233	H	83.17190	97.03033	64.37654	3441.93887	1781.56942	-594.88815	1
16234	H	84.48031	97.02250	65.54901	-1622.54300	-566.46084	-1331.66439	1
16235	C	84.27686	98.92129	64.44344	-104.85739	-578.83089	-676.91193	1
16236	H	83.27526	99.49644	64.23579	3703.41745	-349.62170	-508.39186	1

16237	H	84.71388	99.40033	65.32302	-2714.62475	-636.47951	980.62095	1
16238	C	84.39155	98.02767	61.23997	-132.68913	-1115.80213	364.77845	1
16239	O	84.71219	97.41437	60.24074	479.34350	225.67916	944.91152	1
16240	N	83.15213	98.51274	61.54876	-14.51084	1401.69440	-1086.68565	1
16241	H	83.21003	98.85622	62.46140	-2476.37317	-944.82614	-2190.82464	1
16242	C	82.62499	99.37257	60.52574	900.95141	-91.13820	-143.62078	1
16243	H	83.31597	99.26189	59.69874	2878.78207	1203.01891	-857.78112	1
16244	C	81.16397	98.73951	60.28284	739.16655	115.87692	-345.53188	1
16245	H	80.64469	98.43669	61.23272	1022.96973	-1813.60900	-1525.63135	1
16246	C	80.26786	99.74295	59.51881	652.99705	159.43754	-1037.68007	1
16247	H	80.25562	100.63931	60.20204	-2149.01902	-700.21344	686.38412	1
16248	H	80.82740	100.06782	58.62618	-2049.26492	2672.83919	-3935.26433	1
16249	H	79.28813	99.40184	59.18230	1246.83606	816.38070	1832.91890	1
16250	C	81.36593	97.38032	59.54744	985.21309	202.91567	-796.39410	1
16251	H	82.25946	96.97668	60.03438	873.43640	1528.31591	1772.17710	1
16252	H	80.58391	96.63811	59.63123	2307.06406	-1856.87196	334.36165	1
16253	H	81.60554	97.49601	58.46586	1204.66714	-173.56820	2117.05120	1
16254	C	82.49666	100.90754	61.08048	-438.71220	-486.16424	53.82993	1
16255	O	82.14818	101.26422	62.21255	-284.47101	226.70978	-56.83954	1
16256	N	82.71244	101.68708	60.03912	356.63177	202.35523	-9.66715	1
16257	H	82.98657	101.18761	59.21184	255.92252	-58.10475	872.31484	1
16258	C	82.40743	103.07532	59.93161	698.71265	393.27417	194.00928	1
16259	H	83.06450	103.45541	60.81622	-2886.32093	-774.86186	2063.45776	1
16260	C	83.09140	103.60488	58.60288	756.14989	-741.25162	-126.57821	1
16261	H	82.66297	103.04606	57.72613	1037.33778	-612.26769	-820.80211	1
16262	H	82.86982	104.67937	58.35734	445.01166	608.26640	-3573.10679	1
16263	C	84.65372	103.44211	58.51961	998.78616	-223.54915	886.89878	1
16264	H	84.82500	102.38133	58.88818	2546.74227	-1202.49577	-2156.99882	1
16265	H	85.01088	103.49608	57.48392	1375.14418	749.49369	1473.86197	1
16266	C	85.32077	104.54558	59.39960	-773.47803	-377.68405	483.75225	1
16267	H	85.13790	104.31231	60.46320	332.85702	132.33576	-212.65521	1
16268	H	86.42175	104.42657	59.40622	58.25927	-817.51755	-2474.75458	1
16269	C	85.05327	106.03308	58.94816	-472.15507	80.96932	-60.14614	1
16270	H	85.70907	106.89408	59.32206	423.01754	1399.37343	3446.44253	1
16271	H	84.90864	106.10003	57.86832	-2827.02512	651.44645	1451.98619	1
16272	N	83.77322	106.40234	59.52386	-79.51839	306.60609	456.62581	1
16273	H	83.75024	106.44449	60.51835	-4251.96929	-3441.77950	1029.55302	1
16274	H	80.38632	103.74416	56.73783	1536.92639	-1616.42231	-4415.77737	1
16275	H	83.25644	107.21215	59.33841	1819.02161	-961.51295	-2764.79432	1
16276	C	80.87349	103.59992	59.93232	-387.72139	-122.29879	404.20927	1
16277	O	80.03924	102.78412	60.26211	90.29187	-397.28391	272.87209	1
16278	N	80.72459	104.92272	59.84944	681.79404	-624.82963	464.58143	1
16279	H	81.55664	105.49159	59.87521	-3127.83767	707.75097	-760.80188	1
16280	C	79.46903	105.51923	59.47961	292.42201	-574.77090	102.22778	1
16281	H	78.69529	105.01610	60.08234	-2410.03615	253.97073	556.39856	1
16282	C	79.66712	107.06496	59.76608	236.16810	-900.40155	95.74377	1
16283	H	80.55957	107.34083	60.37454	-1761.18950	1119.89803	-3035.74645	1
16284	H	79.71608	107.57973	58.75981	-585.77745	-344.55727	1259.26572	1
16285	C	78.36382	107.41578	60.50866	1553.12343	19.48528	512.25725	1
16286	H	78.26815	106.85485	61.47060	650.51850	341.37276	1108.91811	1
16287	H	78.36209	108.52622	60.75500	980.19195	2439.26019	-853.41596	1
16288	C	77.16149	107.13280	59.52131	-538.14053	230.49658	-620.44816	1
16289	H	77.46749	107.47825	58.48610	-1054.18199	1138.52679	1868.06819	1
16290	H	77.11936	105.99053	59.38985	3079.27981	669.97561	3165.86332	1
16291	C	75.83990	107.72422	60.10869	65.25852	-1044.97190	-257.63870	1
16292	H	75.88985	108.71192	60.62424	-414.83167	-2259.17487	835.71129	1
16293	H	75.02842	107.67533	59.38251	438.82153	-821.13278	-312.27419	1
16294	N	75.34379	106.71139	61.15472	606.70725	66.42431	-103.51959	1
16295	H	75.98363	106.53931	61.98744	1999.33240	-838.93814	-2138.87202	1
16296	H	74.28543	106.86152	61.61324	163.71500	191.31831	2069.61450	1
16297	H	75.32317	105.70499	60.77602	-437.88890	-1337.80677	793.51988	1
16298	C	79.22183	105.21184	57.87946	334.66878	110.13205	-193.01462	1

16299	O	79.93154	105.73144	57.04817	270.82803	65.09019	190.53391	1
16300	N	78.06963	104.59027	57.77015	-178.51499	-309.68068	749.43481	1
16301	H	77.61667	104.39424	58.69712	1463.94583	-287.84447	1676.20941	1
16302	C	77.86513	103.32094	57.04507	-255.13356	-375.92436	-208.27489	1
16303	H	77.86436	103.52881	55.95509	-661.12812	-126.07949	-2204.91199	1
16304	C	78.92771	102.20884	57.24699	250.51679	395.40838	-644.03368	1
16305	H	79.08582	101.98660	58.28785	457.52531	-426.62601	-80.13490	1
16306	O	80.64470	102.76413	56.89944	421.72193	-339.23833	0.86135	1
16307	H	80.82028	102.82089	57.87042	1782.73375	569.24372	4327.32478	1
16308	C	78.29843	101.00473	56.55693	597.76639	-613.06814	100.78897	1
16309	H	78.71529	100.03894	56.87568	-3941.00200	2201.07113	2928.27887	1
16310	H	77.17142	101.02185	56.84932	-1270.18660	790.95516	1402.94930	1
16311	H	78.49040	101.17068	55.42540	-93.88312	2473.40703	2847.16179	1
16312	C	76.37130	102.81137	57.56699	171.57418	-124.50597	-143.81606	1
16313	O	75.45645	102.76192	56.79728	-793.32506	192.26880	-498.03969	1
16314	N	76.43442	102.52576	58.89219	159.07721	405.89639	-488.25838	1
16315	H	77.35845	102.73080	59.28421	-938.68620	720.70179	517.29721	1
16316	C	75.26567	103.10523	59.54455	-501.10703	757.45770	-368.98481	1
16317	H	75.03257	103.87933	58.76162	455.24700	-557.15030	1728.66878	1
16318	C	73.95273	102.13701	59.63776	1267.40284	200.04970	-1024.67055	1
16319	H	73.14028	102.72891	60.15768	186.13320	-1024.41966	-1950.13102	1
16320	H	73.49278	102.05703	58.60276	-383.88938	485.39237	-1161.56783	1
16321	C	74.14005	100.80581	60.32741	660.73561	-313.74477	-9.76780	1
16322	C	73.31551	100.32408	61.38331	274.37329	-228.70314	-1088.09518	1
16323	H	72.41580	101.00463	61.66805	42.41140	342.95304	-1226.06402	1
16324	C	75.43458	100.19786	60.12594	-642.28612	318.18411	530.96068	1
16325	H	76.22523	100.66034	59.48011	-2525.62334	-1118.94463	-624.87971	1
16326	C	73.69011	99.16674	62.10153	129.14073	435.27490	287.86645	1
16327	H	73.12514	98.79831	62.92295	938.39233	250.36455	2343.38297	1
16328	C	75.78543	99.11135	60.89559	-164.22167	482.40975	1166.87996	1
16329	H	76.77522	98.57074	60.79038	-159.44472	-956.89329	1655.89719	1
16330	C	74.96544	98.62260	61.95322	762.81830	160.17438	-974.64446	1
16331	O	75.46602	97.66862	62.78854	-23.28898	226.94599	283.29923	1
16332	H	74.76404	97.62629	63.50063	2321.32759	301.83428	-728.71568	1
16333	C	76.00388	103.71552	60.78114	908.85832	158.97098	-366.67812	1
16334	O	77.09319	104.34290	60.73976	24.18303	200.34513	264.04992	1
16335	N	75.30117	103.73679	61.97408	106.55194	191.78883	-25.46753	1
16336	H	74.46771	103.19717	61.66988	1023.36631	-988.51537	593.01662	1
16337	C	75.88926	103.26582	63.17516	359.28280	-1057.55800	-754.49140	1
16338	H	74.96849	103.05507	63.78870	-109.89070	-806.89119	-481.31643	1
16339	C	76.69812	101.91708	62.95659	-11.09960	71.14552	-895.71995	1
16340	H	76.44071	101.22907	63.81022	2263.00237	-1609.62756	1282.26617	1
16341	H	76.21731	101.41589	62.10920	-56.41862	-2126.77042	1388.27625	1
16342	C	78.19002	102.20830	62.61459	719.01027	-377.24419	88.40132	1
16343	H	78.40442	102.31785	61.54390	-1591.52915	-1349.40425	-2823.18173	1
16344	H	78.65750	103.06601	63.02009	0.54174	2928.66524	1326.06467	1
16345	C	79.13066	101.02786	63.19751	261.52347	529.05501	-275.91472	1
16346	H	78.72046	100.02493	62.97110	1188.09100	-3551.51206	-3351.97586	1
16347	H	80.21342	101.11870	62.82104	152.13412	-1842.46282	-870.45532	1
16348	N	79.06199	101.21192	64.57137	-693.27974	-332.99022	-89.16227	1
16349	H	78.16284	101.22967	64.98367	1177.89284	-679.59692	-566.83198	1
16350	C	80.07668	101.49981	65.33371	-406.45456	981.27672	1317.55777	1
16351	N	81.40311	101.46606	64.90682	-1040.92044	-223.67762	101.15722	1
16352	H	81.64556	101.19222	63.93488	-2881.25519	-2352.76302	-4022.11905	1
16353	H	82.30954	101.48041	65.48771	947.64782	2745.64354	-3085.86801	1
16354	N	79.51437	101.75431	66.59217	-46.10065	-297.34990	246.44718	1
16355	H	78.55988	101.44600	66.91816	1144.51031	1428.19015	-578.47790	1
16356	H	80.21203	101.80292	67.36585	-793.48504	-2918.55154	581.37837	1
16357	C	76.74773	104.36398	64.00709	-383.99807	-211.32475	-588.50364	1
16358	O	76.47900	104.49574	65.21943	-338.77579	-523.18577	224.56717	1
16359	N	77.49778	105.14206	63.29017	-251.08213	-774.26493	-360.88647	1
16360	H	77.54738	104.97911	62.20180	-273.33061	612.42307	318.83286	1

16361	C	78.43778	105.86468	64.05504	-142.75694	13.63197	654.69188	1
16362	H	78.37047	105.38304	65.07818	467.21922	-1963.42946	202.96931	1
16363	C	79.89132	105.71379	63.42271	-139.36899	-685.81380	-681.52335	1
16364	H	79.90963	105.81995	62.32694	2087.71806	-347.76096	191.19842	1
16365	C	80.67498	107.00450	63.95072	-720.96469	-901.68226	-170.72225	1
16366	H	81.70322	107.24683	63.50544	-1011.21434	-1977.72466	-360.06500	1
16367	H	80.03802	107.85373	63.81428	1472.90762	480.78872	1775.07659	1
16368	H	80.78881	106.87599	65.06319	870.75738	-1379.52425	2162.94828	1
16369	C	80.60298	104.40481	63.87105	679.89594	-374.52772	-342.99011	1
16370	H	80.74631	104.25554	64.96436	-1924.00216	571.90582	-43.14740	1
16371	H	79.96838	103.48557	63.64758	-789.36383	-2302.39650	728.63817	1
16372	H	81.60020	104.27062	63.39638	1195.93750	534.62498	2117.46949	1
16373	C	77.81859	107.41232	64.02865	-35.35368	36.89518	290.98737	1
16374	O	77.26530	107.93316	63.09479	-393.96390	432.05117	443.09884	1
16375	N	78.05813	107.95425	65.25690	-423.70687	-805.19983	-150.52447	1
16376	H	78.61584	107.47966	65.96336	1452.80897	387.90202	-2933.16825	1
16377	C	77.30738	109.24080	65.30987	-476.47555	-539.60426	-428.91969	1
16378	H	77.48980	109.77839	64.32884	717.38212	-172.54951	-2939.69383	1
16379	C	75.80319	108.93601	65.63904	147.94614	221.02709	106.72537	1
16380	H	75.48278	107.91874	65.39595	1519.24790	-606.24593	-252.63727	1
16381	H	75.77153	108.86133	66.74326	210.73079	-2260.06422	-2014.08383	1
16382	C	74.85161	110.06423	65.08175	1132.76005	719.19945	562.39199	1
16383	H	75.29278	111.03766	65.04397	335.90178	-1466.17012	-1592.58777	1
16384	C	74.62163	109.61522	63.59025	237.19811	1001.85028	-150.70054	1
16385	H	74.18628	108.46039	63.41733	1919.75565	-424.45483	-1807.18785	1
16386	H	73.77566	110.19888	63.10277	-967.89615	1528.23105	-1380.19928	1
16387	H	75.54573	109.75644	62.92469	-2532.90746	825.69813	-1485.61024	1
16388	C	73.53105	110.12627	65.96867	476.91522	-503.32664	-146.02202	1
16389	H	72.94738	111.06301	65.89890	-1493.92496	-423.09094	833.97670	1
16390	H	72.80935	109.28293	65.76251	-187.62506	-4198.14817	216.81384	1
16391	H	73.88928	110.12289	67.02412	-981.63032	-1016.86802	2461.07099	1
16392	C	78.05917	110.03820	66.46014	-245.53494	-1190.76085	254.46138	1
16393	O	77.47913	110.82597	67.16261	210.73592	626.07478	-115.04493	1
16394	O	79.43233	109.88032	66.63945	982.47930	137.08680	-184.84980	1
16395	H	79.45779	108.86762	66.36124	1195.06599	1009.36810	-1220.48611	1
16396		5463						
16397		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000***** 150.0000	600000
		0.2500	400.00	0.00	0.00	0.00	-25968.6443	0.2260
							400.0000	
16398	N	56.89626	95.57464	59.13306	-557.38581	-17.49034	-3.32113	1
16399	H	55.95529	95.45373	58.65470	-146.20111	1246.10345	263.18944	1
16400	H	56.70089	95.33070	60.10419	69.15400	-161.14811	-690.99910	1
16401	H	65.70894	98.56003	55.89386	-366.78221	-752.48188	-687.48827	1
16402	C	58.08326	95.13849	58.52436	-654.10271	-754.59577	1094.62111	1
16403	H	58.92011	95.33394	59.27374	-1362.86718	-1844.83096	1667.65027	1
16404	C	57.98420	93.56915	58.49874	-241.50629	394.32326	662.42641	1
16405	H	58.72382	93.08548	57.80090	249.42288	737.94557	-948.31717	1
16406	H	56.95155	93.21064	58.25692	-685.66817	-3376.46504	1035.60041	1
16407	C	58.28538	92.98844	59.89087	-31.88408	412.79135	-412.51421	1
16408	H	57.53428	93.35949	60.66932	-2188.16566	1088.94687	-170.29896	1
16409	H	59.25719	93.36643	60.28090	-3047.62956	-895.25311	-3215.26811	1
16410	S	58.13802	91.17503	59.44883	290.64741	-248.31217	-459.58966	1
16411	C	58.82355	90.45308	60.88192	-393.75621	-388.14848	105.21194	1
16412	H	58.17716	90.27504	61.72139	4800.10782	-2824.23901	95.88675	1
16413	H	59.30240	89.41666	60.80523	-1452.86706	-583.85290	-534.84448	1
16414	H	59.61789	91.03770	61.38416	984.26251	194.48730	1089.22469	1
16415	C	58.27305	95.86314	57.02057	193.00798	-291.54091	-373.59479	1
16416	O	57.51962	95.77795	56.08748	-376.88495	-279.00221	118.97871	1
16417	N	59.31260	96.65183	57.17312	662.90771	565.00599	-15.48908	1
16418	H	59.69455	96.65272	58.15725	1359.46583	-2229.28723	1711.45600	1
16419	C	60.29342	96.70948	56.10103	833.79480	-621.02986	-3.78711	1
16420	H	59.56218	96.76183	55.23368	-301.03378	1014.74819	-845.35422	1
16421	C	61.35625	97.88696	56.34848	-608.48857	-24.53425	864.23220	1

16422	H	60.87803	98.85183	56.03750	3654.38166	2932.79240	-1189.46892	1
16423	H	61.51266	97.97372	57.49309	643.41383	-1993.63145	-686.16087	1
16424	C	62.61736	97.70245	55.46988	156.09396	178.96371	409.32698	1
16425	H	62.45564	98.01693	54.41822	429.35024	-895.18023	-4579.62262	1
16426	H	62.80235	96.55503	55.39454	260.11825	-710.04947	-3163.14582	1
16427	C	63.86795	98.36565	56.10051	-1089.40299	15.51936	-224.30299	1
16428	O	63.98888	98.91531	57.16733	-979.26821	487.63216	-492.49436	1
16429	O	65.03539	98.21953	55.26191	-257.52061	358.38389	-1095.03913	1
16430	C	61.13174	95.27783	56.02276	-16.95876	-263.85879	580.31458	1
16431	O	61.41366	94.79700	54.95619	326.06071	-124.78801	634.15389	1
16432	N	61.44948	94.79221	57.21306	-629.52912	291.01851	-645.42839	1
16433	H	61.21057	95.36614	58.02363	-378.97591	-1693.75629	1246.46013	1
16434	C	62.11249	93.54316	57.21950	651.72508	186.60636	977.96134	1
16435	H	61.83015	93.09263	56.19835	-331.71106	572.35852	-733.49360	1
16436	H	61.67153	92.90192	58.11012	1510.60550	-593.27013	638.25601	1
16437	C	63.78806	93.55051	57.51426	-29.08753	-1086.40390	-593.96101	1
16438	O	64.46930	92.49649	57.57900	78.10073	-213.60748	121.81433	1
16439	N	64.19454	94.78596	57.45366	-344.55385	-624.17399	609.77162	1
16440	H	63.33575	95.39554	57.28402	1672.39210	2016.60782	-618.37395	1
16441	C	65.38932	95.07138	58.22620	118.97607	176.82571	1370.27053	1
16442	H	65.86901	94.07013	58.44994	-3061.20289	-341.72622	52.28402	1
16443	C	66.21788	95.92828	57.17842	593.90667	259.90124	793.54276	1
16444	H	65.57858	96.71691	56.73356	-1245.22357	2910.34222	2068.86632	1
16445	C	67.46840	96.69311	57.73480	68.29410	-891.20749	-218.09041	1
16446	H	67.94682	97.27233	56.90054	-3753.86927	65.17796	-691.05859	1
16447	H	68.25523	96.07886	58.22553	-1852.38770	-2471.37943	437.21459	1
16448	H	67.20833	97.49456	58.56706	462.83882	-2.58878	1184.86043	1
16449	C	66.59676	94.89937	56.03279	-51.77645	106.08887	515.43741	1
16450	H	65.92929	94.01590	55.89496	-4056.03581	382.61553	-357.23513	1
16451	H	67.55468	94.44229	56.33364	-327.41633	-3858.16680	1657.67516	1
16452	C	66.69684	95.62553	54.65098	-3.06388	-908.53502	-361.11275	1
16453	H	67.12155	94.96182	53.81365	-318.84372	-1008.04752	-864.71942	1
16454	H	67.28105	96.51574	54.78350	-916.00877	-2863.71984	-1283.99434	1
16455	H	65.74519	95.88064	54.23519	-922.54548	415.26980	-867.98897	1
16456	C	65.00075	95.97386	59.51736	-166.29284	174.85830	-359.77360	1
16457	O	65.83501	95.97748	60.41501	105.96092	-176.65221	-35.06897	1
16458	N	63.90609	96.71650	59.35889	37.48310	-509.10572	398.81244	1
16459	H	63.44249	96.76834	58.46132	3391.73442	-129.97089	-2118.98282	1
16460	C	63.27474	97.33331	60.50335	-553.02484	-289.33181	-65.65625	1
16461	H	64.09714	97.95450	60.85020	2049.78438	1503.11183	778.14397	1
16462	C	61.92789	98.04658	60.18444	80.49973	-364.90201	150.17084	1
16463	H	61.68648	98.53571	61.19595	-1037.51804	-3858.93338	1913.87132	1
16464	H	62.11789	98.87171	59.46173	1241.82000	-5029.89393	3323.93650	1
16465	O	60.75923	97.29245	59.69007	-443.10227	178.24016	-23.82335	1
16466	H	60.57577	96.80947	60.49211	621.83666	-1210.06585	2275.13106	1
16467	C	62.83938	96.25619	61.70446	71.79655	328.99300	-590.55528	1
16468	O	62.41426	96.75161	62.72277	168.11353	-179.41953	50.78405	1
16469	N	63.01838	95.01601	61.33196	188.54205	17.27262	468.38201	1
16470	H	63.45709	94.99004	60.40590	2588.03991	22.69720	-792.36463	1
16471	C	62.77198	93.79968	62.04376	-529.94925	568.60569	-243.08362	1
16472	H	63.08591	93.04760	61.29460	-16.61856	-997.18520	1791.57536	1
16473	C	63.73671	93.69122	63.31849	-575.41143	416.69731	-103.41024	1
16474	H	64.04641	94.70957	63.63707	-1791.19320	2271.94319	-4799.50060	1
16475	C	63.04784	93.01048	64.52839	-425.74708	-115.96161	-126.74967	1
16476	H	63.70124	93.08045	65.36668	159.14607	-1283.94918	3434.03760	1
16477	H	62.13589	93.64311	64.76748	-1727.62014	-2021.28138	1903.08701	1
16478	H	62.70266	91.91672	64.38450	655.39312	-1219.15873	106.04142	1
16479	C	65.08053	92.92714	62.98739	1194.54602	974.46518	426.24975	1
16480	H	64.95741	91.95356	62.43178	782.28758	2123.98221	1598.59525	1
16481	H	65.62412	92.48799	63.85449	-403.60810	1912.30268	1176.77801	1
16482	C	65.96868	93.96894	62.20981	339.56276	679.30867	45.34317	1
16483	H	65.97731	95.06304	62.56603	-164.82918	1678.56002	-2379.58509	1

16484	H	67.08861	93.71007	62.10315	1329.77106	-1066.08884	1116.23293	1
16485	H	65.70598	93.90455	61.20521	607.86824	-394.30130	-1173.95814	1
16486	C	61.17291	93.48300	62.23056	-781.95997	-138.61592	-338.97442	1
16487	O	60.85523	92.48541	61.55155	922.03039	179.49281	-187.72580	1
16488	N	60.48536	94.26556	63.06147	-424.97580	-138.40748	-28.61334	1
16489	H	61.24166	94.89395	63.41917	-1803.30934	-43.25018	-1677.23502	1
16490	C	59.12283	94.21849	63.34944	42.50100	-971.36810	-11.22690	1
16491	H	58.80114	93.28219	62.91020	-527.21475	999.33625	766.33253	1
16492	C	58.96768	94.54661	64.90798	186.30948	-608.93374	318.36542	1
16493	H	59.46728	95.51859	65.09270	-1311.48805	-851.36288	225.45598	1
16494	H	59.49803	93.80541	65.54370	1104.18120	1347.87502	-1483.93469	1
16495	C	57.50813	94.43788	65.40366	306.33990	589.66576	1887.23579	1
16496	C	56.97079	93.18904	65.85545	109.28414	580.19011	354.79690	1
16497	H	57.67115	92.30371	65.88040	-1018.03512	1554.62367	1293.65093	1
16498	C	55.66613	93.03047	66.30485	-751.66059	574.23223	-11.96037	1
16499	H	55.32161	92.09617	66.67735	-221.57487	-649.36303	-468.32154	1
16500	C	54.72082	94.07738	66.21333	23.72649	-714.64850	345.29559	1
16501	O	53.34406	93.91314	66.50555	-510.58495	-438.20981	-120.72704	1
16502	H	53.28143	92.93867	66.37791	2794.77724	2007.49370	456.44890	1
16503	C	56.59480	95.50882	65.35024	642.34445	-585.49951	-824.44448	1
16504	H	56.97830	96.49411	64.97891	-1953.04931	2870.48959	-2926.16010	1
16505	C	55.25963	95.24505	65.65170	-275.92987	881.81542	158.66540	1
16506	H	54.49954	96.03492	65.56740	660.98908	-712.05217	-1723.89135	1
16507	C	58.37577	95.49918	62.65909	331.76398	-852.12651	607.71508	1
16508	O	57.14916	95.49014	62.65290	636.67679	-1168.74408	-108.98532	1
16509	N	59.13559	96.31866	61.93493	210.22370	-1021.03542	-120.05921	1
16510	H	60.11017	96.00335	62.08676	-47.88242	999.87442	-367.46618	1
16511	C	59.02726	97.75681	62.09437	570.23184	957.34876	552.29950	1
16512	H	60.00614	98.05714	61.56558	528.19066	-273.26409	-2267.85386	1
16513	C	57.81291	98.43753	61.27173	245.87175	-49.62034	1163.25852	1
16514	H	57.79923	99.54646	61.43618	1171.58520	-2439.58390	2339.82547	1
16515	O	56.52979	97.93803	61.67237	-971.76406	-81.48787	189.79629	1
16516	H	56.88948	96.99548	61.93823	2135.38642	596.28314	592.72021	1
16517	C	58.31550	98.38677	59.79253	-251.17435	185.35809	-41.58013	1
16518	H	58.58111	97.35914	59.43042	1734.52235	3232.11245	-1218.59791	1
16519	H	57.62311	98.88105	58.99315	-566.23693	-613.95212	2332.89938	1
16520	H	59.26988	98.99061	59.69638	1069.67356	-1618.82928	-1456.73176	1
16521	C	59.09542	98.13926	63.61792	-247.47772	-57.33670	245.15125	1
16522	O	58.65961	97.61904	64.63463	-520.14465	-246.90390	-202.92270	1
16523	N	59.57371	99.44548	63.63793	-29.48321	-513.71126	-225.83901	1
16524	H	59.89278	99.84107	62.72688	510.26256	2217.58330	-1044.14314	1
16525	C	59.20306	100.20023	64.86200	-65.69904	613.44497	110.49391	1
16526	H	58.17116	99.82395	65.05037	1249.17672	1877.16432	-3146.66176	1
16527	C	60.23472	99.76721	66.00334	-824.39443	546.62389	383.87379	1
16528	H	59.78775	99.87764	66.99687	679.35366	-394.02229	1476.24180	1
16529	H	60.69295	98.70504	65.80746	-2947.92249	-1614.69293	383.68579	1
16530	O	61.56899	100.52672	65.96416	-464.06718	-42.95869	-132.53108	1
16531	H	61.51186	101.18222	66.62178	-269.96979	601.04082	-414.99879	1
16532	C	59.23462	101.73879	64.65312	-390.69855	-501.69002	-27.88811	1
16533	O	59.08345	102.24026	63.55017	-226.64929	18.08224	558.30683	1
16534	N	59.17133	102.31435	65.88905	-315.19664	346.74146	66.34025	1
16535	H	58.95416	101.69396	66.73979	1886.12640	-210.98255	-140.54997	1
16536	C	58.58884	103.67927	66.09805	-613.55181	228.70427	278.66336	1
16537	H	57.77483	103.52687	65.32269	3595.06906	-128.93330	-3131.25114	1
16538	C	58.10475	103.83233	67.55952	236.09609	628.45527	-11.06997	1
16539	H	57.33204	104.59712	67.68859	-2643.30237	755.01883	-1139.64075	1
16540	H	58.99680	104.22048	68.08087	2080.04272	896.29588	866.48085	1
16541	C	57.54230	102.56090	68.33374	165.68073	-311.20192	276.09635	1
16542	O	56.81604	102.84324	69.29779	129.26629	-62.72717	86.67639	1
16543	O	58.10827	101.46264	68.13969	529.18391	175.20875	763.09665	1
16544	C	59.72814	104.77525	65.67512	-474.07139	381.48940	721.09064	1
16545	O	59.45515	105.85190	65.18831	482.04028	98.69285	-477.42576	1

16546	N	60.95729	104.32973	65.88797	-30.44241	105.88609	232.21080	1
16547	H	61.08197	103.43322	66.35885	3248.54173	867.78993	2825.78755	1
16548	C	62.08697	105.07883	65.40505	795.56866	-279.33570	438.35346	1
16549	H	61.79017	106.13841	65.22016	746.01988	-1940.52881	2753.19986	1
16550	C	63.08601	105.04667	66.61158	-69.56878	-486.01718	1096.60308	1
16551	H	62.63820	106.03397	66.99448	1162.54389	1807.81905	2237.19975	1
16552	H	64.16124	105.20355	66.31807	1214.35334	1103.03010	-1400.98035	1
16553	C	63.31626	103.82215	67.58153	-296.84514	-120.05084	-368.71269	1
16554	O	62.38132	103.00704	67.69560	25.10274	-179.02504	-398.89381	1
16555	N	64.52648	103.73186	68.15055	584.61378	-322.33789	1079.22486	1
16556	H	64.73340	103.01720	68.90022	927.47894	645.71800	1268.43735	1
16557	H	65.35785	104.41044	68.02367	-594.88225	1713.35964	-2825.93581	1
16558	C	62.70647	104.21330	64.14632	-183.16356	-464.47442	-71.62656	1
16559	O	63.59845	104.74714	63.52497	-298.06402	-502.59831	310.70154	1
16560	N	62.17969	103.01969	63.88152	198.55506	853.35995	343.01036	1
16561	H	61.44245	102.69861	64.41452	-47.02263	1605.52232	-300.52299	1
16562	C	62.86303	102.28094	62.82017	386.89941	-172.06084	290.60627	1
16563	H	63.85520	102.53194	63.08951	1396.72393	290.53568	2159.91053	1
16564	C	62.51919	100.76170	62.95441	41.35664	-678.82057	-294.65167	1
16565	H	62.05857	100.57267	63.96494	-2413.27788	-370.59393	2717.88941	1
16566	H	61.74077	100.50625	62.11580	-1725.11490	714.90270	-758.85754	1
16567	C	63.78296	99.85220	62.79269	542.15162	-1103.40968	-169.27587	1
16568	C	64.67636	100.01448	61.73208	718.57080	58.98288	-36.44285	1
16569	H	64.44452	100.63827	60.83596	-1593.48103	3310.78951	3773.16641	1
16570	C	65.95564	99.41805	61.87483	-157.51055	845.09521	-1287.59318	1
16571	H	66.72908	99.62818	61.16437	235.42468	-4727.83420	-1282.07996	1
16572	C	66.36714	98.54365	62.88632	280.89798	-906.85531	842.29216	1
16573	O	67.71583	98.03439	62.87338	465.39596	-250.13208	-418.84928	1
16574	H	67.66597	97.29438	63.54336	-244.88683	2051.76169	3339.01561	1
16575	C	64.09697	98.86988	63.79225	-313.60670	306.87955	-34.24641	1
16576	H	63.35909	98.44136	64.45869	-85.39310	-1306.68509	-1471.42898	1
16577	C	65.31760	98.21473	63.80310	225.70677	-453.81425	221.68643	1
16578	H	65.41669	97.53107	64.63707	-886.13427	2072.31585	446.54929	1
16579	C	62.49387	102.77103	61.33118	286.27193	-508.45038	367.06033	1
16580	O	63.25861	102.51197	60.41965	790.33428	36.46047	89.08264	1
16581	N	61.35311	103.50169	61.33802	-684.13234	43.39255	265.45642	1
16582	H	60.76952	103.51685	62.20460	384.91371	722.49558	-213.78469	1
16583	C	60.54294	103.30436	60.17669	36.39742	512.34345	-72.56943	1
16584	H	61.27688	102.90410	59.43069	468.25769	-1697.52301	-1386.99801	1
16585	C	59.39141	102.24207	60.47984	1155.57635	-123.83284	288.72658	1
16586	H	58.50612	102.70159	61.02655	178.60887	611.89961	1768.62433	1
16587	O	59.85098	101.05499	61.28502	631.39311	20.45591	-220.21417	1
16588	H	59.37361	101.27631	62.13974	-854.14314	-261.02497	-1561.46333	1
16589	C	58.94593	101.86827	59.03562	707.11500	-178.00889	-528.35737	1
16590	H	57.99645	101.19291	59.03344	1863.39157	1670.66300	-362.74498	1
16591	H	59.76253	101.32665	58.44366	149.18707	396.87851	1282.33534	1
16592	H	58.65963	102.81006	58.61692	1725.84070	-2032.47194	383.70354	1
16593	C	59.96064	104.75646	59.64314	-451.30409	1218.30941	360.51511	1
16594	O	58.92584	104.81460	59.00140	-442.35593	194.08466	-122.33218	1
16595	N	60.86005	105.72467	59.92832	273.00644	-548.23255	-281.71778	1
16596	H	61.66555	105.15740	60.20269	-398.84105	-727.96690	-2216.40724	1
16597	C	60.41956	106.87157	60.66418	194.75432	76.92231	-453.87447	1
16598	H	59.54112	107.33357	60.05047	2837.26419	-74.28541	-244.62744	1
16599	C	59.93409	106.48274	62.13472	-648.07942	-613.29988	769.10644	1
16600	H	60.41221	105.54244	62.46289	-158.49719	3684.67927	2513.61096	1
16601	H	60.20806	107.18280	62.91860	1013.67418	-235.97280	1846.63097	1
16602	C	58.40886	106.28322	62.12032	45.95243	-148.81200	-606.09974	1
16603	H	58.05810	105.62497	61.29559	3711.75202	1243.48714	2260.31164	1
16604	H	58.06927	105.88637	63.12223	-2096.95150	1630.74685	-824.76154	1
16605	C	57.76639	107.74957	61.80835	-384.75829	-511.02353	-387.98206	1
16606	O	56.54869	107.89125	61.83051	723.52213	906.69058	-185.16217	1
16607	O	58.62880	108.67052	61.59338	-412.99260	107.86462	67.85582	1

16608	C	61.61269	107.92442	60.71468	-1026.96221	116.28534	-427.45210	1
16609	O	62.73893	107.63339	60.33844	-28.85372	-349.36452	365.21319	1
16610	N	61.25507	109.14033	61.23800	673.11493	411.70839	2.80171	1
16611	H	60.22776	109.30945	61.50240	-50.87113	2465.27792	234.16696	1
16612	C	62.23055	109.84063	62.08174	-183.23620	275.30334	116.08983	1
16613	H	63.07146	109.77687	61.35284	905.79173	-792.75168	-1864.33553	1
16614	C	61.55547	111.25345	62.32576	559.93901	9.06031	327.79254	1
16615	H	60.65449	111.12419	62.97028	1063.43765	2250.88313	-1951.43458	1
16616	H	61.13258	111.70541	61.40014	-256.16538	2217.70956	-1015.11596	1
16617	C	62.58669	112.23221	62.97052	-427.53567	-690.01755	-171.03273	1
16618	H	62.11309	113.23562	63.05806	-465.40679	-745.12553	1407.06903	1
16619	H	62.80044	111.88616	63.98009	-2723.61116	974.33704	-605.64258	1
16620	C	63.89707	112.30129	62.01719	-685.35978	-711.24551	109.12013	1
16621	O	64.62704	111.27808	62.20890	-422.84843	211.03667	-241.11091	1
16622	O	64.07759	113.26270	61.28506	-372.32429	276.58662	657.79859	1
16623	C	62.52630	108.91204	63.38983	-157.86663	-65.26538	480.55360	1
16624	O	61.69612	108.14788	63.82764	97.12113	-191.66313	-480.77224	1
16625	N	63.82854	109.21074	63.67897	-636.04777	-72.51403	-31.36939	1
16626	H	64.27027	110.00296	63.17830	1672.27955	1547.44331	-778.48867	1
16627	C	64.51637	108.26150	64.39799	237.27335	625.88001	-672.22773	1
16628	H	63.68872	107.84061	65.02468	184.72901	-2757.60385	2117.88309	1
16629	C	65.18513	107.27856	63.33759	-325.28459	1.91397	-54.35058	1
16630	H	64.43112	106.81866	62.60371	19.78365	-1814.64208	-307.83021	1
16631	H	65.96860	107.77617	62.67376	-399.10971	847.14873	290.50253	1
16632	C	66.00254	106.24358	64.17485	-255.25949	898.91680	-562.14318	1
16633	H	65.31932	105.73247	64.92674	1596.25355	1676.85188	-954.13740	1
16634	H	66.80892	106.75835	64.82083	-1626.12065	184.97367	-100.16414	1
16635	S	66.64526	105.05340	62.87642	436.08190	421.41602	322.36505	1
16636	C	65.35153	105.14462	61.47679	362.39171	-731.32999	-233.84866	1
16637	H	64.41182	104.61104	61.77266	-299.95608	-315.13473	1344.65970	1
16638	H	65.71786	104.68335	60.52954	872.31149	711.14279	-1761.27246	1
16639	H	65.00507	106.14420	61.11482	-1451.26591	1596.58656	-3318.00824	1
16640	C	65.60777	109.16729	65.23335	483.45020	-719.78453	562.89594	1
16641	O	65.72385	109.07040	66.44881	-890.29891	-425.43599	380.42389	1
16642	N	66.36727	109.94816	64.47830	-864.53237	453.45326	-629.95754	1
16643	H	66.20283	109.88471	63.52077	-605.29354	-815.82930	-416.42577	1
16644	C	67.44246	110.70171	65.09075	-73.33987	703.95567	-69.51546	1
16645	H	67.66473	111.61415	64.49436	-787.09080	937.36539	755.55015	1
16646	H	67.09887	110.91717	66.21304	-345.38764	508.96640	-1614.67615	1
16647	C	68.87232	109.89183	65.10464	240.37238	261.78133	143.95915	1
16648	O	69.62386	109.98020	66.05622	147.35589	568.92508	0.74467	1
16649	N	69.01960	109.14329	63.99213	16.40628	-604.89577	302.84493	1
16650	H	68.12652	109.08432	63.47050	-2009.84128	1343.12054	723.55955	1
16651	C	69.69406	107.84966	64.06517	-182.10891	565.81060	479.81406	1
16652	H	69.11638	107.27857	64.85712	-1603.60586	-1620.44133	7.28437	1
16653	C	69.60331	107.31293	62.58632	492.85999	873.53277	-44.05171	1
16654	H	70.50458	107.94002	62.25013	1441.44207	-703.60465	384.61702	1
16655	H	69.99625	106.28914	62.52515	-1857.30759	-361.86608	545.94786	1
16656	O	68.38369	107.53874	61.84634	-688.56942	912.87822	155.06858	1
16657	H	67.93527	106.54976	61.95381	-2592.71034	-1804.59312	863.92345	1
16658	C	71.30075	107.95241	64.28042	218.06589	817.01461	391.04881	1
16659	O	72.14806	108.63812	63.73212	76.11425	23.91142	-91.10208	1
16660	N	71.43085	106.99462	65.25626	238.05026	-581.91770	-261.12713	1
16661	H	70.54139	106.51776	65.35953	-850.52128	225.69146	796.17120	1
16662	C	72.67147	106.22509	65.23595	-403.00425	533.54432	17.35662	1
16663	H	72.85813	105.83235	64.20164	1748.94909	3801.35721	3522.06644	1
16664	H	73.32810	107.16513	65.47344	509.03081	1215.01461	-1943.44860	1
16665	C	72.60771	105.03346	66.30335	-275.47947	-585.93710	-325.58662	1
16666	O	71.85091	105.01854	67.25931	-341.53526	-15.65986	-163.98051	1
16667	N	73.59024	104.10943	66.10654	755.11415	-293.34566	-171.85222	1
16668	H	73.90790	104.26529	65.13655	2060.94843	-1907.55666	459.53756	1
16669	C	73.33812	102.76189	66.54801	-458.78004	226.42119	508.25246	1

16670	H	72.46930	102.57561	65.84694	-1462.09813	-1781.42662	3641.02449	1
16671	C	74.54185	101.81874	66.25274	304.86431	-308.95630	-204.67902	1
16672	H	74.47616	100.98878	66.98186	-962.98759	-2798.06623	-2460.30570	1
16673	H	75.49229	102.37899	66.47806	-1924.76730	1920.72906	987.02771	1
16674	C	74.34305	101.47728	64.70204	673.59892	469.97120	826.24340	1
16675	O	75.33659	100.95662	64.16978	406.83762	-554.70371	-333.80926	1
16676	O	73.24957	101.71473	64.15370	893.21325	-344.68313	1042.21363	1
16677	C	73.31531	102.51887	68.19652	-326.90180	21.64330	-467.02801	1
16678	O	72.98561	101.44963	68.65510	873.32278	-147.59107	-302.06029	1
16679	N	73.54453	103.68340	68.80657	738.85130	-34.94649	450.93424	1
16680	H	73.82096	104.47504	68.20601	-458.04961	3199.76997	-782.33598	1
16681	C	72.85828	103.93224	70.02254	635.70090	666.00437	-374.22409	1
16682	H	72.77011	102.91553	70.50567	2056.44727	-2730.11269	1715.44712	1
16683	C	73.46699	105.14225	70.89554	348.84064	-864.30292	-591.85766	1
16684	H	72.55793	105.81640	71.16286	1441.14775	-70.12563	-29.70861	1
16685	H	74.07702	105.74410	70.26842	-277.14760	-1031.24247	249.34743	1
16686	C	74.29466	104.67961	72.07851	1031.30416	520.63558	-1392.81774	1
16687	C	73.63059	103.88534	73.05916	71.86088	314.97254	404.54180	1
16688	H	72.54749	103.71685	72.97334	-2196.01784	1974.37984	2229.36948	1
16689	C	74.45950	103.31226	74.01672	-1003.20569	304.91103	161.52920	1
16690	H	74.10322	102.73835	74.87105	-1792.92099	430.48565	-446.10504	1
16691	C	75.88105	103.39741	74.06823	223.11739	-101.10478	-83.42847	1
16692	O	76.62319	102.76500	75.06024	-770.09972	207.34482	202.93646	1
16693	H	77.54736	102.99957	74.72307	-2903.02119	-838.97615	3956.03794	1
16694	C	75.69469	104.92985	72.24564	32.47228	88.88401	-21.23463	1
16695	H	76.15896	105.72674	71.62544	414.75661	-3352.04754	1588.76376	1
16696	C	76.51720	104.31961	73.20341	358.35540	-468.56085	-1028.15928	1
16697	H	77.58851	104.58357	73.36082	-516.16350	-460.17511	25.51905	1
16698	C	71.32889	104.38620	69.79759	-729.22244	-387.97292	71.95862	1
16699	O	70.82352	105.45812	70.11099	-1093.81401	-40.12395	-101.01599	1
16700	N	70.62768	103.31817	69.34346	888.55092	-483.51376	185.22862	1
16701	H	71.19526	102.56289	68.97631	-195.05198	-2476.20648	2516.97523	1
16702	C	69.25921	103.36844	69.01544	-544.55136	209.81993	406.13405	1
16703	H	68.86897	104.22852	69.56921	1160.09036	-2261.65819	-700.01123	1
16704	C	69.25631	103.75429	67.51652	688.50672	-522.65037	109.38825	1
16705	H	70.22316	104.33900	67.27313	-2744.77715	1238.05916	-1405.35445	1
16706	H	69.24705	102.85021	66.93004	-816.44216	350.94358	-2521.24543	1
16707	C	67.93713	104.54661	67.01644	-325.26185	153.90186	-582.74894	1
16708	O	67.92818	105.28054	66.03176	180.78169	373.50058	510.67464	1
16709	O	66.89848	104.32693	67.71336	515.80258	153.66876	-596.61908	1
16710	C	68.69139	101.76596	69.25883	-898.61557	91.15021	-104.57001	1
16711	O	69.19643	100.70379	68.95766	675.30422	1201.38906	-331.84701	1
16712	N	67.51796	102.02744	69.82771	-847.80803	-117.95212	-48.63510	1
16713	H	67.46241	103.01970	70.12945	-1557.80766	-2636.37236	91.15102	1
16714	C	66.73540	101.05320	70.51826	-346.24551	681.91437	-23.63304	1
16715	H	67.45651	100.34225	71.04760	-135.04215	2464.69057	131.80053	1
16716	C	65.74176	101.81832	71.48005	167.73009	205.52264	-801.17616	1
16717	H	65.03469	100.94423	71.75973	377.98022	1603.89479	1272.63218	1
16718	H	65.08644	102.57083	70.85700	2678.14100	386.94081	1029.46649	1
16719	O	66.25912	102.46254	72.60259	152.04610	-315.34439	592.60462	1
16720	H	66.76660	101.67299	73.04167	1135.92428	-1976.27848	4.49808	1
16721	C	65.79645	100.34514	69.37586	163.38817	-373.86424	430.21561	1
16722	O	64.59897	100.36693	69.45881	-351.33404	-876.67864	403.33032	1
16723	N	66.64338	99.86282	68.43561	-753.79079	-266.15095	24.85628	1
16724	H	67.62615	99.93380	68.61994	-703.26672	-1508.78987	1553.12352	1
16725	C	66.03893	98.84882	67.61195	-229.25618	932.50221	-347.64314	1
16726	H	65.16854	98.41359	68.23546	-1658.51306	1417.28515	2261.10130	1
16727	C	65.56327	99.82478	66.39428	-866.09485	-543.60060	-538.65386	1
16728	H	64.94747	99.24782	65.71149	1135.00287	569.06473	-704.33726	1
16729	H	64.93109	100.65842	66.77367	-82.06692	1120.75510	-2111.42621	1
16730	C	66.89733	100.27844	65.73677	599.97698	-434.34652	312.87396	1
16731	H	67.56229	100.76218	66.50054	208.56501	-4494.40144	-2155.68838	1

16732	H	67.45856	99.37640	65.46747	379.80719	3187.13824	-3171.21955	1
16733	S	66.29469	101.23518	64.33474	260.47920	763.82462	140.11302	1
16734	C	65.56029	102.76702	64.97845	-284.62446	-853.08178	14.58074	1
16735	H	65.00880	102.54702	65.87723	-2.00341	176.35471	2372.24257	1
16736	H	66.20986	103.59189	65.24513	-97.56901	-2293.83517	-1314.23393	1
16737	H	64.60290	103.05117	64.35758	315.42937	-387.67694	1125.42171	1
16738	C	67.14002	97.83533	67.07508	19.37317	-409.73532	-299.16302	1
16739	O	68.35943	98.03768	67.11282	683.31704	-391.54469	741.48423	1
16740	N	66.51202	96.79727	66.46310	280.69557	-306.37998	6.89100	1
16741	H	65.53450	96.73442	66.71365	1571.81268	-351.05677	-1464.94975	1
16742	C	67.37249	95.61699	66.59696	643.15406	202.54511	1220.11452	1
16743	H	67.99797	95.84948	67.45285	1248.01172	340.86054	-2927.74435	1
16744	C	66.56531	94.28243	66.77365	777.06781	-23.62190	42.04573	1
16745	H	65.59489	94.35969	66.25190	1981.22227	-1923.43748	1859.31317	1
16746	H	67.18975	93.47296	66.21032	696.58643	2284.36150	1155.12835	1
16747	C	66.07898	93.98976	68.23652	799.10070	-429.61345	417.26542	1
16748	H	65.02842	93.73071	68.24747	-761.86919	-31.41097	-3275.63971	1
16749	H	66.26195	94.93084	68.88983	-322.75689	973.70774	2535.14284	1
16750	C	66.92688	92.77829	68.74952	-681.88801	255.55644	-77.86483	1
16751	H	68.04424	92.83320	68.56052	881.36423	-809.12693	-2057.59076	1
16752	H	66.51941	91.77655	68.46974	-332.95090	-1732.01473	-1938.46496	1
16753	C	66.78920	92.99287	70.32440	-1129.48412	-797.76563	226.94999	1
16754	H	66.80257	92.03600	70.92848	-1147.82593	5.24557	-1506.47194	1
16755	H	65.83521	93.40147	70.43246	2920.31645	848.88754	891.74807	1
16756	N	67.75994	94.00305	70.77892	-117.54733	358.38882	-30.92568	1
16757	H	67.88999	94.12850	71.87707	-1260.72612	340.42257	2633.63631	1
16758	H	68.93916	93.84114	70.49376	-122.24195	4650.85899	-2753.00281	1
16759	H	67.56313	94.98466	70.52752	-659.86533	-703.55130	148.15418	1
16760	C	68.13127	95.52504	65.15802	317.13222	135.58876	-256.07916	1
16761	O	67.81125	94.68120	64.33766	-853.70197	295.34277	-818.12160	1
16762	N	69.07175	96.42744	65.09945	441.26937	401.18963	-239.42523	1
16763	H	69.09297	97.18430	65.74422	-1658.22273	3096.56425	3297.29939	1
16764	C	70.22985	96.25019	64.19874	262.94851	863.95445	-914.12569	1
16765	H	70.38611	95.18111	64.33947	-737.96263	-967.61249	-3087.52032	1
16766	C	70.00049	96.55368	62.67078	-39.20471	657.00871	-69.39166	1
16767	H	69.11821	95.93427	62.26851	2373.24614	-1056.03702	-1275.33307	1
16768	H	69.67879	97.60915	62.44553	2389.69104	-2823.70844	1240.49616	1
16769	C	71.24581	96.04906	61.87748	-270.66804	618.39761	-234.15396	1
16770	H	71.59033	94.97936	62.21531	-294.51202	-2098.79398	-2584.38108	1
16771	H	72.07123	96.73726	62.11329	3413.06976	-342.66404	1503.88456	1
16772	C	70.88945	96.10666	60.28490	-709.46429	-115.20191	-120.52643	1
16773	O	70.75104	95.11145	59.57535	118.51721	457.99255	-486.18061	1
16774	O	70.54867	97.28084	59.98441	-329.98966	657.76009	-55.47746	1
16775	C	71.42925	97.22272	64.67402	-1086.59584	135.81440	724.90375	1
16776	O	72.57630	96.95302	64.27750	-148.33013	598.57568	215.58301	1
16777	N	71.02892	98.32238	65.35449	662.37351	-261.99506	161.65860	1
16778	C	70.21780	99.33414	64.77800	-277.01354	882.61318	601.26118	1
16779	H	69.16859	99.02650	65.00382	-913.83871	-2028.01705	-2209.17383	1
16780	H	70.41992	99.46758	63.67101	793.19977	-3094.28410	576.42107	1
16781	C	72.09020	98.75552	66.27449	-303.48005	-518.72467	317.28721	1
16782	H	73.02823	98.90988	65.59078	-3040.51522	56.14189	-453.67783	1
16783	C	71.35445	100.05533	66.77784	-733.47038	294.73686	-472.19175	1
16784	H	72.08049	100.67321	67.45333	-68.67302	850.71078	213.17596	1
16785	H	70.50597	99.71744	67.53231	500.17572	186.28908	1174.19537	1
16786	C	70.65232	100.67673	65.55591	527.57469	-24.05043	-96.69770	1
16787	H	71.37937	101.32180	65.01004	853.74106	-2854.39821	-3000.44118	1
16788	H	69.82997	101.38760	65.79590	1311.33042	-2464.18588	3148.18640	1
16789	C	72.38277	97.70768	67.43274	-102.63284	-800.84377	636.25749	1
16790	O	71.84687	97.84123	68.52788	-297.91075	-337.91877	599.04609	1
16791	N	73.29755	96.68790	67.07989	346.50561	-13.41379	-661.29797	1
16792	H	73.37967	96.64168	66.00972	271.21587	-3183.03270	-592.07820	1
16793	C	73.00173	95.47170	67.79635	1034.96316	-349.72178	756.38592	1

16794	H	72.49863	95.76519	68.78233	-1597.94001	-1014.03773	-2612.90953	1
16795	C	72.09999	94.41854	66.98326	1108.12509	375.96174	215.08300	1
16796	H	72.02869	94.87639	65.93242	3144.30016	1276.82178	2644.95802	1
16797	H	72.67190	93.47082	66.73595	-964.84469	974.96671	518.66610	1
16798	S	70.47181	94.30773	67.77522	229.25065	-340.66088	196.56034	1
16799	C	74.39364	94.66266	67.98736	580.46867	-2.19579	-277.37681	1
16800	O	74.38256	93.52629	68.39065	-94.63681	745.59311	1112.32844	1
16801	N	75.51532	95.36869	67.64777	572.24330	44.22511	1133.48122	1
16802	H	75.54278	96.33463	67.25484	1614.90169	-1356.43462	3923.57691	1
16803	C	76.73277	94.65529	68.10306	-735.01300	202.73425	654.41566	1
16804	H	76.67087	93.62098	67.76543	-2374.16193	2244.75140	-436.23556	1
16805	C	77.93780	95.61419	67.65966	-615.68889	-165.98520	-124.67952	1
16806	H	78.80331	95.19237	68.27708	2701.83340	-335.59129	-316.81301	1
16807	H	77.60378	96.60686	67.96078	924.14485	206.91243	3576.53807	1
16808	C	78.24107	95.64368	66.15797	457.72839	-857.23951	1110.11248	1
16809	C	79.33973	94.89087	65.69840	475.55702	-297.64372	-938.38046	1
16810	H	80.00350	94.33356	66.44136	3185.81589	1520.05364	-2974.14674	1
16811	C	79.65129	94.77727	64.35917	-613.43882	-397.71098	50.83852	1
16812	H	80.51514	94.19267	64.13211	-105.26438	381.96035	-166.21830	1
16813	C	79.04523	95.57129	63.32869	1012.28234	619.49351	265.84150	1
16814	H	79.39776	95.54748	62.29801	2439.98075	-304.17379	1378.11498	1
16815	C	77.50249	96.25587	65.12686	385.50578	89.21093	28.34215	1
16816	H	76.50787	96.68745	65.31018	223.80593	-286.42392	-228.19483	1
16817	C	77.96926	96.31381	63.80737	-574.45900	408.82585	-730.22137	1
16818	H	77.44610	96.81531	63.03138	874.93887	1000.05752	-2785.06360	1
16819	C	76.69396	94.61208	69.71908	-112.60482	203.36115	-873.24702	1
16820	O	76.64160	95.68359	70.33417	668.63633	-435.75042	181.01347	1
16821	N	76.72384	93.39165	70.24285	-264.74004	-748.47989	-155.18083	1
16822	H	76.67830	92.62767	69.58980	2466.92030	478.91409	162.67478	1
16823	C	76.15715	93.21567	71.58934	-523.26034	-414.28652	-211.70066	1
16824	H	75.22065	93.81969	71.42773	631.45053	3871.90905	-1998.62470	1
16825	C	75.84835	91.63583	71.41862	629.63086	-153.03014	35.82514	1
16826	H	76.39036	90.89312	72.03561	2705.13761	-968.85380	118.88824	1
16827	H	75.96662	91.26455	70.37459	-476.58995	-505.31292	-433.55912	1
16828	C	74.46449	91.20580	71.97051	-242.08674	-76.43187	169.11688	1
16829	H	73.57920	91.74064	71.53172	2835.52438	1020.61886	-228.87344	1
16830	H	74.32316	90.06989	71.71414	-4.66392	1939.61174	-216.69488	1
16831	C	74.46650	91.35134	73.58232	508.25822	-17.60247	195.81692	1
16832	H	75.11841	92.17855	73.93163	-2542.86554	454.30299	514.54105	1
16833	H	74.66671	90.27145	74.00135	-154.36676	-931.08177	1679.39836	1
16834	N	73.16639	91.69956	73.87231	129.23040	-312.69450	-588.19079	1
16835	H	73.14279	92.68940	74.22037	-426.30683	-2870.91805	2260.01716	1
16836	C	72.11006	91.00444	73.67444	195.44825	30.64325	-594.03861	1
16837	N	72.12061	89.66294	73.33680	-655.10545	40.19026	-78.18207	1
16838	H	72.91676	89.09985	73.21252	-2208.34155	-1992.64353	-588.12984	1
16839	H	71.22470	89.11898	73.31495	-1605.53722	-570.90944	1652.55954	1
16840	N	70.98800	91.79674	73.89560	367.92025	-455.15043	-1033.24919	1
16841	H	71.16604	92.74811	74.19489	-533.57602	1761.72453	2184.84068	1
16842	H	69.95260	91.50616	73.91924	-1354.15654	1581.50798	-952.26891	1
16843	C	77.15778	93.66804	72.73597	-312.86870	992.36347	-669.07757	1
16844	O	76.87689	93.24924	73.89384	119.30897	74.22788	331.11539	1
16845	N	78.25172	94.33014	72.43631	53.79319	306.48171	264.82220	1
16846	H	78.29554	94.55120	71.45547	-22.72617	1829.19197	889.88597	1
16847	C	78.73853	95.33374	73.43505	-581.91295	693.29770	-1114.79771	1
16848	H	79.45168	96.06514	72.87588	1191.73363	-380.49558	-969.04028	1
16849	C	77.49190	96.22917	73.96004	677.56417	288.85512	46.64060	1
16850	H	76.61086	95.63847	74.13376	-89.55322	1101.03684	2473.80386	1
16851	H	77.65889	96.75614	74.91937	-4298.17827	342.63115	1690.28803	1
16852	C	77.35260	97.28064	72.82598	628.34349	490.10926	-64.91694	1
16853	H	76.67922	98.04741	73.12371	1047.36336	774.39414	2505.98537	1
16854	H	76.89661	96.77696	71.89798	1965.81370	1997.00564	2095.86484	1
16855	C	78.80842	97.87954	72.42271	186.56202	574.41528	286.26810	1

16856	O	79.25348	98.56476	73.34262	-64.78327	-134.15483	-632.83149	1
16857	O	79.33772	97.74556	71.27429	6.62007	-233.47997	64.55851	1
16858	C	79.47880	94.50657	74.56714	725.71238	947.93486	-317.78230	1
16859	O	79.82965	93.37897	74.39132	204.03351	-806.20766	-274.41381	1
16860	N	79.80379	95.26800	75.65846	696.02311	-182.60543	72.38528	1
16861	H	79.41562	96.20403	75.94799	-1948.90667	-1552.86390	1005.23863	1
16862	C	80.66838	94.57736	76.60456	-570.78439	-62.84086	-512.70834	1
16863	H	80.39158	93.48543	76.60774	-1322.55359	3749.75597	-327.22643	1
16864	C	82.18783	94.57390	76.10206	-694.52153	-1039.35155	-500.46993	1
16865	H	82.57012	95.57715	75.84802	474.72325	-4312.30108	-73.05685	1
16866	H	82.11944	93.91199	75.21482	365.26230	1283.07669	-972.29176	1
16867	C	83.05290	93.97035	77.23277	-90.47290	145.19916	-752.06623	1
16868	H	82.88254	94.48507	78.20542	1184.61068	837.16479	1122.31580	1
16869	H	84.13898	94.12907	77.02320	2016.66958	-2659.76404	107.39558	1
16870	C	82.84723	92.37489	77.22469	-173.18454	301.56483	-295.83004	1
16871	O	83.39321	91.68353	76.36442	141.78114	571.28069	-416.70171	1
16872	O	81.89783	92.00586	77.91505	-155.45550	-442.15076	542.57905	1
16873	C	80.23993	95.29288	77.98790	188.85426	-41.19961	-199.21121	1
16874	O	79.68539	96.40618	77.97261	-359.43197	-266.26244	123.74395	1
16875	N	80.72011	94.71939	79.04641	253.76364	-953.23669	-519.81307	1
16876	H	81.27248	93.79901	78.94166	3435.38620	-1525.22321	3901.72589	1
16877	C	80.49934	95.34091	80.32125	240.84720	280.56499	-302.97509	1
16878	H	80.26197	96.49436	80.20493	459.63365	-466.20654	-2065.89516	1
16879	C	79.27620	94.46605	80.89796	-634.49280	412.76792	-123.03054	1
16880	H	79.47198	93.38563	80.87189	911.95721	-1767.71123	-635.48852	1
16881	H	78.44737	94.69559	80.12393	-1814.26770	-3825.75115	859.45341	1
16882	C	78.75871	94.89074	82.33001	860.24517	-376.73690	-286.55597	1
16883	O	78.64465	96.00510	82.78201	-788.98952	-77.70931	-292.78749	1
16884	N	78.42073	93.68416	82.86263	-398.33592	-402.55200	39.11168	1
16885	H	78.55608	92.71525	82.48763	-591.81176	-986.84276	-122.99786	1
16886	H	78.08500	93.63352	83.82563	-293.21061	158.15056	-1224.78519	1
16887	C	81.87452	95.14456	81.21943	-797.42278	-108.30001	-87.87926	1
16888	O	82.66171	94.26414	81.04165	189.71623	328.24472	467.54530	1
16889	N	81.83460	96.15208	82.17348	-112.85927	-1056.88308	-130.59809	1
16890	H	80.94275	96.74417	82.10163	1149.21866	-1386.31832	-4384.99016	1
16891	C	83.00366	96.37397	82.95118	34.38635	248.68124	-211.28083	1
16892	H	83.83572	95.84213	82.35952	-3346.08176	1261.50086	-1801.80736	1
16893	C	83.13469	97.93596	83.16668	502.61969	-674.04822	-138.54659	1
16894	H	83.14034	98.47323	82.17270	1165.24698	2634.12989	-218.95436	1
16895	H	82.38015	98.38629	83.82522	-1069.96827	2381.02555	3307.41680	1
16896	H	84.12863	97.94422	83.72122	-1241.14467	1138.86560	-838.45291	1
16897	C	82.98580	95.36257	84.30585	1059.19409	578.49387	-447.92562	1
16898	O	84.08137	94.97246	84.63114	-506.50774	94.40387	21.98443	1
16899	N	81.79941	95.09358	84.75406	-376.40977	39.65804	-999.95278	1
16900	H	80.96760	95.58132	84.32650	919.08364	260.81981	2474.74462	1
16901	C	81.68715	94.79185	86.15871	-10.63745	179.39547	683.61827	1
16902	H	82.77736	94.86851	86.32208	-187.83313	-706.77753	327.12621	1
16903	C	80.94906	95.87780	87.00263	125.20273	-253.81698	55.78024	1
16904	H	81.35897	96.03702	88.03705	528.12333	-445.24162	3245.58846	1
16905	H	79.89145	95.53450	87.21799	-1242.35041	4723.94812	1550.77846	1
16906	C	80.75043	97.14153	86.06903	642.52764	-369.96915	-693.10819	1
16907	O	81.57036	98.01091	85.96251	-2.16582	1.22737	-76.57100	1
16908	N	79.53555	97.01197	85.48462	-530.39240	541.53532	388.17157	1
16909	H	78.92631	96.17777	85.68345	1350.11478	-292.25566	-3135.26720	1
16910	H	79.27179	97.62761	84.70390	3691.52655	-2520.19329	-1178.13744	1
16911	C	81.11143	93.28641	86.45699	-161.82070	140.84977	-619.90457	1
16912	O	81.34500	92.92963	87.59301	-388.93832	374.10864	310.17815	1
16913	N	80.77540	92.54022	85.41791	-695.94677	-20.07681	15.70625	1
16914	H	80.72051	93.03196	84.53569	1418.32714	3218.47433	836.95759	1
16915	C	80.31567	91.17247	85.64705	129.35103	322.50524	-297.11911	1
16916	H	80.37487	90.86937	86.71921	-293.46886	-1207.40545	-37.22426	1
16917	C	78.83190	90.96962	85.06141	39.07133	-166.39333	-246.33033	1

16918	H	78.49705	89.88676	85.10546	268.67776	293.53790	1720.88845	1
16919	H	78.86098	91.33855	84.03006	-1129.91489	-399.60933	-1401.67032	1
16920	C	77.84192	91.85554	85.84388	1003.65486	-514.35439	-403.26797	1
16921	C	76.67408	91.91836	85.01878	165.38845	-9.77294	23.69672	1
16922	H	76.65509	91.31722	84.04400	-249.79440	2999.94573	-1560.58362	1
16923	C	75.59691	92.55402	85.65983	-797.42135	322.98265	-1654.43742	1
16924	H	74.61344	92.57110	85.17663	1219.14366	2872.23763	-3204.35282	1
16925	C	75.69441	93.33991	86.82584	-508.14367	-170.72283	127.82195	1
16926	H	74.82638	93.91406	87.17869	395.07247	-1087.55211	606.22931	1
16927	C	77.99990	92.47316	87.12556	-40.79024	-115.32467	-253.87383	1
16928	H	78.87744	92.39397	87.79223	200.56404	2309.99138	1445.72161	1
16929	C	76.96462	93.33181	87.50445	86.60067	36.43801	-458.68773	1
16930	H	77.17166	94.03829	88.29759	591.46851	881.64280	544.58340	1
16931	C	81.31367	90.32947	84.71929	-1382.36948	635.55991	-508.58940	1
16932	O	81.94724	89.40075	85.23596	-615.92089	72.31679	-305.42133	1
16933	N	81.31582	90.79617	83.48844	795.60640	-463.57689	-468.01848	1
16934	H	80.69445	91.54535	83.24203	-1703.17958	-2731.33617	-1078.08713	1
16935	C	81.89570	90.12390	82.36033	481.56398	-164.71486	-43.99374	1
16936	H	81.48277	89.09089	82.43146	2629.92851	-3051.84728	215.99213	1
16937	C	81.70325	90.83800	80.92829	117.00335	-189.53562	-213.40400	1
16938	H	82.12552	90.20854	80.07476	1598.01465	-1663.93969	76.55506	1
16939	H	82.37213	91.73581	80.97342	445.97396	651.39649	-2726.05912	1
16940	C	80.22847	91.33147	80.75503	29.46073	-115.82488	-174.92437	1
16941	O	79.40769	91.36878	81.67751	-157.60026	-242.99053	-584.81451	1
16942	N	79.99188	91.62187	79.47366	52.88030	-166.09579	-351.31180	1
16943	H	80.69525	91.35499	78.68891	-806.84592	1296.95033	2467.06898	1
16944	H	79.11750	92.01659	79.10956	2279.12041	-2082.33854	384.74379	1
16945	C	83.59660	90.05061	82.51533	509.41642	-354.51492	-153.84341	1
16946	O	84.23982	89.20577	81.86154	-321.15852	-510.03559	-147.19596	1
16947	N	84.11971	91.11480	83.06551	522.34963	1319.53979	96.04218	1
16948	H	83.40127	91.66671	83.50342	706.76195	-777.10404	-1114.28245	1
16949	C	85.52749	91.22681	83.22069	-154.53740	-303.34839	-285.76291	1
16950	H	85.96465	90.57116	82.42204	-2088.68366	-1383.41809	661.66520	1
16951	C	85.99320	92.73107	83.28296	-280.12391	0.24295	-531.36639	1
16952	H	87.08083	92.90596	83.17290	-838.12057	2758.55045	-1881.36974	1
16953	H	85.73025	93.04649	84.32555	2365.19144	817.62767	85.36814	1
16954	C	85.29488	93.59924	82.11730	-518.18490	147.12674	-389.83816	1
16955	H	84.22732	93.80828	82.31081	1910.80461	413.74630	-302.25833	1
16956	H	85.36429	93.04860	81.13917	273.54861	-761.33141	51.36207	1
16957	C	86.02498	94.97951	82.07608	594.86815	595.48664	-472.00892	1
16958	H	87.13302	94.88674	82.25744	2816.61626	-2285.41274	-1173.84435	1
16959	H	85.84832	95.54696	83.01022	3615.54637	-996.11535	-2568.93890	1
16960	C	85.57763	95.55266	80.62846	1833.74784	129.68729	-547.05505	1
16961	H	84.47595	95.71265	80.48702	1715.19390	-516.48603	482.86096	1
16962	H	86.20306	96.47321	80.52656	941.62239	-988.60080	-3386.73549	1
16963	N	86.04292	94.73041	79.54110	-30.79118	385.81792	-193.72275	1
16964	H	86.92556	94.29391	79.64010	-2283.64800	-128.32525	-2529.91277	1
16965	H	85.46275	93.89238	79.45707	1079.67963	-798.82768	-234.48174	1
16966	H	82.54069	96.74105	79.59778	-867.32183	709.74612	1090.09172	1
16967	C	85.95286	90.82914	84.75554	539.03864	-258.55540	140.51659	1
16968	O	87.09501	91.02687	85.10325	424.36737	384.43876	760.36527	1
16969	N	84.97625	90.35100	85.55486	82.01282	-304.55593	-501.23489	1
16970	H	84.05087	90.36461	85.21963	-253.39154	1293.12727	90.88336	1
16971	C	85.15313	90.43464	86.95753	247.74787	-66.57409	-149.94006	1
16972	H	86.23124	90.79950	87.18240	-280.51524	-2398.10983	271.45374	1
16973	C	84.03903	91.41132	87.47070	-1192.22377	632.25501	-276.29587	1
16974	H	83.02874	91.31117	87.03496	-2725.86540	-548.28886	2221.33308	1
16975	C	83.88719	91.37403	89.01071	-470.41032	-177.92762	636.51081	1
16976	H	84.79983	91.64440	89.57912	1602.50438	-171.56485	1768.99515	1
16977	H	83.66799	90.25275	89.18077	-1984.07197	2286.57891	987.44897	1
16978	H	82.93023	91.87037	89.27530	-76.81970	-1103.49022	10.14613	1
16979	C	84.36510	92.88694	86.99128	-492.15010	778.79830	-211.71715	1

16980	H	84.28147	93.02374	85.89125	926.22788	-2175.77855	-3631.70776	1
16981	H	83.60169	93.49668	87.50617	557.87496	-3066.91038	1242.77568	1
16982	C	85.80984	93.36487	87.42153	-480.80550	33.04189	-68.11889	1
16983	H	86.59396	92.86801	86.83881	-960.79324	354.22997	-1216.40844	1
16984	H	85.90540	94.46210	87.14999	-1292.18258	980.53191	1088.26226	1
16985	H	85.96258	93.27439	88.53894	1455.10401	552.91977	1985.63330	1
16986	C	84.83719	88.91419	87.62546	-306.04808	385.94429	219.69450	1
16987	O	85.73198	88.32499	88.18615	883.14849	561.74173	214.03561	1
16988	N	83.54256	88.67830	87.46423	8.74703	630.59512	-522.92858	1
16989	H	82.92152	89.11440	86.74946	-1590.70485	66.77681	-429.45219	1
16990	C	83.04836	87.39748	87.83480	1160.20712	382.12223	75.83100	1
16991	H	83.51510	87.13156	88.85173	1309.73818	-732.05341	5220.47295	1
16992	C	81.44589	87.51917	88.02698	-381.43053	-15.04779	480.51111	1
16993	H	80.94840	87.86543	87.10484	-3020.45193	-1484.83749	2084.51526	1
16994	H	81.36926	88.35861	88.80879	1676.76509	-5264.19828	482.77079	1
16995	C	80.87769	86.18136	88.47620	977.89747	-546.91621	46.99303	1
16996	C	80.04334	85.53342	87.57188	-150.56583	-542.57721	-56.41739	1
16997	H	79.92040	85.98528	86.56192	1365.99711	428.19691	-3693.73271	1
16998	C	79.40000	84.34180	88.00890	144.47270	-887.62377	-155.87244	1
16999	H	78.84100	83.76780	87.28590	-328.20360	-2959.33355	1021.19185	1
17000	C	79.47800	83.93480	89.35490	-642.70599	451.43486	-466.81034	1
17001	H	78.96900	83.02580	89.64090	-635.63027	-442.27836	3049.76432	1
17002	C	81.09330	85.72442	89.79197	596.26004	377.80357	-274.59613	1
17003	H	81.87395	86.18361	90.43206	-90.28449	-2248.10444	936.93919	1
17004	C	80.30600	84.65280	90.26790	21.13127	-626.18118	-664.90332	1
17005	H	80.48200	84.28180	91.26690	-2377.19387	-1194.15714	-1686.65329	1
17006	C	83.43773	86.37917	86.63979	-13.36156	-624.58042	241.96852	1
17007	O	83.89729	85.28819	86.84201	364.17403	242.96924	-70.88379	1
17008	N	83.20828	86.98825	85.43837	-411.97118	-372.19449	579.13573	1
17009	H	82.57957	87.81226	85.28015	222.44419	1592.01624	784.46400	1
17010	C	83.37053	86.00024	84.43059	336.72533	451.72163	486.80248	1
17011	H	82.75595	85.21460	84.89847	-2902.37568	61.13080	3341.78213	1
17012	C	82.79620	86.49903	82.97916	350.13491	-246.86179	958.23443	1
17013	H	83.00858	85.78749	82.22097	-960.09760	1043.95432	4208.47078	1
17014	H	83.46536	87.33653	82.60865	-1910.97738	-2591.35975	-1584.49925	1
17015	C	81.35851	86.81659	83.10103	1344.99795	614.45109	44.08718	1
17016	H	81.34234	87.92376	83.43424	1420.11616	-503.26292	-2588.19946	1
17017	C	80.52409	86.73087	81.81508	274.55105	308.40224	521.50134	1
17018	H	80.85400	87.46680	81.00247	440.60867	-1477.96874	432.12199	1
17019	H	79.44837	87.07428	82.12016	2427.09964	1076.78580	-1315.34185	1
17020	H	80.45787	85.70909	81.39384	321.75356	-1637.46334	-311.77878	1
17021	C	80.70679	85.85372	84.11820	-353.64791	-344.88549	304.77696	1
17022	H	80.63688	84.85447	83.71867	1533.38465	-751.89139	1820.61527	1
17023	H	79.68218	86.17213	84.31058	-1173.40567	2087.21942	-856.27582	1
17024	H	81.15334	85.87883	85.10105	2868.34488	4784.46044	389.54994	1
17025	C	84.89418	85.38544	84.27479	-745.50358	-41.64789	-688.93231	1
17026	O	84.87300	84.21580	83.92590	484.78819	-232.13709	572.07571	1
17027	N	85.96175	86.14178	84.36158	123.54411	53.25714	-238.66256	1
17028	C	86.09988	87.50514	84.85773	365.47642	593.57332	586.00848	1
17029	H	85.49953	87.84010	85.73434	-883.92831	130.04870	-18.62159	1
17030	H	85.72043	88.20108	83.99343	-2203.73739	291.38644	-1986.45573	1
17031	C	87.26254	85.49221	84.26374	-460.66260	338.36669	-360.76761	1
17032	H	87.36000	84.75980	83.39390	-1956.53740	-1725.16788	-1765.99997	1
17033	C	88.30247	86.65814	84.13280	532.55355	450.04133	218.11163	1
17034	H	88.29077	87.00633	83.12365	2175.17987	-1680.77782	2307.72374	1
17035	H	89.29873	86.41391	84.56172	130.70397	-1987.21918	1226.27880	1
17036	C	87.64629	87.67076	85.16553	902.10408	-407.40678	402.26241	1
17037	H	87.87664	87.43805	86.21956	-4113.62137	-791.26557	-354.04681	1
17038	H	87.97305	88.78875	85.04566	1246.10989	897.95928	63.92804	1
17039	C	87.49300	84.44880	85.47990	481.17713	-770.68342	-26.39082	1
17040	O	88.17500	83.43780	85.31690	662.28783	338.86154	-256.54544	1
17041	N	86.94800	84.79480	86.61690	-355.77024	360.43447	-679.89734	1

17042	H	86.35221	85.65655	86.58018	6536.77701	-59.93697	322.94936	1
17043	C	86.99100	84.05980	87.81290	748.44016	418.03311	-302.26836	1
17044	H	88.04200	83.90580	88.00490	-1286.35492	1354.34724	-2536.24087	1
17045	C	86.54200	84.90880	89.03390	418.38191	558.35263	-585.25714	1
17046	H	85.56812	85.48050	88.83566	-2124.34058	3005.03087	1084.80342	1
17047	O	87.55116	86.19057	89.16198	166.15675	-196.33519	148.69930	1
17048	H	87.00274	86.90875	88.79760	-3785.59398	-1206.29802	-1757.64155	1
17049	C	86.58800	84.13880	90.31390	-283.70739	860.17132	100.11513	1
17050	H	86.42200	84.88380	91.12190	-1795.94078	1435.55542	2147.21644	1
17051	H	87.58000	83.65880	90.45790	-435.86088	1217.30768	2865.37132	1
17052	H	85.87300	83.28880	90.33790	847.17946	-2925.10475	789.94646	1
17053	C	86.28000	82.71080	87.71290	348.70998	-610.39722	-581.61753	1
17054	O	86.82200	81.66680	88.07090	487.52202	-368.28329	-500.33258	1
17055	N	85.01900	82.70380	87.12790	147.88702	116.27934	-824.53825	1
17056	H	84.59100	83.60380	87.13890	-2674.73959	1532.87730	-646.48648	1
17057	C	84.34600	81.49680	86.73990	-173.64911	895.38896	-18.27396	1
17058	H	84.30700	80.75780	87.52590	2626.33703	724.73484	-1569.57992	1
17059	C	82.88500	81.78680	86.44690	472.40232	489.18323	601.57630	1
17060	H	82.91900	82.67580	85.78090	-1567.70870	-1396.99338	2344.15697	1
17061	C	82.17700	80.62380	85.67890	-686.10317	-556.20421	-242.24390	1
17062	H	81.07800	80.71880	85.54690	598.41109	-2089.90955	-2275.59134	1
17063	H	82.70400	80.35880	84.73790	461.08637	2498.75301	-1856.94623	1
17064	H	82.32100	79.72080	86.31090	1404.57528	-2171.67960	1786.11393	1
17065	C	82.07000	82.12980	87.72690	829.91579	-260.36295	260.76104	1
17066	H	81.10200	82.37580	87.23990	2005.26066	-1846.06125	-1568.82272	1
17067	H	82.53400	83.06080	88.11890	1997.51249	-773.18170	2299.81178	1
17068	C	81.94500	81.05480	88.81990	-714.77797	295.25802	-489.47011	1
17069	H	82.88100	80.59980	89.20790	-591.02561	3050.46585	-490.56526	1
17070	H	81.31400	80.20680	88.47790	2815.64469	-509.29682	1298.78701	1
17071	H	81.40000	81.55980	89.64590	-697.87421	-1644.06384	2590.27197	1
17072	C	85.05200	80.71580	85.59890	-8.53369	117.84609	-907.35201	1
17073	O	85.24900	79.52680	85.71490	28.89394	785.85224	67.89789	1
17074	N	85.49400	81.43280	84.53190	-394.64883	-637.49170	-394.75551	1
17075	H	85.40200	82.42480	84.48490	-917.73706	-3005.42708	-172.11869	1
17076	C	86.03100	80.79380	83.32290	-685.05291	-509.53067	325.44447	1
17077	H	85.31500	80.12480	82.86790	2087.93761	-1749.15828	1563.17221	1
17078	C	86.55300	81.83280	82.24690	-285.42760	680.70566	-543.31346	1
17079	H	87.16500	81.34780	81.45690	-406.93343	1249.33627	2856.78426	1
17080	H	87.19100	82.46680	82.89890	-1420.16195	-2746.04582	586.62255	1
17081	C	85.50700	82.73980	81.58390	-387.37410	-516.39031	-648.51176	1
17082	C	84.15500	82.39380	81.53690	8.37560	738.15855	534.98096	1
17083	H	83.79200	81.55280	82.10890	-1976.71996	-503.22493	-2401.95861	1
17084	C	83.21100	83.32080	80.93390	-813.75607	351.40567	-239.32063	1
17085	H	82.15600	83.09880	80.98090	2035.65888	1768.92256	-1615.98393	1
17086	C	83.64600	84.52480	80.37890	772.34234	-27.95156	472.41300	1
17087	O	82.61489	85.32259	79.66166	185.06485	129.57855	-573.92468	1
17088	H	81.83700	84.81180	79.82390	-1080.08605	-2322.12039	1828.02480	1
17089	C	85.92600	83.94280	80.96390	6.05711	-903.27024	-110.87849	1
17090	H	86.96400	84.21780	81.07890	2829.27439	-598.86941	-1226.46106	1
17091	C	84.98800	84.82180	80.36790	-678.00518	496.60885	-369.86313	1
17092	H	85.44105	85.66017	79.78998	-2915.48703	244.22891	-2438.63971	1
17093	C	87.28100	79.90080	83.70090	-602.48169	658.69385	-208.30911	1
17094	O	87.52500	78.85780	83.08590	-549.44032	561.74256	109.17800	1
17095	N	88.11400	80.46780	84.61090	642.96512	513.19753	-179.98725	1
17096	H	87.81200	81.38580	84.85490	554.47561	2851.08366	1205.19199	1
17097	C	89.22100	79.75680	85.24590	-801.90495	437.56083	62.18517	1
17098	H	89.95300	79.50280	84.49390	-1464.51312	-2546.38990	1124.84143	1
17099	C	89.96200	80.65580	86.28690	-458.29519	-343.52332	707.42201	1
17100	H	90.83200	80.05380	86.62590	2283.07377	-336.40392	-2139.03685	1
17101	H	89.32800	80.96580	87.14490	931.33406	2257.02425	-1986.55878	1
17102	O	90.43900	81.84080	85.66990	610.32611	92.12801	483.01903	1
17103	H	89.67500	82.42080	85.62090	2369.02049	-1179.21299	1691.04846	1

17104	C	88.73400	78.47380	85.93690	-909.04626	101.73149	39.15022	1
17105	O	89.25800	77.41880	85.68690	452.12303	480.50776	425.07062	1
17106	N	87.62200	78.53080	86.72490	-701.95005	282.62632	-385.82932	1
17107	H	87.11900	79.38180	86.85290	1745.97851	2397.36485	-1047.62160	1
17108	C	87.01300	77.34680	87.36090	-113.26819	694.01660	575.81346	1
17109	H	87.78600	76.78980	87.87090	2151.54835	2266.77734	334.12137	1
17110	C	85.83700	77.64780	88.31690	-573.33049	-363.66500	-616.67497	1
17111	H	85.15200	78.26580	87.69790	2170.45817	953.65837	2060.27926	1
17112	C	85.23200	76.35180	88.91690	-584.42856	628.39546	-316.18304	1
17113	H	84.85900	75.70780	88.09290	1913.26524	866.71986	-2344.55790	1
17114	H	85.99500	75.79680	89.50290	-1848.14339	-1493.28883	2060.17481	1
17115	H	84.35600	76.61180	89.54990	-674.86039	3069.33543	124.10768	1
17116	C	86.39100	78.49780	89.48490	354.02269	771.95453	-330.31748	1
17117	H	87.06500	79.27980	89.07290	1427.84035	-2198.47053	-1742.42291	1
17118	H	87.08200	77.89680	90.11390	-991.08893	-1148.86745	2752.86447	1
17119	C	85.32100	79.24980	90.26490	548.11549	-645.98527	-339.45320	1
17120	H	85.66100	79.80480	91.16590	-1839.58327	-1095.46754	2304.62952	1
17121	H	84.50800	78.55480	90.56390	2588.94393	367.32088	-1748.92652	1
17122	H	84.81600	79.99880	89.61990	942.94869	-1655.61062	-2506.74063	1
17123	C	86.59100	76.33380	86.29590	37.20179	705.09135	-582.03551	1
17124	O	86.87600	75.13580	86.32990	263.40507	-247.17595	-706.70502	1
17125	N	85.94400	76.86980	85.20790	-715.74336	-4.18375	448.95949	1
17126	H	85.63800	77.81680	85.14890	838.32427	1784.43455	-2455.06733	1
17127	C	85.54400	75.97380	84.09090	-589.85106	56.62431	-701.66531	1
17128	H	84.97100	75.16780	84.52390	-590.84555	-2292.32178	-2078.06839	1
17129	C	84.70500	76.68680	83.02590	812.00035	-153.54614	-379.98876	1
17130	H	85.34800	77.43880	82.51990	-2032.51842	-1169.11159	-2105.97809	1
17131	C	84.27500	75.71480	81.91990	385.98328	-7.71678	819.03347	1
17132	H	85.09700	75.06980	81.54390	-1047.85130	1847.31625	-2329.86050	1
17133	H	83.47900	75.04880	82.31590	-1135.20078	2167.35756	1976.83175	1
17134	H	83.83700	76.40380	81.16690	-1221.64390	-1777.21280	-2296.52661	1
17135	C	83.45000	77.48980	83.55590	415.02904	385.08012	708.60650	1
17136	H	82.97200	77.88180	82.63290	2751.84028	500.29216	1428.17904	1
17137	H	83.89400	78.25780	84.22490	-2555.14716	-1013.25557	-1541.31490	1
17138	C	82.33100	76.72480	84.30590	-573.33093	-645.33268	-305.08700	1
17139	H	81.47300	77.36780	84.59690	621.70489	408.45907	3052.63070	1
17140	H	82.01000	75.87880	83.66190	-2558.93167	-332.97762	1801.47885	1
17141	H	82.78500	76.35380	85.24990	1982.50157	2424.49246	-276.77835	1
17142	C	86.82000	75.33080	83.39190	633.64313	7.37543	645.91442	1
17143	O	86.93000	74.10180	83.14490	-603.25143	514.93996	22.36745	1
17144	N	87.87300	76.12580	83.05390	-668.26296	292.10033	-438.63187	1
17145	H	87.78700	77.10580	83.21590	964.78945	2390.24356	1798.08006	1
17146	C	89.14600	75.69580	82.51290	626.46137	150.81961	-647.37545	1
17147	H	88.77200	75.17380	81.64490	1618.39587	-2060.16562	-1741.49121	1
17148	C	89.90200	76.92480	82.03590	424.59801	564.74533	-580.80130	1
17149	H	89.27500	77.50780	81.32890	-1811.25018	1035.66443	2354.13974	1
17150	H	90.24800	77.70980	82.74190	964.18930	-2105.74945	2119.73999	1
17151	C	91.23100	76.59480	81.38190	330.76457	-775.30707	330.92615	1
17152	C	91.21500	76.27080	80.01490	-28.59772	910.50041	79.53944	1
17153	H	90.34000	76.17680	79.38890	-472.92306	-1957.49942	-2421.96958	1
17154	C	92.38300	75.83580	79.33690	118.94082	106.98705	890.39808	1
17155	H	92.23500	75.47680	78.32890	1776.04172	-2559.66751	-397.81678	1
17156	C	93.59700	75.74780	79.99190	624.25308	-211.62993	-631.08708	1
17157	H	94.46100	75.44580	79.41890	-286.74729	2950.04185	1059.05801	1
17158	C	92.48600	76.63880	82.03490	847.11558	317.80017	-86.34671	1
17159	H	92.45700	76.91580	83.07890	1214.48412	-2333.47331	1713.23095	1
17160	C	93.65300	76.24480	81.37190	115.99903	622.16726	651.06787	1
17161	H	94.58100	76.33180	81.91690	2963.59074	-681.12503	779.80069	1
17162	C	89.91100	74.63880	83.25790	-903.35201	-96.10774	108.68106	1
17163	O	90.31700	73.58680	82.77890	109.23489	594.74348	-516.45866	1
17164	N	90.07200	74.84380	84.60690	-68.67408	765.07853	-360.08800	1
17165	H	89.75100	75.72580	84.94490	-1906.82177	2504.33977	93.67718	1

17166	C	90.99200	74.14780	85.47890	172.71877	834.47793	317.70845	1
17167	H	91.87600	73.95580	84.88990	-1942.47029	1232.11708	2142.81582	1
17168	C	91.44100	74.96580	86.68890	169.75461	895.44451	-32.20202	1
17169	H	90.54900	75.39680	87.18990	1716.23254	-1244.50565	-2328.82035	1
17170	H	91.98500	74.47680	87.52490	-143.93812	3114.14148	-434.24383	1
17171	C	92.29500	76.20180	86.29890	-752.76381	-253.55780	446.41399	1
17172	H	91.81200	76.81980	85.51190	2489.39924	790.71973	-1755.28764	1
17173	C	92.49600	77.08680	87.49090	612.60728	-40.83853	664.57138	1
17174	H	93.34000	76.67480	88.08490	-647.51045	2185.19990	-2176.92106	1
17175	H	92.75900	78.11980	87.17690	-2283.80133	-591.50604	-2091.43735	1
17176	H	91.62000	77.10680	88.17290	-2016.74418	1687.67690	1724.41877	1
17177	C	93.63900	75.80880	85.71290	-666.17844	-596.80161	179.52286	1
17178	H	94.39500	76.62280	85.73390	2421.79571	-1272.66991	-1553.85365	1
17179	H	94.08800	74.94380	86.24590	214.75996	-1963.48001	2439.94516	1
17180	H	93.51200	75.52980	84.64590	2276.70286	1360.53574	-1695.68753	1
17181	C	90.49500	72.83780	85.92890	-814.14824	-84.26131	400.54954	1
17182	O	91.27500	71.96380	86.38890	-132.46349	-268.58705	722.86785	1
17183	N	89.19100	72.60280	85.69690	-255.16401	122.08979	789.17282	1
17184	H	88.59100	73.30280	85.31790	39.89389	-3144.60655	-66.45142	1
17185	C	88.45900	71.35680	85.94490	723.48278	-371.94380	398.59829	1
17186	H	89.12800	70.64180	86.40090	2330.53934	-2080.58670	343.46997	1
17187	C	87.22600	71.64880	86.78490	628.93547	105.95190	641.74511	1
17188	H	86.71000	70.67580	86.92890	-1832.19757	1647.43117	1951.24989	1
17189	O	86.29500	72.52080	86.19690	718.99266	-294.92835	116.77926	1
17190	H	86.60700	73.42780	86.23990	269.56486	493.91441	-3101.48944	1
17191	C	87.61600	72.22880	88.17090	-738.48817	-496.03654	-217.47822	1
17192	H	86.73200	72.42180	88.81590	-1087.52799	2935.07605	310.64735	1
17193	H	88.12700	73.21380	88.10690	-37.72906	-1909.23681	2493.87076	1
17194	H	88.25200	71.51380	88.73390	1025.24679	2136.63130	-2074.96968	1
17195	C	88.17800	70.69480	84.65590	-50.45776	572.17860	-716.90844	1
17196	O	88.41700	69.53780	84.41390	232.33051	-360.22923	-669.87632	1
17197	N	87.69700	71.45480	83.66790	-645.41248	347.13244	-432.94398	1
17198	H	87.49600	72.42580	83.77290	2619.81576	493.36611	1658.26441	1
17199	C	87.33000	70.99180	82.32790	-518.85451	-528.09049	-541.94431	1
17200	H	86.87200	71.79880	81.77690	-1052.25888	-1586.80486	2498.18214	1
17201	H	86.53900	70.25880	82.39390	3133.90996	-192.42974	116.21042	1
17202	C	88.38800	70.38780	81.46990	-134.42879	-887.79751	-158.04236	1
17203	O	88.07800	69.34780	80.89690	-373.16759	-566.26035	396.88793	1
17204	N	89.50700	71.10180	81.21690	-382.56945	-571.82143	481.75427	1
17205	H	89.71200	71.85980	81.82990	-624.86721	-1575.02937	2642.79307	1
17206	C	90.54000	70.62380	80.30890	-326.05866	684.89496	504.16750	1
17207	H	90.04700	70.37080	79.38190	2545.99165	-1528.54897	1014.57343	1
17208	C	91.49700	71.77680	80.00190	-689.53880	-166.98733	569.17932	1
17209	H	90.87200	72.69580	80.01990	-280.02924	2907.79365	-1184.42513	1
17210	C	92.63800	71.97780	81.09890	357.68200	827.09032	136.09454	1
17211	H	93.11400	72.96780	80.93290	-1450.60608	-648.23368	2708.93437	1
17212	H	93.41500	71.18380	81.09390	-1779.50368	-142.04318	-2602.43373	1
17213	H	92.18000	72.00080	82.11090	2932.36592	-375.46993	1055.84134	1
17214	C	92.06200	71.74980	78.55590	277.79333	-287.01938	808.22593	1
17215	H	91.23500	71.68480	77.81690	-1773.01643	2094.85048	1541.24861	1
17216	H	92.43600	72.79180	78.45790	-1700.52523	2130.76431	1572.99887	1
17217	C	93.19900	70.75380	78.20890	621.50515	-557.64419	-360.59341	1
17218	H	94.09500	70.93880	78.83990	-2529.67869	389.04233	-1846.44203	1
17219	H	93.64100	70.73480	77.18990	897.29307	-2274.97275	1962.54830	1
17220	H	92.87200	69.72480	78.47090	-2542.31628	637.72588	1739.11216	1
17221	C	91.19200	69.33780	80.85890	-849.95865	43.45862	328.99050	1
17222	O	91.46200	68.34780	80.13890	-217.10709	678.60722	-358.65655	1
17223	N	91.48600	69.32480	82.18790	-416.88690	596.93588	-443.17047	1
17224	H	91.23100	70.17480	82.64090	2764.92366	-1189.20059	893.24514	1
17225	C	91.91500	68.12480	82.90290	671.36736	-2.87476	-623.06226	1
17226	H	92.79300	67.74880	82.39990	1133.56769	2477.29230	1564.60967	1
17227	C	92.25100	68.54980	84.34890	-626.76818	-215.90569	618.92128	1

17228	H	91.36300	68.83680	84.95190	2028.09572	-2132.98964	-1113.19804	1
17229	C	92.93000	67.35280	85.13090	-40.91579	546.89107	719.26604	1
17230	H	93.39500	67.66780	86.08990	2814.39815	786.43232	-1170.73680	1
17231	H	93.59900	66.86780	84.38790	680.66775	2167.50407	2166.50194	1
17232	H	92.08600	66.72380	85.48590	-1299.95203	-2084.63292	-1976.25914	1
17233	C	93.12200	69.81780	84.36490	-85.87097	-711.85949	-571.20768	1
17234	H	92.59100	70.79080	84.28690	414.67910	-1823.40109	-2537.36238	1
17235	H	93.47800	69.79780	85.41690	-1802.65629	612.34957	-2516.71922	1
17236	H	93.92400	69.74080	83.59990	-2113.48540	-1556.20673	-1746.88212	1
17237	C	90.88500	67.01480	82.85490	-560.17604	643.61302	-340.86267	1
17238	O	91.19100	65.97680	82.31990	575.22684	277.24387	-472.22652	1
17239	N	89.59800	67.27880	83.21290	524.26395	509.00915	411.22306	1
17240	H	89.33800	68.17280	83.56890	-3104.29147	-448.44894	272.40266	1
17241	C	88.50800	66.28280	83.31090	-546.36324	555.93347	468.75313	1
17242	H	87.63400	66.81180	83.66190	-1061.58852	-2934.61204	389.35155	1
17243	H	88.77800	65.52880	84.03490	10.55105	2346.86330	2086.70722	1
17244	C	88.13700	65.55880	82.06790	310.85332	-559.78602	-655.74751	1
17245	O	88.04400	64.34280	82.03790	297.99695	-575.60490	436.46325	1
17246	N	87.94300	66.29480	80.94490	-137.00757	642.44250	-543.31416	1
17247	H	88.08700	67.28080	80.99990	-2816.45071	981.16264	-1023.44780	1
17248	C	87.72000	65.63780	79.67190	409.75527	-523.64252	-628.67610	1
17249	H	87.02600	64.82080	79.79990	1055.26269	209.07024	2945.60613	1
17250	C	86.96700	66.60780	78.71390	-96.50363	174.73197	-899.78714	1
17251	H	87.46400	67.58080	78.50890	3100.41132	83.77961	492.40403	1
17252	H	86.78100	66.01880	77.79090	2244.79463	362.51811	-2179.42405	1
17253	C	85.61000	66.79680	79.39290	253.03182	779.73252	-410.17787	1
17254	O	84.83300	65.81480	79.48890	37.47156	745.08190	256.45328	1
17255	N	85.34400	67.99780	79.87490	288.96529	778.85602	145.97078	1
17256	H	86.08300	68.66580	79.96190	-2090.44743	-1477.05993	1824.28030	1
17257	H	84.39500	68.15680	80.14790	-3078.34110	132.10681	648.47374	1
17258	C	88.89800	64.98780	79.03490	725.56730	379.20971	-407.24982	1
17259	O	88.72200	64.04280	78.34190	-697.68038	357.86740	-140.39072	1
17260	N	90.14400	65.40080	79.46790	206.17005	-788.69204	-214.25132	1
17261	H	90.25700	66.25580	79.96790	-1065.98865	2023.85267	-2174.79194	1
17262	C	91.31700	64.73480	79.05890	93.71269	519.29579	734.58953	1
17263	H	91.30700	64.62180	77.98490	-2931.29772	1154.91559	-86.26070	1
17264	H	92.21500	65.29480	79.27790	1058.09386	-1921.96269	2239.17693	1
17265	C	91.40100	63.43180	79.75790	307.19372	-793.67896	-327.48745	1
17266	O	91.82500	62.42080	79.26990	-580.71505	335.53104	412.68605	1
17267	N	91.02800	63.38680	81.05790	657.76904	157.06926	-513.16336	1
17268	H	90.80500	64.21680	81.56290	-2520.77814	1604.09448	-1008.37858	1
17269	C	90.91800	62.15580	81.79590	272.45577	-732.55007	-476.09448	1
17270	H	91.86200	61.64080	81.70190	-1069.04265	2392.46453	1734.04641	1
17271	C	90.82800	62.40680	83.27890	329.01022	-793.01168	288.14551	1
17272	H	90.54300	61.55180	83.92790	1675.42279	2646.15876	286.61107	1
17273	H	89.92600	63.04680	83.38890	-2288.58946	-1672.21465	1356.64915	1
17274	C	92.01900	63.17780	83.96190	-509.76875	-339.68900	-688.14800	1
17275	H	92.39400	64.07880	83.43090	2369.14348	459.71170	2004.19969	1
17276	C	91.67700	63.61180	85.38990	-429.89384	656.53258	456.35901	1
17277	H	91.21000	62.80180	85.98990	-2954.60133	-361.20843	-1035.64947	1
17278	H	92.58900	63.86880	85.96890	1881.86793	-747.02512	-2417.75690	1
17279	H	90.99500	64.48680	85.45990	-1865.52047	1325.49624	-2172.38385	1
17280	C	93.24800	62.26580	83.90690	393.27022	144.47070	796.69234	1
17281	H	93.04800	61.32980	84.47190	2317.86464	-1499.53353	1491.55401	1
17282	H	94.12500	62.84280	84.26990	-1441.26038	1876.80917	-2088.92882	1
17283	H	93.55700	61.98580	82.87690	1526.72314	1894.80110	1981.84056	1
17284	C	89.83700	61.22880	81.39190	-673.56171	392.29999	-491.00902	1
17285	O	90.05200	60.01880	81.38790	778.59487	-101.80623	35.24678	1
17286	N	88.67800	61.73480	81.04490	327.52024	-212.84915	735.04661	1
17287	H	88.46700	62.70780	81.09490	-1224.48454	-2122.30223	1962.12456	1
17288	C	87.67100	60.85880	80.39390	537.35759	463.01271	560.59986	1
17289	H	87.32000	60.08580	81.06090	-2112.67471	422.44166	-2307.29397	1

17290	C	86.36900	61.62080	80.15290	433.87130	380.64547	694.38434	1
17291	H	86.66700	62.53680	79.59990	-935.20663	-1903.33518	2312.79831	1
17292	C	85.41000	60.79180	79.24990	-43.61770	142.25521	-910.99776	1
17293	H	85.78800	60.71980	78.20790	-341.41829	2236.52582	2178.93898	1
17294	H	84.42100	61.27980	79.11590	-2235.95014	1459.15621	1660.75727	1
17295	H	85.21300	59.82180	79.75490	-1558.88322	-962.09369	-2570.00536	1
17296	C	85.66900	62.05280	81.46790	56.95089	166.44982	884.42928	1
17297	H	84.86800	62.78280	81.22090	2285.82367	-973.61446	-1935.38889	1
17298	H	85.26400	61.20280	82.05790	1415.76207	-210.19905	-2810.85385	1
17299	H	86.41700	62.61580	82.06690	1683.88527	1797.32319	-1967.03297	1
17300	C	88.14800	60.21080	79.10090	-464.01205	410.83459	661.23382	1
17301	O	87.98300	59.02080	78.84890	-681.96966	364.92232	-191.34311	1
17302	N	88.93200	60.97080	78.26790	599.50119	-481.08076	-349.45192	1
17303	H	88.88200	61.95180	78.43890	946.20447	-2007.23967	-2236.91977	1
17304	C	89.63900	60.42180	77.09990	721.30426	370.11921	401.85220	1
17305	H	88.99200	59.82980	76.46890	-2641.09457	-774.16600	-1541.37773	1
17306	C	90.13200	61.55680	76.21090	-249.73876	332.90145	-826.21242	1
17307	H	90.77500	62.20780	76.84090	2383.78880	1979.62664	-553.06215	1
17308	C	91.04800	61.07380	75.04890	-458.90769	-400.75647	-690.82362	1
17309	H	91.94600	60.50580	75.37390	-1643.60510	-2667.34882	252.83678	1
17310	H	91.50200	61.91580	74.48490	2373.47000	2040.78215	301.13448	1
17311	H	90.55600	60.35680	74.35590	-889.18090	-323.61543	-3013.67162	1
17312	C	89.00800	62.48180	75.66090	2.41465	571.42336	702.92004	1
17313	H	88.47400	61.93980	74.85190	2608.02503	-1680.09225	-494.18834	1
17314	H	88.14100	62.60780	76.34490	-2635.58262	-1486.42667	-879.13109	1
17315	C	89.53000	63.78780	75.11390	-558.13061	-410.42923	583.44340	1
17316	H	90.19400	63.52080	74.26490	937.78538	-2995.70759	55.39792	1
17317	H	88.68400	64.35180	74.66590	-2111.45304	2271.08343	-580.65405	1
17318	H	89.97900	64.42080	75.90890	-2577.15885	1659.78578	-746.17560	1
17319	C	90.77300	59.45680	77.46190	329.05637	-605.52153	-603.74000	1
17320	O	90.96700	58.38780	76.89490	-36.89162	742.63305	264.66326	1
17321	N	91.47500	59.73380	78.58890	-209.46183	-458.02523	663.27245	1
17322	H	91.42900	60.64380	78.99590	1673.14064	1715.00203	2026.56494	1
17323	C	92.46700	58.82380	79.17890	-728.08068	-472.04575	-296.01746	1
17324	H	93.13400	58.59180	78.36190	-2157.87647	2202.47670	-663.86227	1
17325	C	93.39400	59.54580	80.25190	-730.45366	-63.40790	532.29891	1
17326	H	93.67500	58.93680	81.13790	-480.11514	1903.19728	2447.81206	1
17327	H	92.68800	60.32980	80.60090	-1888.57015	2442.64555	-638.24877	1
17328	C	94.60100	60.20980	79.64990	-3.17038	139.77363	-915.12005	1
17329	H	94.23900	60.46180	78.62990	-1497.82791	2213.14065	-1682.09542	1
17330	C	95.06300	61.43480	80.47190	178.10144	820.46697	-374.98231	1
17331	H	95.28300	61.04180	81.48790	-1714.68042	-2400.28468	1078.48133	1
17332	H	94.26400	62.20680	80.47790	-1642.19514	-1985.67416	-1817.20160	1
17333	H	96.00300	61.82780	80.02690	786.27561	-1751.03237	2475.87270	1
17334	C	95.76500	59.20580	79.52190	-727.03968	518.79853	191.27898	1
17335	H	96.08900	58.91780	80.54590	-2582.50637	1683.27393	635.04484	1
17336	H	95.53700	58.21280	79.07790	1394.79679	-2449.70895	1372.41442	1
17337	H	96.53300	59.68580	78.87890	588.50767	-2902.94354	1033.01070	1
17338	C	91.86500	57.57880	79.69390	-585.46378	-299.95709	-646.33610	1
17339	O	92.42900	56.49880	79.48290	532.95971	-21.51262	-593.94772	1
17340	N	90.65400	57.56080	80.28190	-384.15772	-693.58104	273.19261	1
17341	H	90.21300	58.42780	80.50190	-2076.92091	2030.04528	-1232.07644	1
17342	C	89.92200	56.39580	80.60690	-271.79873	-30.09409	-884.24767	1
17343	H	90.56100	55.73180	81.16890	2607.64521	-681.42523	-1632.40807	1
17344	C	88.72200	56.64380	81.52490	-258.24014	820.33596	-323.89875	1
17345	H	88.11700	57.51680	81.19890	-2203.02400	-869.90295	2059.72808	1
17346	C	87.81900	55.37180	81.65790	-272.15218	310.67785	-827.90045	1
17347	H	87.24900	55.30580	80.70590	-1681.65973	2607.81144	524.33392	1
17348	H	88.39100	54.44580	81.87890	2323.15910	1311.67298	-1680.44588	1
17349	H	87.10100	55.43280	82.50390	1539.72277	-1894.79062	-1994.62403	1
17350	C	89.30500	57.08480	82.90890	-337.14599	788.76436	-328.88430	1
17351	H	89.91800	58.00280	82.78290	2330.12044	611.44628	-2034.77314	1

17352	H	89.92900	56.23680	83.26390	-1970.49449	1710.20878	1747.79753	1
17353	H	88.39800	57.27180	83.52290	-1982.06179	-1725.43340	-1743.61534	1
17354	C	89.44700	55.63980	79.32990	-362.02130	579.39707	594.58887	1
17355	O	89.89800	54.49180	79.18290	-452.31241	651.48165	18.98527	1
17356	N	88.71500	56.24380	78.37590	-690.63293	365.25085	-343.51006	1
17357	H	88.39800	57.18380	78.48190	-1685.49488	-206.93043	-2663.24163	1
17358	C	88.13600	55.43780	77.35890	478.36241	-511.56873	-591.56564	1
17359	H	87.98700	54.42380	77.69790	2164.42108	1548.30737	-1691.41299	1
17360	C	86.80000	55.99480	76.89190	514.99122	-65.87512	733.87699	1
17361	H	86.79700	57.04880	76.53890	-1147.62899	2799.00795	-893.68217	1
17362	H	86.30400	55.48680	76.03690	1251.33634	2537.35880	-1393.27456	1
17363	C	85.67600	55.90280	77.97190	-487.62758	-147.45835	744.92118	1
17364	H	86.01400	56.61080	78.75890	1868.93221	1230.59661	2198.00104	1
17365	H	85.62800	54.90080	78.44890	-2221.71982	1005.34716	1979.39634	1
17366	S	83.95900	56.24880	77.57990	-408.26724	-141.71723	343.17326	1
17367	C	84.12800	58.00880	77.20090	-200.84187	-506.55809	-741.40743	1
17368	H	83.24300	58.67880	77.24590	-417.77200	-2977.18794	908.17125	1
17369	H	84.54900	58.20380	76.19090	407.55617	2086.46621	-2333.35067	1
17370	H	84.85200	58.45580	77.91490	2083.96667	1036.17712	-2126.57726	1
17371	C	89.02800	55.25480	76.12090	448.45100	-399.40198	-695.23347	1
17372	O	88.67300	54.33880	75.34490	-486.05266	221.26994	-600.58136	1
17373	N	90.17100	55.99680	75.92590	-671.16278	-218.14259	452.58388	1
17374	H	90.45000	56.78180	76.47390	1344.22147	2731.26508	-816.79921	1
17375	C	91.03600	55.84080	74.74190	-893.83321	196.54963	-68.61397	1
17376	H	91.33000	56.77180	74.28090	-1591.12168	302.17210	-2714.27866	1
17377	H	90.59400	55.18780	74.00390	-576.40564	2947.00891	943.08605	1
17378	C	92.32500	55.26980	75.05690	633.10786	-635.66830	108.59183	1
17379	O	92.92800	54.78180	74.07790	-203.32699	-693.29440	294.05873	1
17380	N	92.85900	55.28180	76.31390	-423.77072	-721.99708	74.73643	1
17381	H	92.39700	55.80080	77.02990	-2182.92949	-317.00795	2231.41823	1
17382	C	94.18600	54.76780	76.54990	-519.65626	741.53402	-163.87150	1
17383	H	94.42000	54.19980	75.66190	2042.92389	2186.73409	-990.76277	1
17384	C	95.24000	55.87480	76.84190	-406.83065	773.69858	-293.62934	1
17385	H	96.23400	55.39980	76.97990	1640.53249	998.87294	-2507.31248	1
17386	H	94.96800	56.43880	77.75990	1804.08947	-533.91802	-2533.35478	1
17387	C	95.32500	56.83880	75.67490	654.95474	604.67323	-210.00064	1
17388	C	94.57400	58.04680	75.56990	731.71339	-400.11289	340.42540	1
17389	H	93.81100	58.35680	76.26890	1621.81396	-2627.07086	559.19251	1
17390	C	94.76300	58.89280	74.47790	-425.21057	-262.96070	-777.13733	1
17391	H	94.19800	59.78980	74.27190	-2214.85488	878.17117	2048.42730	1
17392	C	95.64700	58.60780	73.44990	412.56078	587.45763	550.72522	1
17393	O	95.87200	59.44180	72.41690	-560.11085	-357.88667	413.39932	1
17394	H	96.32200	59.00280	71.69190	1955.31868	-1688.47311	1768.93106	1
17395	C	96.26800	56.58880	74.66090	-711.29179	-522.03013	-245.19670	1
17396	H	96.92000	55.72780	74.64290	-1396.08723	234.46085	-2827.95862	1
17397	C	96.40200	57.42980	73.55890	239.36014	-857.17333	-178.26183	1
17398	H	97.07000	57.15380	72.75690	1810.66320	1092.18531	-2344.28853	1
17399	C	94.25100	53.70880	77.63690	514.36361	686.42840	-329.84905	1
17400	O	94.75800	52.60880	77.40090	-419.00787	-618.77781	-265.43881	1
17401	N	93.66100	53.96080	78.80590	254.13132	-668.26441	426.01780	1
17402	H	93.27600	54.86780	78.95390	-1236.76060	-2600.59858	1246.98660	1
17403	C	93.44100	53.00680	79.89090	-601.81432	604.19439	-349.06548	1
17404	H	94.35700	52.47780	80.10790	1825.75358	1578.63553	2002.46595	1
17405	C	92.94400	53.62880	81.25290	443.80576	-393.77199	-705.11153	1
17406	H	92.05600	54.20480	80.91490	1526.44231	1905.07992	1970.59790	1
17407	H	92.64800	52.84180	81.97990	1216.13596	899.36378	2742.98059	1
17408	C	93.94700	54.46080	82.04690	-395.24330	818.29969	91.04556	1
17409	H	94.47900	55.07880	81.29190	-1518.71544	-2747.20600	171.08257	1
17410	H	94.64500	53.84780	82.65590	2441.23361	-1925.35655	446.86464	1
17411	C	93.27700	55.39580	83.02990	-568.93645	45.01388	697.67726	1
17412	O	92.47900	54.97380	83.85390	277.08816	-652.90903	327.84141	1
17413	N	93.52300	56.72180	82.88790	-589.21039	-84.00996	585.73711	1

17414	H	94.41900	57.02380	82.56290	-2099.22431	47.95983	-2359.45524	1
17415	H	92.86000	57.35880	83.28190	1727.88598	366.51408	-2616.65426	1
17416	C	92.57700	51.86780	79.50590	307.03237	599.38574	600.81571	1
17417	O	92.78500	50.65780	79.79990	-588.61236	398.43318	-367.87454	1
17418	N	91.47300	52.18080	78.75590	358.64088	365.81277	655.88441	1
17419	H	91.20800	53.14080	78.70990	2026.38491	266.84928	2374.73414	1
17420	C	90.61600	51.17280	78.07990	622.80050	-485.14990	433.00641	1
17421	H	90.80800	50.23680	78.58390	-2146.65397	-1357.71144	-1872.82504	1
17422	C	89.08300	51.53180	78.20090	474.89020	-646.62861	410.05360	1
17423	H	88.90900	52.51580	77.71390	-2986.90579	-810.46801	559.95488	1
17424	H	88.49600	50.75480	77.66490	385.07431	2813.55053	1345.41743	1
17425	C	88.66600	51.54680	79.65090	-18.59448	730.56480	533.97343	1
17426	H	89.15400	52.39480	80.17690	1410.85715	2459.48343	-1381.03279	1
17427	H	89.07300	50.61780	80.10390	2468.82731	-1052.29292	-1652.96547	1
17428	C	87.13900	51.48180	79.68990	-434.68627	-793.38035	-118.26329	1
17429	H	86.76700	52.34880	79.10290	819.63088	-1656.38513	2529.15828	1
17430	H	86.88900	50.48680	79.26190	-2962.05142	807.77855	684.02838	1
17431	C	86.57500	51.74980	81.08890	624.52108	584.56640	-330.56326	1
17432	H	86.92000	52.73180	81.47690	-1472.39118	2540.31383	-1150.99503	1
17433	H	86.98500	50.92780	81.71390	426.78497	-2562.75313	-1786.33586	1
17434	N	85.12500	51.68880	81.07790	-327.65326	635.94393	-466.28001	1
17435	H	84.77400	50.75480	80.78390	2059.62684	2254.53092	-772.57995	1
17436	H	84.69900	52.02580	81.96490	-2255.66064	-2169.92629	-334.00927	1
17437	H	84.83800	52.34680	80.32490	2700.67518	849.04682	-1383.60262	1
17438	C	90.95300	50.94980	76.60790	-794.82222	419.33478	162.82826	1
17439	O	90.98900	51.89480	75.82090	-480.24644	-339.16292	-542.84198	1
17440	N	91.05100	49.72080	76.17790	-652.42125	402.56880	347.06871	1
17441	H	90.96200	48.97080	76.82890	1455.59256	2352.58446	-1519.18408	1
17442	C	91.29900	49.34780	74.85290	-199.67264	857.49545	240.30770	1
17443	H	91.82800	50.10280	74.28990	806.87489	-479.31523	-3017.74564	1
17444	C	92.38200	48.18380	74.82990	-235.56528	673.22905	-592.82728	1
17445	H	92.07000	47.34480	75.48790	1994.94448	898.40063	2242.64783	1
17446	H	92.30400	47.74580	73.81190	-1465.24917	-2624.07662	902.06909	1
17447	C	93.85500	48.62380	74.83190	-427.43123	622.41207	502.45541	1
17448	H	94.07900	49.05780	73.83490	-1536.79240	-1549.85098	-2281.87548	1
17449	H	94.46100	47.69280	74.87390	-1015.85140	-903.76807	-2854.69531	1
17450	C	94.33100	49.57380	75.99790	-126.33383	754.23628	487.29172	1
17451	H	93.81300	50.55380	75.93290	2513.79348	1869.68758	277.35752	1
17452	H	94.18600	49.06480	76.97490	-1089.28768	2944.09369	-293.96816	1
17453	C	95.82100	49.84980	75.84490	659.12768	340.02034	512.35935	1
17454	H	96.00100	50.55280	75.00390	1606.27959	-835.05304	2551.70036	1
17455	H	96.33200	48.90480	75.56290	-1868.93442	2260.54528	1135.13105	1
17456	N	96.36400	50.35680	77.12790	81.20232	-835.21473	-23.09563	1
17457	H	95.93900	49.92380	77.97290	364.39057	-1843.26879	-2537.64610	1
17458	H	96.24700	51.38080	77.26290	-215.43952	-2413.36853	-2018.75078	1
17459	H	97.39300	50.20580	77.11590	2218.23074	1042.91871	1953.89131	1
17460	C	90.00100	49.00580	74.10290	-649.43109	-428.40477	458.87613	1
17461	O	90.08300	48.49180	72.98190	-112.65898	635.89307	446.27918	1
17462	N	88.81000	49.29580	74.67490	642.13307	-286.88294	443.47643	1
17463	H	88.70200	49.78880	75.53390	-1339.66650	-686.17315	2747.20915	1
17464	C	87.55400	48.97680	74.08890	807.40947	337.23074	236.54092	1
17465	H	87.68600	49.00780	73.01690	1257.58492	-2804.72326	625.85089	1
17466	C	87.15200	47.53380	74.50490	192.69265	-367.55207	-825.43390	1
17467	H	87.00100	47.55280	75.60590	624.95393	-2726.71050	1414.33315	1
17468	H	88.03400	46.90580	74.25790	-297.94061	1842.96608	2519.41907	1
17469	C	85.88800	46.98380	73.78190	-517.72163	-671.48744	-346.92766	1
17470	H	85.04600	47.70380	73.87690	2156.37604	2132.35386	825.17355	1
17471	C	86.19700	46.73680	72.27590	509.88814	-385.04054	628.24096	1
17472	H	86.97300	45.94380	72.21590	754.15993	1558.26217	-2646.15083	1
17473	H	86.79000	47.58380	71.86990	-2373.73063	8.06651	2052.89856	1
17474	H	85.32100	46.35980	71.70490	1416.40800	2205.52311	-1760.23517	1
17475	C	85.44900	45.69380	74.43390	-575.59521	-683.72804	156.05618	1

17476	H	86.17400	44.86080	74.31090	-2599.21855	1299.81467	1198.89010	1
17477	H	84.50200	45.40480	73.93090	-2901.17415	-258.25554	-1211.83336	1
17478	H	85.30700	45.81980	75.52790	-2860.55318	-599.22074	1152.23141	1
17479	C	86.58300	49.95080	74.48290	467.10690	40.38841	765.05519	1
17480	O	86.54200	50.31480	75.64190	-591.60520	473.35718	-253.86202	1
17481	N	85.76300	50.38280	73.53390	70.85480	-808.54208	198.73130	1
17482	H	85.97600	50.05580	72.61690	1801.88911	1550.27901	2046.56587	1
17483	C	84.62100	51.21080	73.67290	-169.02506	-438.56183	-793.81836	1
17484	H	84.52300	51.36680	74.73690	-1670.48822	2606.29968	-604.10162	1
17485	C	84.88700	52.61880	73.07790	867.09297	228.53306	-163.98279	1
17486	H	83.94100	53.16780	72.88390	1366.84042	587.76508	2757.73719	1
17487	H	85.25400	52.43280	72.04590	-1943.23716	-81.37147	-2490.07071	1
17488	C	85.88700	53.42880	73.88690	641.21360	-636.33986	52.33474	1
17489	H	86.80800	52.87480	74.16590	-296.71855	2776.83533	-1472.81840	1
17490	H	85.38700	53.70380	74.83990	-224.50653	2919.51661	-1175.67359	1
17491	C	86.28500	54.67180	73.14490	-50.67725	-647.09072	-649.04509	1
17492	H	85.41500	55.31380	72.88890	967.76638	2325.71282	-1901.62633	1
17493	H	86.96800	55.30180	73.75390	1562.55506	2005.23223	1841.94832	1
17494	N	87.02500	54.16280	71.89790	-613.51596	357.87667	452.82345	1
17495	H	86.52100	54.27380	71.04090	2251.03426	2194.33652	-154.74492	1
17496	C	88.26400	53.66480	71.80990	-574.32393	369.15566	-626.42116	1
17497	N	89.10000	53.50980	72.82190	573.46650	615.66775	-96.05201	1
17498	H	88.79100	53.70980	73.75190	-331.83540	2641.13313	1671.42228	1
17499	H	90.04200	53.23980	72.62390	2820.03680	636.37764	1219.55910	1
17500	N	88.74400	53.35480	70.59690	239.09338	-458.47432	646.66656	1
17501	H	88.15000	53.32880	69.79290	588.76453	-1071.18775	-2909.93942	1
17502	H	89.71700	53.20780	70.42090	1550.59835	2704.32568	432.95304	1
17503	C	83.32200	50.61480	73.20590	-631.25281	-474.40471	-470.44823	1
17504	O	83.24600	50.07780	72.10590	154.16955	81.40065	755.61937	1
17505	N	82.30300	50.67980	74.02090	285.13236	-353.75363	-721.81545	1
17506	H	82.47000	51.01780	74.94390	-1320.51972	2084.15193	1944.69055	1
17507	C	80.90500	50.41080	73.69990	210.07684	865.93215	193.90642	1
17508	H	80.90700	49.61780	72.96590	2618.24816	1230.87924	1218.80562	1
17509	C	80.09800	49.91280	74.88890	887.87873	102.98276	152.46396	1
17510	H	80.65700	49.07480	75.35590	-613.28966	2741.78292	-1437.77795	1
17511	H	79.13500	49.50380	74.51390	-1337.39175	-2451.62466	-1459.22698	1
17512	O	79.93000	50.94380	75.84990	401.92725	680.62285	12.17402	1
17513	H	80.78600	51.10580	76.25190	2042.19612	-1931.06415	1391.89319	1
17514	C	80.20200	51.63780	73.09290	-294.67002	464.99592	718.26769	1
17515	O	80.82500	52.67380	72.89290	2.14290	-665.84704	404.90586	1
17516	N	78.90600	51.49280	72.63190	800.15382	-240.89606	64.27737	1
17517	H	78.46200	50.61780	72.45690	1962.54868	2036.12175	1366.55138	1
17518	C	78.10900	52.61380	72.12490	-43.08762	-518.84935	-757.77133	1
17519	H	78.62900	53.02480	71.27190	566.72532	3042.40369	574.85855	1
17520	C	76.74700	52.13880	71.62190	-6.00748	690.83885	588.36671	1
17521	H	76.16900	52.99880	71.21990	956.16082	-1450.21470	2607.71660	1
17522	H	76.18700	51.79780	72.51890	-1766.91820	-2487.23243	-776.41636	1
17523	C	76.84800	51.01580	70.56590	-680.31760	336.20169	502.41519	1
17524	H	75.93000	51.16180	69.95690	960.34794	1597.10047	2524.16015	1
17525	H	77.66100	51.23680	69.84290	2352.98473	469.80657	2018.28403	1
17526	S	76.94200	49.31380	71.19890	337.19909	412.75368	154.65424	1
17527	C	75.79700	48.59480	69.95690	822.81620	249.88131	282.45155	1
17528	H	75.35400	47.67380	70.39290	2060.74359	-2366.09647	-132.47549	1
17529	H	76.40800	48.33680	69.06590	-364.61826	-2319.87485	2075.47209	1
17530	H	75.08300	49.32480	69.51890	1732.48659	1351.75257	-2263.39407	1
17531	C	77.92300	53.80080	73.01490	-220.98370	641.16344	603.70978	1
17532	O	78.11000	54.94380	72.61990	507.20748	-571.98677	-184.01056	1
17533	N	77.71000	53.58280	74.34390	112.45206	-796.61967	231.54239	1
17534	H	77.59800	52.67680	74.74290	-1360.67478	-1229.55302	2544.89250	1
17535	C	77.68700	54.67680	75.33990	-682.04171	-106.36014	-610.49811	1
17536	H	76.94800	55.38980	75.00390	-1210.53135	2908.43475	23.36828	1
17537	C	77.20500	54.32980	76.79390	469.29062	13.13921	-790.83834	1

17538	H	77.72800	53.41580	77.14590	2370.63613	-1296.24041	-1617.01128	1
17539	O	75.76300	54.21780	76.78490	246.74145	-472.35287	-590.27785	1
17540	H	75.63300	53.42280	76.26290	3026.59544	-800.63023	-281.48693	1
17541	C	77.39900	55.42680	77.81890	-568.97019	427.32721	564.12234	1
17542	H	76.81700	55.15480	78.72490	2377.70020	2040.06093	265.30622	1
17543	H	78.42900	55.46880	78.23490	220.82873	3109.80303	-446.85938	1
17544	H	77.11100	56.36280	77.29590	-11.43411	-3026.81523	840.02012	1
17545	C	78.99300	55.41280	75.48290	697.95757	-573.76628	-89.93018	1
17546	O	79.01200	56.64380	75.52890	-63.11175	-772.43755	-146.97250	1
17547	N	80.04200	54.60680	75.54790	-402.26277	514.11675	-552.84201	1
17548	H	79.91100	53.62580	75.42390	-2352.64599	2069.82402	318.70266	1
17549	C	81.45000	55.05880	75.60490	203.28338	640.59352	-630.52741	1
17550	H	81.54600	55.60980	76.52890	628.71135	-639.37924	-3026.00901	1
17551	C	82.49400	53.85080	75.62690	595.14304	400.57143	-574.32955	1
17552	H	83.54200	54.17680	75.80090	-2235.84851	-1657.68567	-1480.77062	1
17553	H	82.40300	53.30880	74.66190	673.19822	2405.60484	-1929.09052	1
17554	C	82.13700	52.85880	76.75290	-373.08063	40.92871	-845.48761	1
17555	O	82.51800	51.66580	76.56390	-354.38605	24.61665	693.37048	1
17556	O	81.53100	53.20380	77.76190	284.12498	77.25823	719.25973	1
17557	C	81.81100	55.96680	74.36290	201.59443	704.83893	-557.48842	1
17558	O	82.31600	57.09180	74.51690	407.19084	420.97399	518.20284	1
17559	N	81.46000	55.58180	73.12090	226.26998	-737.12114	-342.84076	1
17560	H	80.97900	54.71980	72.97790	2573.21982	1051.39428	1457.15659	1
17561	C	81.68400	56.29980	71.95890	384.57750	-164.97618	-818.36243	1
17562	H	82.73300	56.54780	72.03390	-1974.24170	1754.81688	-1731.48162	1
17563	C	81.30300	55.39580	70.72990	-586.61785	328.70786	-635.13016	1
17564	H	81.29600	56.08680	69.85890	-2347.84998	-2027.08644	516.75439	1
17565	H	80.24900	55.09180	70.90490	-2706.22542	1288.96343	964.54968	1
17566	C	82.34400	54.32980	70.40590	40.27656	-674.19040	593.67127	1
17567	H	82.91800	54.03380	71.31090	-1069.05665	1990.54140	2183.64709	1
17568	H	83.11200	54.74680	69.71990	-617.05995	-2633.90841	1586.03922	1
17569	C	81.85800	53.05580	69.67590	655.61508	-561.97280	256.89264	1
17570	H	81.45300	53.35580	68.68590	-2522.32768	-602.87286	1774.03817	1
17571	H	81.02700	52.73880	70.34090	-291.10079	-1814.87670	-2562.77661	1
17572	C	82.96900	51.98280	69.53090	-519.84914	-510.12782	534.16558	1
17573	H	83.51800	51.86480	70.48990	1852.32208	1399.27427	2109.45388	1
17574	H	83.71600	52.20480	68.73890	1296.71898	-1527.63214	2405.11738	1
17575	N	82.51400	50.65680	69.16890	530.42691	534.02625	370.02555	1
17576	H	82.10400	50.74380	68.21690	-174.42471	2207.89161	-2254.88183	1
17577	H	83.32800	50.00980	69.15490	-697.52425	2022.61341	2299.10532	1
17578	H	81.81100	50.26080	69.82490	-1895.70458	-2330.05748	916.87689	1
17579	C	80.96500	57.63780	71.82890	826.33937	-331.71141	153.65811	1
17580	O	81.52700	58.63680	71.43890	523.16986	50.70035	-595.67242	1
17581	N	79.66900	57.69580	72.21290	62.45139	409.56300	-748.05525	1
17582	H	79.23700	56.80280	72.31390	1047.96918	-1318.90113	2642.40019	1
17583	C	78.91900	58.95380	72.34290	668.93466	8.64760	604.37743	1
17584	H	79.04000	59.54580	71.44790	-1801.46544	2274.28975	1223.80510	1
17585	C	77.45800	58.71880	72.77690	812.28507	-345.45887	-213.28381	1
17586	H	76.82600	59.62580	72.87990	-1464.45585	-658.36634	2698.36901	1
17587	H	77.44500	58.21880	73.76890	-2755.11863	1063.15487	1090.38235	1
17588	C	76.64300	57.82380	71.87090	565.68760	-81.69041	696.34826	1
17589	C	76.58300	58.10480	70.48090	191.17442	-840.35040	-289.80430	1
17590	H	77.12200	58.96280	70.10690	-2027.91211	1447.77085	-1939.83156	1
17591	C	75.81100	57.35880	69.59390	-626.25240	-139.62751	642.60311	1
17592	H	75.76500	57.60680	68.54390	-1780.74170	-1779.93218	-1896.43867	1
17593	C	75.22600	56.17080	70.00690	502.67737	-711.06597	237.11467	1
17594	O	74.53900	55.28780	69.16190	631.47124	29.23568	456.27273	1
17595	H	74.41500	54.44180	69.59890	-1234.33470	-2724.01531	-980.30574	1
17596	C	75.90500	56.70580	72.30390	-442.83426	-215.54464	759.17842	1
17597	H	75.83900	56.41280	73.34090	-1393.61831	2307.76743	1620.77316	1
17598	C	75.30900	55.81680	71.36490	-143.38104	491.05271	-768.48538	1
17599	H	74.94300	54.87280	71.74090	1870.61073	1909.21757	-1669.14605	1

17600	C	79.49600	59.91880	73.36590	310.03549	-622.19152	573.62197	1
17601	O	79.75100	61.08780	73.13790	161.29134	38.24882	-780.40413	1
17602	N	79.82100	59.45580	74.55290	-645.59120	-337.18352	-440.57348	1
17603	H	79.68400	58.49580	74.78390	2765.67771	-1450.35858	-344.06181	1
17604	C	80.44200	60.30880	75.56290	-734.28892	362.26782	-421.75171	1
17605	H	79.90500	61.24580	75.55490	-2792.31292	-897.72575	-1155.65992	1
17606	C	80.24100	59.73180	76.98690	329.07937	554.50571	-654.93185	1
17607	H	80.77400	60.48080	77.61190	2462.34126	127.12950	1939.85042	1
17608	H	80.74600	58.75980	77.17490	-1131.41524	2485.96200	-1578.84657	1
17609	C	78.72500	59.53680	77.40490	-659.15040	472.49354	-434.86651	1
17610	H	78.16700	60.42180	77.03090	2658.64920	1563.65188	-618.41456	1
17611	H	78.24300	58.62080	77.00190	-2103.48584	-1944.98981	1292.83512	1
17612	C	78.50600	59.36680	78.91590	28.64145	200.53876	879.83748	1
17613	H	78.94700	58.43680	79.33590	-77.54784	2294.75625	2142.82964	1
17614	H	77.42800	59.16480	79.09190	-1973.69052	-1071.09530	2196.37425	1
17615	N	79.05000	60.55680	79.71390	-232.92205	497.60710	634.13661	1
17616	H	79.41200	61.35180	79.22890	829.62815	-2922.84523	-815.56267	1
17617	C	79.10800	60.62180	81.05290	121.67880	-646.72468	-638.70515	1
17618	N	78.65600	59.79180	81.93890	-680.33710	-278.22122	409.58322	1
17619	H	78.00100	59.08680	81.66790	-1758.51946	-2223.70049	1356.87274	1
17620	H	78.68000	60.11080	82.88590	-1985.72939	-1569.31999	-1880.29613	1
17621	N	79.61200	61.72080	81.54490	-337.58761	-584.30655	-517.00108	1
17622	H	79.92100	62.44280	80.92490	-1565.41979	1492.86060	2278.79114	1
17623	H	79.73600	61.78780	82.53490	-1798.38855	1793.76216	-1868.53441	1
17624	C	81.91100	60.65180	75.26890	612.34580	443.77764	-517.12508	1
17625	O	82.34700	61.74380	75.64890	404.44469	677.51636	-55.80654	1
17626	N	82.63500	59.80580	74.56990	-194.80445	74.07543	-829.93939	1
17627	H	82.35300	58.85480	74.46790	-2534.09818	1466.87656	1155.08720	1
17628	C	83.96700	60.27580	74.06590	575.73276	-678.33284	157.97618	1
17629	H	84.51900	60.58080	74.94290	-2020.08267	-266.09556	2389.94338	1
17630	C	84.76500	59.15580	73.29790	802.63368	-158.23136	-402.30804	1
17631	H	84.27400	58.99080	72.31490	-1309.67093	1430.43942	-2494.03726	1
17632	H	84.62400	58.26080	73.94190	-1614.59018	2706.35416	64.72486	1
17633	C	86.25700	59.33680	73.14890	-741.70812	202.46992	487.94101	1
17634	H	86.42000	60.38280	72.81090	2277.59375	-2075.12710	-611.22370	1
17635	C	86.99400	59.10380	74.43890	-137.29936	763.25162	-500.00913	1
17636	H	88.03400	59.42780	74.21690	2311.67705	2064.42048	527.50779	1
17637	H	86.66200	59.73080	75.29390	1760.34186	-1717.90148	1942.49574	1
17638	H	86.94000	58.03480	74.73590	1613.83236	1951.69980	1855.41381	1
17639	C	86.78800	58.36680	72.08090	-38.09675	295.79315	851.64547	1
17640	H	86.63600	57.36080	72.52590	-1367.98749	2400.07169	-1530.64046	1
17641	H	87.88400	58.53880	72.02790	-267.64055	2655.86362	1662.64344	1
17642	H	86.34700	58.51580	71.07190	-2547.99560	1748.39836	617.68570	1
17643	C	83.83400	61.42680	73.15390	-354.64480	-407.89906	-744.37542	1
17644	O	84.63000	62.37580	73.26490	648.14062	411.87515	-185.96437	1
17645	N	82.85300	61.48880	72.22890	-702.02783	-438.82468	-184.48865	1
17646	H	82.23800	60.70680	72.16490	2551.70259	1722.72296	-649.34929	1
17647	C	82.51100	62.67080	71.40490	-180.44389	898.20725	-67.92951	1
17648	H	83.43700	63.02080	70.97290	2736.15189	942.16660	1216.01058	1
17649	C	81.45100	62.39580	70.30990	648.58985	637.19681	52.60743	1
17650	H	80.52300	61.97280	70.74890	-1130.53842	1220.42489	2666.10188	1
17651	H	81.11100	63.34480	69.84290	-1243.55693	-1028.19869	2692.91121	1
17652	N	83.07400	62.04880	68.49190	-72.09256	-817.92844	160.36765	1
17653	C	81.94000	61.60380	69.18490	547.48863	-716.85763	39.39778	1
17654	C	83.07900	61.30880	67.38090	-162.73829	807.53689	-417.27807	1
17655	H	83.93400	61.31080	66.70590	2700.42262	1608.11270	65.40617	1
17656	N	82.06700	60.43080	67.32990	21.15065	698.20229	-493.46019	1
17657	H	81.96900	59.68080	66.67590	2116.59453	2326.94943	-96.22663	1
17658	C	81.28500	60.67180	68.46190	745.64159	350.07244	-394.10703	1
17659	H	80.30900	60.21780	68.57990	2033.02284	196.50651	2378.51407	1
17660	C	81.99700	63.82580	72.29390	-165.90970	-887.54285	-106.51993	1
17661	O	82.45800	64.95180	72.13090	-748.05413	56.91983	-273.20362	1

17662	N	81.10700	63.58780	73.24290	-512.30371	-351.85098	564.88451	1
17663	H	80.64000	62.70880	73.29990	2256.16195	587.08714	-2116.98066	1
17664	C	80.62600	64.63480	74.15290	535.62813	423.97319	593.90494	1
17665	H	80.25900	65.41980	73.50690	1099.07169	2679.89010	-1239.77150	1
17666	C	79.51400	64.01580	75.02690	482.42299	682.57672	356.16106	1
17667	H	78.93200	63.32680	74.37890	1776.31344	-1447.63628	2141.04153	1
17668	H	80.05900	63.34980	75.72990	2042.83635	2141.45031	-1073.18334	1
17669	C	78.65200	64.92580	75.86790	146.11829	896.21227	-111.29981	1
17670	H	79.32500	65.43280	76.59190	1572.66026	-162.20736	-2724.55262	1
17671	C	77.84300	65.91680	75.11090	397.68066	398.06485	-723.21153	1
17672	H	78.40300	66.58380	74.41990	-2086.64999	-2126.87440	-1020.86725	1
17673	H	77.04300	65.37980	74.55790	1421.83921	-2277.51256	1623.99252	1
17674	H	77.34800	66.57180	75.85890	469.35220	679.65577	-3042.08427	1
17675	C	77.73700	63.96780	76.62590	173.72059	-633.55352	-636.05472	1
17676	H	78.25600	63.31880	77.36390	-2273.11237	-1444.05636	1622.53117	1
17677	H	77.23500	63.24180	75.95090	-2034.98824	-468.30590	-2364.38132	1
17678	H	77.01400	64.60180	77.18190	1032.40119	2970.78737	-112.01456	1
17679	C	81.76100	65.29180	74.99290	338.51371	303.40417	781.50850	1
17680	O	81.80900	66.50180	75.10190	441.91437	532.16493	372.24414	1
17681	N	82.73700	64.49880	75.49490	-438.71074	390.93270	-620.66337	1
17682	H	82.74800	63.51180	75.35190	2662.66134	-1430.57157	-860.87617	1
17683	C	84.02000	64.94880	76.06590	570.07449	-676.82637	185.98102	1
17684	H	83.77900	65.63080	76.86790	-1568.41220	1468.68089	2294.83952	1
17685	C	84.77200	63.73480	76.76590	591.31833	-679.25247	-111.61653	1
17686	H	85.81700	64.05580	76.96690	-1294.43509	2329.36057	1670.94555	1
17687	H	84.71000	62.84780	76.09990	2122.06918	2037.89727	-1122.36510	1
17688	O	84.15300	63.55380	78.01490	481.99624	-40.08419	-630.29644	1
17689	H	84.37800	64.25280	78.63390	-1791.30470	2066.63923	1554.08905	1
17690	C	84.93100	65.67980	75.13190	-668.65983	-284.45105	546.13060	1
17691	O	85.56500	66.64980	75.53790	-593.22646	-509.33452	-128.31155	1
17692	N	85.05100	65.29680	73.86190	-264.97826	746.65147	298.61939	1
17693	H	84.70800	64.42780	73.51290	-2112.12096	-134.96352	2323.26722	1
17694	C	85.69500	66.04380	72.82190	567.18923	371.70183	-616.07252	1
17695	H	86.70800	66.33380	73.05990	2758.97835	-1496.28405	-16.80281	1
17696	C	85.74100	65.15480	71.54090	-139.12277	-863.66209	-250.56710	1
17697	H	84.87900	64.46080	71.44990	142.62428	2094.40964	-2357.14046	1
17698	C	85.79600	65.94080	70.19390	448.09140	-357.51663	692.87889	1
17699	H	84.86900	66.50480	69.95490	2545.26475	-1360.53258	1223.72822	1
17700	H	85.96200	65.21880	69.36590	-1483.02878	-28.50688	-2787.29310	1
17701	H	86.63500	66.66980	70.17690	-1298.62715	2551.36513	1314.32383	1
17702	C	87.01400	64.26180	71.59490	-398.47848	628.50707	528.07633	1
17703	H	86.82200	63.39980	72.26990	-897.36194	-2480.49486	1699.58092	1
17704	H	87.92700	64.84480	71.84190	309.69020	-2967.42149	969.38262	1
17705	H	87.23900	63.84180	70.59090	-3029.74422	-812.69627	282.55922	1
17706	C	84.98600	67.39680	72.55390	-388.20567	-802.29636	-191.53180	1
17707	O	85.69000	68.41580	72.40690	204.00267	-510.67779	551.72119	1
17708	N	83.64700	67.48780	72.47490	209.88712	-309.53405	-760.88718	1
17709	H	83.09500	66.66380	72.57690	1587.35745	333.16398	2684.92746	1
17710	C	82.92000	68.76280	72.32790	-522.12723	261.97688	-713.72885	1
17711	H	83.22900	69.31680	71.45390	2017.85139	1696.18342	-1721.77106	1
17712	C	81.43200	68.40580	72.15790	642.18654	-297.34433	558.50114	1
17713	H	80.91900	69.33580	71.83390	-1732.04280	1320.60283	-2284.41409	1
17714	H	80.92200	68.18880	73.12090	-1763.10117	-1739.80244	1934.58287	1
17715	H	81.28100	67.60480	71.40290	-744.24462	1524.10081	2647.34867	1
17716	C	83.14400	69.72080	73.44490	-401.56651	816.77359	116.76247	1
17717	O	83.43900	70.90080	73.25090	533.44374	563.95410	-145.61397	1
17718	N	83.00700	69.24380	74.69190	-39.97664	577.49679	-625.50195	1
17719	H	82.62000	68.33680	74.84090	2961.24189	977.11794	378.73485	1
17720	C	83.27700	70.00580	75.90190	868.18360	27.95767	253.05356	1
17721	H	82.61000	70.85480	75.90990	-2618.14610	-281.83495	1723.37295	1
17722	C	83.12800	69.09680	77.13590	-194.20103	-628.26331	623.09979	1
17723	H	83.48300	69.52780	78.09690	-434.75185	1739.98287	2580.57913	1

17724	H	83.61800	68.12180	76.92790	547.37166	-3045.50053	-553.82756	1
17725	C	81.58900	68.79880	77.42290	501.38341	748.89580	-142.27043	1
17726	O	80.75700	69.59680	76.91990	629.39047	471.66334	27.60771	1
17727	O	81.33500	67.81580	78.15690	-685.65551	-126.81589	-385.37380	1
17728	C	84.71100	70.58080	75.95190	712.37272	56.03895	552.77983	1
17729	O	84.86800	71.75680	76.30490	-398.58340	-423.74005	528.83059	1
17730	N	85.74100	69.79480	75.67590	-420.60342	269.36334	-693.03326	1
17731	H	85.60700	68.83480	75.43990	2131.55193	-2196.38932	691.72991	1
17732	C	87.13300	70.09780	75.63590	-194.25664	-885.16984	-78.06735	1
17733	H	87.32400	70.52680	76.60790	1086.47113	-2112.86238	2048.01621	1
17734	C	87.91400	68.77880	75.41390	484.11481	-588.49556	481.71557	1
17735	H	87.59900	68.21680	74.50790	694.43447	2655.17981	1535.04643	1
17736	H	87.63200	68.11480	76.25890	-2487.21738	1386.93921	1342.35916	1
17737	C	89.44000	68.82480	75.48290	687.32333	574.92272	-170.45234	1
17738	H	89.72900	69.58180	74.72290	292.40196	-1741.75538	2591.10961	1
17739	C	89.94100	69.29480	76.88690	176.79026	685.55266	569.03778	1
17740	H	89.75800	68.53080	77.67190	2538.41880	1853.64798	-97.31015	1
17741	H	91.05200	69.32680	76.88190	1541.41723	714.58211	2636.97240	1
17742	H	89.44900	70.26980	77.09490	2908.37514	811.39892	861.79164	1
17743	C	89.95100	67.43480	75.03090	-440.37549	-435.26089	660.29917	1
17744	H	89.65900	67.25180	73.97490	-2235.33346	-1200.65278	1854.09040	1
17745	H	91.05800	67.51580	75.08490	-2352.04345	2042.37497	-499.88046	1
17746	H	89.58900	66.62280	75.69590	2312.84618	2119.59863	216.90221	1
17747	C	87.46200	71.14180	74.60090	237.27872	-510.70131	704.40633	1
17748	O	88.19800	72.07180	74.83790	236.08794	-369.12582	644.87549	1
17749	N	86.84400	71.04980	73.39090	-212.52087	-785.72387	204.69509	1
17750	H	86.17000	70.32580	73.26190	-2335.64399	-1640.93104	1320.51084	1
17751	C	87.01800	71.85880	72.20590	-804.01431	-379.60713	-225.11485	1
17752	H	88.03400	71.65880	71.90090	-1375.31846	-1174.71095	-2582.66918	1
17753	C	86.05600	71.26180	71.07990	-551.52472	-635.70301	344.33956	1
17754	H	85.03600	71.30180	71.51890	1892.07259	-2212.96784	1164.10830	1
17755	H	86.42000	70.23180	70.88090	-1163.07643	-2073.46781	2051.08699	1
17756	C	86.06000	71.96180	69.68690	-564.94187	622.88925	-381.50936	1
17757	H	85.52600	72.93580	69.71790	1889.54724	-325.31404	2481.59483	1
17758	C	87.48200	72.28980	69.17990	214.81475	-623.62407	-627.25981	1
17759	H	88.21400	71.45680	69.22790	750.41205	3051.66438	220.99950	1
17760	H	87.92000	73.10780	69.79090	-681.47380	2380.22746	-1958.58845	1
17761	H	87.44600	72.71180	68.15290	1930.44647	1434.77548	2018.60962	1
17762	C	85.20100	71.16880	68.59090	65.77431	-584.21557	683.83865	1
17763	H	85.60800	70.14180	68.47390	351.36567	-2854.66222	1250.49403	1
17764	H	84.15200	71.20580	68.95590	-2365.75256	2035.65280	-474.34324	1
17765	H	85.20300	71.73380	67.63390	1735.96716	-20.55441	-2625.03691	1
17766	C	86.64900	73.30080	72.42790	165.30275	-752.36931	470.79021	1
17767	O	87.45100	74.21280	72.17190	115.49290	-364.28724	-693.18047	1
17768	N	85.50800	73.52580	73.11090	155.62338	-283.42482	-782.65226	1
17769	H	84.97100	72.71180	73.31890	2615.16069	-1508.59074	-863.22509	1
17770	C	85.11500	74.80280	73.59690	620.33716	-472.37695	453.51387	1
17771	H	85.32400	75.60080	72.90090	1523.65794	1538.97562	-2285.95655	1
17772	C	83.55300	74.85180	73.84290	669.18378	209.29702	571.77076	1
17773	H	83.38800	74.05380	74.59790	-1791.68459	-1113.73741	2331.73852	1
17774	H	83.04800	74.70080	72.86490	-1456.48194	-2333.06436	1522.17870	1
17775	C	83.06600	76.20680	74.31390	-323.30774	794.82781	321.32763	1
17776	C	83.49400	77.39480	73.61290	-690.60474	359.11199	484.34991	1
17777	H	84.09300	77.25680	72.72490	-734.44688	2297.76149	-2032.06310	1
17778	C	83.02700	78.64780	74.04590	586.02348	-649.52679	-231.87825	1
17779	H	83.34500	79.53480	73.51790	2483.77400	412.76260	1874.51630	1
17780	C	82.11700	78.73280	75.12690	-73.83237	798.97442	-444.16364	1
17781	H	81.80600	79.73380	75.39090	-2030.52580	287.53404	2389.53778	1
17782	C	82.25700	76.31380	75.36790	509.74574	695.25257	-298.40294	1
17783	H	81.88900	75.42480	75.85690	-289.64877	3132.02664	-176.40238	1
17784	C	81.80600	77.52180	75.83390	154.49631	-644.86573	-624.20506	1
17785	H	81.02300	77.59480	76.57490	1610.36273	1953.48617	1862.27773	1

17786	C	85.85600	75.28680	74.89890	551.94871	-315.04845	640.82202	1
17787	O	86.21200	76.46780	74.94090	-623.64636	-325.34870	361.28744	1
17788	N	86.17100	74.39980	75.83690	359.74186	185.71876	732.92331	1
17789	H	86.02200	73.41680	75.76590	-969.78659	626.62849	2923.25589	1
17790	C	86.82000	74.75980	77.14490	87.08210	-704.36475	561.27531	1
17791	H	86.15300	75.48880	77.57990	-2696.71457	374.29449	1581.84553	1
17792	C	86.94000	73.58780	78.11590	405.49713	704.80430	-419.12917	1
17793	H	87.14500	72.68280	77.50590	2422.94955	1809.77411	852.52307	1
17794	C	88.11000	73.73880	79.17790	427.75013	-781.61778	-175.53223	1
17795	H	89.11200	73.50380	78.75790	-2807.49405	12.10367	-1437.13632	1
17796	H	87.89000	73.00680	79.98390	1684.44889	-2018.36985	1713.69353	1
17797	H	88.01200	74.79180	79.51590	-2370.35484	1459.51705	-1483.39932	1
17798	C	85.60400	73.41880	78.88190	484.05100	393.94197	656.55445	1
17799	H	85.67200	72.50580	79.51190	2300.45982	1922.04758	-954.59843	1
17800	H	85.36200	74.27280	79.54890	1145.11528	-2921.78123	-160.98052	1
17801	H	84.74200	73.40480	78.18090	843.48751	-2265.93803	2001.66877	1
17802	C	88.17300	75.40380	76.92690	263.90865	-695.14568	-525.71419	1
17803	O	88.54300	76.32780	77.61390	216.98731	-470.56935	-596.62610	1
17804	N	88.89700	74.85580	75.91890	-243.60281	-510.54149	-631.90316	1
17805	H	88.53000	74.08180	75.40890	-407.24081	2260.88654	2148.80142	1
17806	C	90.29200	75.32580	75.66290	-234.73417	-240.18219	841.54056	1
17807	H	90.89600	75.29980	76.55790	2240.11415	1864.98748	-1186.14884	1
17808	C	90.95300	74.41080	74.56690	334.87763	769.82144	353.55324	1
17809	H	90.23300	74.14880	73.76190	2547.48593	1657.75648	795.47200	1
17810	C	92.24400	75.00980	73.95790	-644.56647	645.23234	116.28143	1
17811	H	92.97600	75.11480	74.78690	-1458.67259	1644.21811	2251.60185	1
17812	H	92.67300	74.27880	73.23890	1795.76073	-2162.47044	1387.94855	1
17813	H	91.99400	75.90680	73.35290	2247.73265	-2186.36975	-104.57226	1
17814	C	91.30800	73.01580	75.20290	574.41658	-208.18284	-677.87929	1
17815	H	90.39500	72.66380	75.72790	-1259.46669	2447.10828	1528.82474	1
17816	H	92.16300	73.06880	75.90890	-2572.27047	-1165.44627	-1401.80332	1
17817	C	91.58000	71.93880	74.11790	-551.05875	728.78144	97.74645	1
17818	H	92.58900	72.13780	73.69690	-1855.94692	1932.00343	1654.80183	1
17819	H	90.83500	71.82580	73.30090	3074.99244	563.03598	295.39384	1
17820	H	91.68900	70.94580	74.60390	1166.42133	2855.07588	-642.34699	1
17821	C	90.27000	76.76580	75.16090	37.40249	534.74287	-746.74704	1
17822	O	91.26100	77.50980	75.35290	-675.93397	-413.21845	-36.48690	1
17823	N	89.15800	77.21180	74.50990	-192.59274	-540.33783	-622.78191	1
17824	H	88.43600	76.60280	74.19090	1194.13194	1548.22509	2458.92348	1
17825	C	89.12800	78.59280	74.10490	377.50393	508.01125	651.07281	1
17826	H	90.03400	78.84180	73.57190	1469.30424	-1257.81007	-2479.54999	1
17827	C	87.93400	78.86780	73.12990	-29.07440	-731.92606	531.65041	1
17828	H	88.03500	79.86580	72.65290	874.83027	-2362.58676	-1878.30949	1
17829	O	86.60800	78.75480	73.78290	494.52937	-520.88501	304.75807	1
17830	H	86.49900	77.90180	74.21090	3133.14724	32.62321	187.58542	1
17831	C	87.97000	77.75680	72.01390	-721.09669	-537.08802	-171.68586	1
17832	H	87.68400	76.74380	72.36890	1930.66671	2474.54389	-219.98785	1
17833	H	87.16200	78.06680	71.31790	1557.84851	-1308.35620	-2396.37134	1
17834	H	88.96600	77.83780	71.52890	194.80847	-1558.04845	2717.03243	1
17835	C	88.96700	79.58880	75.24390	-553.02543	-593.71890	-423.33659	1
17836	O	89.33600	80.75080	75.13190	-480.33427	-511.35593	-369.58633	1
17837	N	88.46200	79.15180	76.40990	-50.08885	-812.88617	-213.00321	1
17838	H	88.27300	78.17780	76.50590	-1758.54857	-1463.49354	-2167.10605	1
17839	C	88.07500	80.00680	77.54090	-28.71935	192.47567	887.54003	1
17840	H	87.30100	80.66680	77.17790	2295.51013	334.11988	-2122.61327	1
17841	C	87.30500	79.28680	78.65090	-600.75589	186.28553	-670.72541	1
17842	H	87.05400	79.85480	79.57290	-2004.71889	1719.40676	-1723.13828	1
17843	H	87.98500	78.45680	78.93890	42.46103	-2585.37115	1782.97069	1
17844	C	85.94700	78.73980	78.20890	-397.08447	316.88538	757.44892	1
17845	H	86.02600	78.13580	77.27990	-2809.43718	1416.73723	-210.73565	1
17846	C	85.44800	77.83980	79.37790	-901.55403	-8.23883	-173.48386	1
17847	H	86.11200	76.94880	79.37190	221.84360	-2791.68866	-1432.60241	1

17848	H	85.48900	78.35180	80.36290	-2616.16425	1752.27728	-142.86320	1
17849	H	84.39600	77.56880	79.14390	-3051.72716	-124.86140	772.55016	1
17850	C	84.96300	79.87180	77.92290	-902.58962	87.58801	141.05840	1
17851	H	85.05400	80.27480	76.89190	2452.58299	1965.27922	39.43196	1
17852	H	85.04300	80.76780	78.57490	-2004.02539	-1894.58962	-1521.98116	1
17853	H	83.95600	79.43980	78.10290	825.88212	-1453.43888	-2665.16199	1
17854	C	89.17800	80.94580	78.08890	-717.73370	495.08186	285.18454	1
17855	O	88.80600	82.04980	78.42590	643.80407	451.28983	9.90323	1
17856	N	90.47200	80.68380	78.13390	-575.46373	-15.62058	618.56191	1
17857	C	90.96500	79.30680	78.36890	-415.30352	-444.98896	-685.51246	1
17858	H	91.18800	78.92780	77.34790	-1625.89174	1659.09059	2124.28766	1
17859	H	90.26700	78.62680	78.90290	-1445.60582	-1853.86634	-2097.26055	1
17860	C	91.54100	81.64680	78.45690	-35.51050	-446.29956	-797.09137	1
17861	H	91.23900	81.98780	79.43590	1750.19217	-1805.57020	-1886.28395	1
17862	C	92.73700	80.82480	78.49790	-848.62530	148.03671	-322.99370	1
17863	H	93.63600	81.30280	78.94390	409.67599	-1805.76782	2534.63577	1
17864	H	93.12400	80.48380	77.51490	9.85446	-2364.30124	-2076.16703	1
17865	C	92.24000	79.53580	79.14890	-352.98667	-208.46490	810.58332	1
17866	H	92.99800	78.74380	78.96890	-2033.07651	2406.98548	-117.87916	1
17867	H	92.10900	79.69280	80.24090	1902.48921	922.23929	-2331.91371	1
17868	C	91.62700	82.88080	77.58990	241.68839	693.14751	-547.06959	1
17869	O	92.02600	83.95080	78.05690	142.54234	-167.16372	752.56465	1
17870	N	91.29900	82.78080	76.30590	-338.32292	600.73457	-501.42521	1
17871	H	91.10600	81.91780	75.84690	1438.75264	2796.77989	-111.68873	1
17872	C	91.14300	83.99380	75.47590	604.84887	-314.06511	-599.28591	1
17873	H	92.02900	84.60980	75.52090	334.23111	2840.27751	1316.20242	1
17874	C	90.89300	83.53080	73.98690	509.73219	-493.75844	-564.53696	1
17875	H	89.88900	83.05780	73.93690	2121.13629	1642.17408	1635.43948	1
17876	H	90.85600	84.47980	73.41090	-1264.53322	2233.67949	-1834.86309	1
17877	C	92.01000	82.69580	73.39690	-555.24922	498.95382	532.79230	1
17878	C	93.29400	83.19280	73.34590	778.46609	-194.97186	411.19007	1
17879	H	93.55400	84.19180	73.66590	2074.07972	1136.03738	-2074.33098	1
17880	C	94.39900	82.58680	72.68290	-626.48512	-283.79687	599.05816	1
17881	H	95.32400	83.13780	72.59590	647.85034	2028.50396	2314.26611	1
17882	C	94.10100	81.35380	72.07090	592.07914	415.31278	546.14982	1
17883	H	94.80900	80.81280	71.46190	2036.91765	-1251.39844	-2038.75525	1
17884	C	91.83500	81.41480	72.88390	-378.45493	-309.66484	-775.77502	1
17885	H	90.85900	80.95880	72.95990	2813.11635	1343.27426	-394.31620	1
17886	C	92.82900	80.73080	72.21990	270.21419	874.56722	-11.72674	1
17887	H	92.53500	79.82280	71.71490	658.77731	-2796.46782	1258.59595	1
17888	C	90.05300	84.85580	75.95490	645.34379	569.61098	-296.01316	1
17889	O	90.18971	86.11386	75.79968	87.20267	16.85860	44.00216	1
17890	N	88.89800	84.23980	76.38290	-75.79354	-682.36849	483.68959	1
17891	H	88.83200	83.24980	76.48090	1524.22391	545.33974	-2697.71222	1
17892	C	87.77100	84.95680	77.05290	-798.32742	72.99855	445.70217	1
17893	H	87.74051	85.88426	76.40874	-2740.25171	-864.68190	2771.23806	1
17894	C	86.55800	84.09580	77.20590	163.11260	499.92033	743.42924	1
17895	H	85.74200	84.75480	77.57290	-20.07454	1991.78310	2436.18207	1
17896	H	86.63600	83.28580	77.96190	-1446.34277	-2244.98917	1662.08304	1
17897	C	85.94200	83.48480	75.94290	-442.36402	-529.88417	-600.01367	1
17898	C	86.43200	82.68380	74.93490	-345.72223	783.60156	328.51514	1
17899	H	87.49000	82.51880	74.79890	2677.19712	-1072.20530	1234.45955	1
17900	N	85.42800	82.11980	74.20990	-293.13340	724.27691	333.44806	1
17901	H	85.59200	81.26780	73.76190	-663.36023	1787.42280	-2511.06987	1
17902	C	84.25200	82.63580	74.59690	741.17339	-445.24619	-264.77802	1
17903	C	84.51500	83.48880	75.69290	560.58922	477.19987	531.73216	1
17904	C	83.41000	84.02980	76.41090	-688.33602	150.84721	586.55691	1
17905	H	83.66700	84.57280	77.30890	-3142.46524	-240.51300	-90.32763	1
17906	C	82.13800	83.76480	75.96090	-662.36626	-462.18708	429.54334	1
17907	H	81.32000	84.18880	76.52390	2392.24601	-856.60585	1843.58505	1
17908	C	82.96000	82.40980	74.11690	-624.28084	-652.82006	137.63412	1
17909	H	82.82800	81.82880	73.21690	3096.63441	-413.09320	291.94873	1

17910	C	81.86200	82.98280	74.83290	-50.54226	657.72889	632.56363	1
17911	H	80.85600	82.74780	74.51690	1524.34316	-1262.00261	2437.87261	1
17912	C	88.11250	85.66270	78.46984	582.26307	474.47936	-84.06955	1
17913	O	87.67886	86.81050	78.64750	155.80029	731.39524	-1009.20929	1
17914	N	88.88700	84.89880	79.22090	-44.81963	143.63465	-834.12364	1
17915	H	89.17100	83.95280	79.08290	-2214.68935	-2227.88938	-214.22198	1
17916	C	89.47333	85.42271	80.42356	-76.49927	-663.67168	132.22853	1
17917	H	88.51118	85.77588	80.96909	-1226.14808	-3715.29199	-655.85850	1
17918	C	90.14400	84.27080	81.25390	374.41713	-501.42978	654.79595	1
17919	H	90.98300	83.74980	80.74590	2218.12834	1542.30109	-1610.19931	1
17920	H	89.46800	83.42280	81.49390	-1283.70864	884.49750	-2739.49382	1
17921	H	90.53800	84.71780	82.19190	-2546.37681	-1852.66993	-59.18317	1
17922	C	90.60299	86.62356	80.23630	-276.53911	810.39040	102.93082	1
17923	O	91.08639	87.26194	81.12492	500.31263	20.01386	-113.11716	1
17924	N	90.82269	86.68932	78.93274	352.68819	725.10123	774.35486	1
17925	H	90.30551	86.06928	78.27972	-3804.53132	-1173.67588	-293.57148	1
17926	C	91.31425	87.93990	78.44570	-554.59652	-611.26210	-859.08885	1
17927	H	91.81120	88.33694	79.38672	1129.23516	-234.03595	-165.03939	1
17928	C	92.41879	87.55224	77.31777	411.84346	-1238.10861	-639.23156	1
17929	H	91.85881	87.43273	76.32478	2830.10716	-1036.41439	1443.46981	1
17930	C	93.44375	88.71781	77.08244	250.31224	-154.04295	458.10917	1
17931	H	92.96764	89.51323	76.36805	2377.39884	-3649.44511	120.56463	1
17932	H	93.69336	89.23088	78.04923	1086.82116	1087.65259	-1956.74787	1
17933	H	94.44577	88.35501	76.76008	1472.85105	-36.61045	1971.51421	1
17934	C	93.45416	86.44893	77.66179	541.12950	913.94389	189.80458	1
17935	H	92.93028	85.45834	77.94442	1698.40023	2628.67304	-1877.72477	1
17936	H	94.08614	86.62428	78.57419	1721.20497	-2538.27093	3586.22592	1
17937	H	94.24449	86.24261	76.87185	463.04164	-1770.38849	-3449.77125	1
17938	C	90.19485	88.97011	77.87532	-251.41248	701.76811	-1450.53174	1
17939	O	90.20409	90.12313	78.27368	-255.18881	531.38496	44.10961	1
17940	N	89.40360	88.48620	76.96130	-282.08563	-237.65783	748.70580	1
17941	H	89.46208	87.45447	76.67788	2132.06572	109.33989	694.82600	1
17942	C	88.63256	89.32498	76.02489	118.40067	-496.17952	-137.74701	1
17943	H	89.30719	90.13975	75.68985	2285.38587	-1705.69828	-572.68422	1
17944	C	88.04891	88.35949	74.99028	-785.49517	308.05316	-165.03608	1
17945	H	88.76175	87.59353	74.61801	1577.33077	1026.39116	-145.10710	1
17946	H	87.19203	87.75888	75.34139	4777.89097	1777.04779	-3513.34210	1
17947	C	87.55147	89.18666	73.68346	1309.11484	-241.47284	-821.51456	1
17948	O	87.01155	88.61836	72.68374	506.36076	532.97625	-210.59339	1
17949	O	87.74370	90.41064	73.80315	-805.67691	181.78340	143.62099	1
17950	C	87.36091	89.98913	76.81020	-119.10251	-359.56626	-240.38877	1
17951	O	87.08342	91.13276	76.54992	540.41530	790.73321	148.34351	1
17952	N	86.67145	89.14055	77.60284	561.85243	-93.18469	1071.43949	1
17953	H	86.97934	88.14052	77.80658	3839.90500	-1552.90408	-2806.16502	1
17954	C	85.62950	89.73777	78.40175	624.84515	526.69899	902.00348	1
17955	H	85.05687	90.21596	77.55453	3048.25692	1801.90274	-3481.69612	1
17956	C	84.87421	88.55481	79.07437	-307.46651	-861.55997	-184.11522	1
17957	H	85.52074	87.64470	79.10855	-1490.06437	-3178.88986	257.56470	1
17958	H	84.49023	88.85085	80.08226	436.60729	261.63669	721.05889	1
17959	H	84.00994	88.20106	78.45113	2713.45942	-1307.04908	-1194.84762	1
17960	C	86.10160	90.92122	79.45161	494.15709	-214.94202	-430.91429	1
17961	O	85.42697	91.88815	79.66492	-522.22375	-28.24627	-760.86030	1
17962	N	87.31370	90.56944	79.95963	-186.67514	-171.07454	-896.18461	1
17963	H	87.75484	89.86481	79.36262	2956.02156	-1554.01934	3040.65651	1
17964	C	88.06027	91.40541	80.88622	-861.81687	61.17332	332.84830	1
17965	H	87.10821	91.75460	81.42864	2370.94363	516.62894	4298.72041	1
17966	C	89.04048	90.50417	81.61332	863.06444	-377.07995	-411.67044	1
17967	H	89.95449	90.46614	80.96104	-1574.30564	4361.59887	1727.11745	1
17968	C	89.34968	91.07914	82.97762	-485.71802	386.74925	-1083.56522	1
17969	H	90.18501	90.54247	83.45140	-5164.31398	-670.71499	-4265.82021	1
17970	H	89.45919	92.17894	83.00721	-1805.34345	-315.20337	2235.66114	1
17971	H	88.49114	90.85598	83.68102	1039.96930	1374.74305	360.42401	1

17972	C	88.67029	89.03547	81.74174	-222.03603	511.32919	-687.95753	1
17973	H	87.59109	88.93463	82.03643	2928.77217	3080.07556	1324.23668	1
17974	H	89.29567	88.55904	82.52501	2632.84222	1037.35044	-2715.54646	1
17975	H	88.86651	88.52085	80.77189	2929.71413	-1133.75620	-1177.17137	1
17976	C	88.64213	92.76926	80.17136	335.97808	1115.42169	26.44809	1
17977	O	88.63592	93.80969	80.82081	-274.96523	-59.48299	446.25934	1
17978	N	89.12386	92.60763	78.96261	-102.62712	-124.43859	-525.51400	1
17979	H	89.03702	91.68339	78.45248	-456.00798	2909.42236	1468.67570	1
17980	C	90.37083	93.32393	78.73995	-262.76160	851.87737	454.36221	1
17981	H	90.02401	94.24269	79.23735	223.70114	1571.13346	2562.31304	1
17982	C	91.62580	92.56469	79.38020	97.58182	-331.15501	821.65267	1
17983	H	91.36062	92.46294	80.42402	-1991.63252	852.74927	-2544.15598	1
17984	H	91.82174	91.52840	78.98462	-4591.94654	-861.78537	-2347.17855	1
17985	H	92.51518	93.18243	79.37581	989.05529	32.26697	1978.65442	1
17986	C	90.80084	93.53644	77.16043	298.91361	521.48346	-340.11987	1
17987	O	90.59829	94.68333	76.78456	313.30831	-343.67448	-65.35558	1
17988	N	91.25513	92.50216	76.49263	-737.78265	-469.34173	-272.93866	1
17989	H	91.31101	91.62583	77.02865	-189.23503	1204.60913	467.52256	1
17990	C	91.30201	92.70332	75.04963	-316.22092	372.63960	393.40931	1
17991	H	90.46128	93.39691	74.90086	1667.06162	-3506.03876	3268.09007	1
17992	C	92.61975	93.51797	74.75283	56.62442	407.79728	145.42060	1
17993	H	92.97039	94.09676	75.54198	-1992.96812	-1761.31849	897.64523	1
17994	H	93.48795	92.88058	74.45991	-3718.89338	-92.91065	-1776.73602	1
17995	C	92.15221	94.47823	73.60693	-1139.92933	604.07790	497.22900	1
17996	O	92.47565	94.21428	72.46828	-106.52238	-18.62015	-697.30529	1
17997	N	91.23393	95.33905	74.10468	-438.85728	14.45410	630.56758	1
17998	H	90.96231	95.54569	75.05172	597.24114	2521.37899	-1125.64991	1
17999	H	90.46397	95.57327	73.49436	-1211.66703	1117.19125	-509.06964	1
18000	C	91.40230	91.24581	74.33410	37.02945	-340.05139	-1042.29606	1
18001	O	91.89065	90.29485	74.90999	-93.36095	-1342.71795	-567.57186	1
18002	N	90.76745	91.20718	73.18845	301.21891	-264.94518	-176.46934	1
18003	H	90.29439	92.05762	72.80011	-1024.92508	899.09098	3173.31003	1
18004	C	90.92062	89.97640	72.42169	-376.91525	62.01310	279.16923	1
18005	H	90.91903	89.20708	73.21843	750.05842	2892.47388	-1457.94475	1
18006	C	89.74197	89.89592	71.30692	-1157.36053	583.35028	582.45485	1
18007	H	90.07140	90.69282	70.62371	-3049.26554	-763.63667	321.04291	1
18008	H	88.72509	90.19009	71.72715	1745.30556	-1093.54994	-2710.70985	1
18009	C	89.74872	88.57999	70.54116	13.31459	-548.89763	16.55385	1
18010	C	90.13860	88.45427	69.19922	313.20633	-414.11072	818.39424	1
18011	H	90.45278	89.25658	68.51117	-1495.58719	-607.74228	2321.39531	1
18012	N	90.17335	87.19110	68.85309	261.40195	141.78996	421.32328	1
18013	H	90.68231	86.97396	67.92879	1488.18454	-206.97056	-2508.61461	1
18014	C	89.77053	86.29948	69.85385	-175.67600	160.73987	163.11679	1
18015	C	89.56696	87.19310	71.01339	447.60664	-191.11620	241.81885	1
18016	C	89.20672	86.60372	72.26206	-183.62999	858.51085	-556.05804	1
18017	H	89.07512	87.25350	73.13576	265.60970	1209.89323	-2722.19641	1
18018	C	89.16062	85.23995	72.35342	654.00769	459.43747	-313.99074	1
18019	H	88.94841	84.74456	73.32390	86.13077	-655.81280	3685.47197	1
18020	C	89.74253	84.88717	69.96105	-91.81283	188.49878	-687.86408	1
18021	H	89.86342	84.25688	69.02274	-815.21786	-3979.33666	3925.90066	1
18022	C	89.26927	84.37466	71.18709	284.44451	119.25482	-1005.72142	1
18023	H	89.24362	83.29448	71.32175	688.60234	2232.57337	-289.70970	1
18024	C	92.27097	90.07932	71.61238	-338.29202	598.80974	418.13859	1
18025	O	92.21724	90.50484	70.44629	170.95617	-479.02104	2.27993	1
18026	N	93.36456	89.70552	72.27728	288.27572	496.36594	-321.39525	1
18027	H	93.27068	89.36506	73.23895	1509.86010	-305.50853	1799.46499	1
18028	C	94.60911	90.21749	71.76312	1001.82537	1232.14595	232.20313	1
18029	H	94.25019	91.19654	71.48558	1997.60996	54.47020	375.80432	1
18030	C	95.76219	90.14945	72.84515	420.64309	312.21290	-650.47958	1
18031	H	95.87642	89.17326	73.28077	-3294.41492	238.06928	-1225.70497	1
18032	H	96.72412	90.30968	72.32310	2496.36546	-1565.26627	2433.77824	1
18033	C	95.55036	91.10360	74.03427	46.01947	-384.30645	-255.42013	1

18034	C	95.39456	90.80572	75.43017	-294.47309	802.96321	-4.75051	1
18035	H	95.33141	89.75108	75.75385	-2330.60759	-1442.57798	-1138.38960	1
18036	C	95.22374	91.84853	76.37600	-192.13453	658.60773	-455.77219	1
18037	H	95.04491	91.55551	77.39766	270.28791	-235.01327	427.64173	1
18038	C	95.34024	93.20257	76.05480	-1044.38047	86.84071	-289.91865	1
18039	O	95.19051	94.27369	77.01179	-132.88024	-305.56544	-513.53433	1
18040	H	95.34829	93.73923	77.83995	1027.14660	125.72802	-4292.82285	1
18041	C	95.44897	92.47991	73.66184	112.14144	-833.65638	-133.23029	1
18042	H	95.54923	92.83823	72.62222	1479.43320	1579.39548	-572.21941	1
18043	C	95.45091	93.45561	74.65894	-249.49110	-174.74416	290.62970	1
18044	H	95.40913	94.49212	74.32573	223.71860	718.86918	1354.34349	1
18045	C	95.28640	89.37406	70.53056	418.89105	317.97813	280.71741	1
18046	O	96.50143	89.30653	70.46849	-55.93856	263.84382	263.22765	1
18047	N	94.37760	88.86277	69.71408	936.21632	-189.58625	268.52146	1
18048	H	93.41046	89.14802	69.97030	2166.45900	3346.10429	-805.57009	1
18049	C	94.49691	87.51606	69.27684	-362.02037	199.68345	-1.51019	1
18050	H	95.53455	87.19084	69.40953	107.04505	-4260.72909	1048.51292	1
18051	C	93.39729	86.63212	70.01050	916.78607	-361.42323	-424.73372	1
18052	H	93.41966	85.69110	69.44678	-723.87842	-3077.05927	1669.39023	1
18053	H	92.34008	86.94246	69.91034	2995.34903	-2057.55411	-460.44602	1
18054	C	93.61949	86.62497	71.53477	-805.51805	-485.64260	-118.54092	1
18055	C	94.91250	86.45474	72.16995	-177.63109	253.72530	-224.32669	1
18056	H	95.73068	86.26055	71.51317	2477.00567	-1289.75983	-2546.13492	1
18057	C	95.02667	86.62197	73.59076	386.56126	783.39960	-196.16647	1
18058	H	96.09415	86.54053	73.98259	-2932.65016	716.25837	1005.60939	1
18059	C	93.85770	86.69309	74.32953	-1117.64472	122.70128	138.08409	1
18060	H	93.96589	86.82871	75.41117	3559.06355	226.01377	-1693.06671	1
18061	C	92.43707	86.59052	72.33759	-346.08844	-82.11274	485.57976	1
18062	H	91.42805	86.63742	71.90990	505.35088	2550.34356	-1199.39227	1
18063	C	92.60297	86.65464	73.73177	514.32110	-573.18643	66.85091	1
18064	H	91.65705	86.57445	74.40480	242.16337	-1007.28692	-112.32411	1
18065	C	94.07552	87.50547	67.64614	-669.94807	-42.02036	-64.08778	1
18066	O	94.54582	86.56077	66.97918	-1113.21630	111.61217	229.27369	1
18067	N	93.15273	88.37522	67.24272	-554.49756	436.79579	-173.84692	1
18068	H	92.96787	89.14824	67.92732	1610.93117	-390.62184	-1863.81443	1
18069	C	92.92197	88.41767	65.82713	-376.39777	-149.98905	139.26976	1
18070	H	93.70403	87.80310	65.31627	-631.29747	1315.98078	1150.62256	1
18071	H	92.80261	89.46392	65.41529	-1803.49254	2467.91967	1496.11085	1
18072	C	91.46998	87.79814	65.42655	658.10369	-41.30199	-446.79654	1
18073	O	90.81593	87.10000	66.23698	-465.89095	361.60019	597.03513	1
18074	N	91.11963	88.25489	64.26631	682.00580	-177.45275	352.87129	1
18075	H	91.76821	88.91001	63.73861	785.47875	3543.70146	1672.28080	1
18076	C	89.89326	87.76738	63.65997	2.25848	11.18585	233.32943	1
18077	H	89.19805	87.72160	64.56961	270.73955	-2931.87266	-1006.24857	1
18078	C	89.64704	88.98812	62.72291	620.01663	-33.38814	-350.14210	1
18079	H	90.42170	89.14613	61.94843	-2126.41445	3302.00244	215.24808	1
18080	H	89.98385	89.83449	63.38424	169.91172	1024.38624	1139.83196	1
18081	C	88.23849	89.02236	62.05917	176.54730	579.85275	106.00525	1
18082	O	87.92249	89.95328	61.28985	317.12435	-661.21520	-319.96123	1
18083	N	87.41460	87.94505	62.34976	-543.60703	311.30408	-224.03429	1
18084	H	87.85558	87.02688	62.58636	849.23509	-1379.10849	-3110.85885	1
18085	H	86.58292	87.63197	61.74790	-204.49259	-519.60077	4113.89955	1
18086	C	90.02378	86.34454	62.89167	-1036.52123	-141.43324	-137.23534	1
18087	O	89.04001	85.73499	62.54673	193.63073	8.13301	556.28008	1
18088	N	91.31507	86.05118	62.58371	503.83042	-342.22445	366.28404	1
18089	H	91.93791	86.52382	63.22151	-2064.13295	-1522.16093	4032.97627	1
18090	C	91.51800	84.51480	62.52590	-314.84111	337.70502	-798.14484	1
18091	H	90.87200	84.13680	61.74790	641.95804	1485.71105	-2704.10817	1
18092	C	92.98800	84.28580	62.01190	-249.79702	379.53540	794.81225	1
18093	H	93.08100	84.82880	61.04690	1073.81968	-2912.30676	-425.43246	1
18094	H	93.75600	84.78580	62.63890	1117.56010	-2194.36978	1936.55402	1
18095	C	93.37900	82.83780	61.76390	597.74732	-543.57805	-397.25737	1

18096	C	93.09300	82.24380	60.53090	-480.21480	-645.51123	-430.08698	1
18097	H	92.55800	82.73080	59.72890	-1619.03187	-1765.70741	-2043.45513	1
18098	C	93.42400	80.89180	60.32490	-636.94378	-642.80439	106.87966	1
18099	H	93.07600	80.44380	59.40590	-1056.96770	1154.29294	2732.81864	1
18100	C	94.15700	80.14080	61.27890	568.92686	676.62414	-233.26303	1
18101	H	94.35300	79.09980	61.07090	1114.18823	-362.83730	2908.08357	1
18102	C	94.09900	82.07280	62.66490	451.91417	-767.14491	-121.50679	1
18103	H	94.24300	82.65980	63.55990	-96.34455	-3117.79203	326.51976	1
18104	C	94.50800	80.76380	62.47290	665.14410	116.30930	-608.71441	1
18105	H	94.97700	80.15980	63.23490	1550.20926	-1609.03405	-2206.55935	1
18106	C	91.15900	83.68080	63.73290	-522.29095	30.86254	750.72521	1
18107	O	90.49700	82.62580	63.60990	154.76027	367.78046	-687.79781	1
18108	N	91.54500	84.08880	64.97890	400.53455	-696.54886	211.82646	1
18109	H	92.25500	84.78180	65.07190	2438.77680	-1682.31607	1016.28561	1
18110	C	91.05900	83.46380	66.12890	-642.19439	227.29730	-623.13309	1
18111	H	90.97300	82.39880	65.96990	-1288.21407	-1114.91791	-2650.26536	1
18112	C	91.97900	83.68480	67.32190	669.53350	299.83802	530.00399	1
18113	H	92.00800	84.76880	67.56390	96.10404	2286.26177	2163.52663	1
18114	H	91.54900	83.17080	68.20790	2781.77159	1233.65436	-781.71507	1
18115	C	93.41300	83.09980	67.07090	454.38664	790.96032	54.79291	1
18116	H	93.86800	83.56380	66.16990	26.52113	2141.86721	2307.74682	1
18117	C	94.41000	83.62580	68.14990	-610.04034	-662.66560	-149.17717	1
18118	H	94.13600	83.23380	69.15290	1332.97300	-1097.92060	-2626.69494	1
18119	H	94.50000	84.72780	68.25790	-2094.18134	2354.61193	-216.93472	1
18120	H	95.41400	83.22980	67.88390	-2823.45447	-41.15834	-1410.96679	1
18121	C	93.41700	81.60480	66.91190	-596.73741	-409.09612	553.78820	1
18122	H	92.78300	81.17580	66.10690	59.99094	-2200.39947	2234.15968	1
18123	H	93.12900	81.18280	67.89790	-696.67920	1514.11090	-2680.35504	1
18124	H	94.45700	81.21880	66.84390	-1165.69871	-2818.67335	748.54857	1
18125	C	89.61400	83.83780	66.42890	-561.39294	-566.52995	-447.25423	1
18126	O	88.85000	83.03980	67.01290	266.17139	-622.83922	384.07104	1
18127	N	89.19563	85.06724	65.94532	-329.04385	-488.94074	57.21887	1
18128	H	89.85326	85.86580	65.66706	-870.24643	-1521.77448	1775.55210	1
18129	C	87.81232	85.33576	66.41155	-379.00394	-525.29042	-1211.54020	1
18130	H	87.86683	85.04774	67.50340	-1432.19517	458.22959	-2404.08017	1
18131	C	87.29175	86.83143	66.15472	-707.49946	-439.51370	86.10100	1
18132	H	87.20104	86.73439	65.05843	-2061.27572	304.79286	-3710.45895	1
18133	H	88.14594	87.56688	66.34075	-1720.55379	19.97106	-4953.02530	1
18134	S	85.85502	86.94398	67.12648	-177.08650	-2.75656	-28.64921	1
18135	C	86.67300	84.54580	65.53490	458.36775	-770.12205	-82.92837	1
18136	O	85.70400	84.06480	66.09490	-64.90151	-663.61914	410.33736	1
18137	N	86.85900	84.23180	64.25690	55.67696	-761.21625	338.14673	1
18138	H	87.68800	84.53680	63.79390	-146.28953	1077.07121	-2958.50408	1
18139	C	86.09400	83.32380	63.49490	119.92114	-821.73656	-355.84907	1
18140	H	85.03600	83.53880	63.49790	2357.78813	-1141.46710	-1724.44075	1
18141	C	86.54900	83.31080	62.03090	101.84808	645.82823	-645.61129	1
18142	H	86.13700	82.48080	61.41790	-315.49305	-3112.58887	-244.61584	1
18143	H	87.65600	83.22380	61.99490	2926.10362	-908.70079	652.02878	1
18144	C	86.19500	84.62180	61.36690	-508.67508	-278.28508	-709.99166	1
18145	H	86.39491	85.46088	62.05793	1387.58023	-1404.09537	-2805.41873	1
18146	H	85.09100	84.55380	61.26190	-2310.29808	-1774.91651	1193.84131	1
18147	C	86.79500	84.65480	59.96290	648.57340	313.57678	-552.93060	1
18148	H	86.34400	83.82380	59.38090	2415.00305	-1982.36036	-199.03186	1
18149	H	87.86800	84.41480	60.12190	-1399.02018	-1530.92573	-2368.60539	1
18150	C	86.54036	85.98677	59.17721	556.62660	245.11807	538.88121	1
18151	H	86.90120	85.98490	58.13746	-294.51088	1705.82467	-1256.13577	1
18152	H	86.78984	86.90891	59.79590	2101.02953	-1486.40310	-1262.60518	1
18153	N	84.99480	86.20170	59.21150	-785.32985	-533.38209	133.29338	1
18154	H	84.50814	86.75773	58.45803	2483.79594	-2106.09666	-395.14558	1
18155	H	84.79740	86.77865	60.16536	-919.90757	-384.44068	-1483.61167	1
18156	H	84.43942	85.27024	59.30386	-917.82285	195.82838	2567.75055	1
18157	C	86.02200	81.92880	64.05690	-35.45080	-722.53953	541.57784	1

18158	O	84.99900	81.30480	64.09590	-679.75656	-136.97610	389.71304	1
18159	N	87.20100	81.39480	64.42590	654.38963	332.12546	-411.37386	1
18160	H	88.05400	81.83980	64.16690	1864.48288	1579.56828	-1982.41481	1
18161	C	87.36500	80.09380	65.00890	-816.41882	414.29532	-129.89564	1
18162	H	86.88200	79.29380	64.46790	-850.08403	751.30029	-2943.60695	1
18163	C	88.86800	79.76980	65.00690	374.43435	420.87789	712.23849	1
18164	H	89.28500	79.59280	63.99190	232.44788	2849.84611	-1334.48981	1
18165	H	88.98400	78.87080	65.64790	-2632.33675	1517.72547	855.23828	1
18166	H	89.43500	80.62280	65.43790	-680.75503	322.01465	-3062.06516	1
18167	C	86.72700	79.92780	66.35090	438.45055	-658.59246	428.58437	1
18168	O	85.95200	79.01880	66.54290	8.87594	-526.44235	577.54551	1
18169	N	86.90000	80.80780	67.33590	43.02836	5.85719	-846.19593	1
18170	H	87.40500	81.66380	67.25290	-644.90563	3081.96811	-206.46889	1
18171	C	86.19000	80.52680	68.62890	-54.01345	-739.30871	518.84194	1
18172	H	86.32400	79.48480	68.87990	2480.69677	-1406.45585	-1309.59407	1
18173	C	86.84000	81.26180	69.83390	889.04089	-103.67968	-119.95892	1
18174	H	86.44200	80.90480	70.80790	1399.88128	2480.91490	1334.30405	1
18175	C	88.33400	81.07680	69.72290	-591.05031	639.38682	-306.80738	1
18176	H	88.48300	79.98080	69.82890	-1218.63648	2656.01997	1184.73515	1
18177	H	88.82500	81.27280	68.74590	-2168.56829	-2201.90570	591.68513	1
18178	H	88.77100	81.69980	70.53290	-2083.93822	-2098.25710	1073.92859	1
18179	C	86.58200	82.78080	69.82590	-592.30484	-475.06658	506.39840	1
18180	H	86.96400	83.25980	70.75290	2204.88349	-173.52341	-2231.24693	1
18181	H	85.55100	83.08380	69.54390	615.76563	2761.99008	1381.09233	1
18182	H	87.13100	83.11580	68.91990	-253.69985	3131.74586	-272.20067	1
18183	C	84.70900	80.73080	68.63990	-632.93376	-114.55297	650.64257	1
18184	O	84.02200	80.17280	69.49290	-246.99726	577.78224	486.75900	1
18185	N	84.24600	81.55880	67.65790	-160.86550	-803.22477	180.42175	1
18186	H	84.91200	81.97480	67.04290	1968.06047	1880.40704	1571.70651	1
18187	C	82.80800	81.69580	67.40890	490.44376	-241.22522	719.07705	1
18188	H	82.37200	81.78180	68.39290	-357.39592	-212.66674	-3121.15642	1
18189	C	82.41500	82.92780	66.52990	732.99075	-24.01000	526.49050	1
18190	H	81.41600	82.87480	66.04590	886.31487	-2277.04131	-1970.62278	1
18191	H	83.13300	83.04280	65.69090	-1156.73282	1814.86041	2303.95039	1
18192	N	83.09257	85.36004	67.44620	-789.21115	-813.88626	-955.33760	1
18193	H	83.77200	85.76976	66.72670	1681.88614	-180.51981	-877.23354	1
18194	C	82.39900	84.15480	67.43290	892.37825	-118.13890	-48.73980	1
18195	C	82.80789	86.22734	68.36828	108.96633	-454.19816	-518.27704	1
18196	H	83.23171	87.28899	68.39648	1748.65740	1495.93687	3895.58814	1
18197	N	81.80824	85.63067	69.08945	-579.99165	-252.50955	-577.32749	1
18198	C	81.65600	84.41580	68.51590	136.32421	-477.04237	-760.27294	1
18199	H	80.87200	83.84280	68.99590	-3030.68003	352.89241	-805.98543	1
18200	C	82.16700	80.46780	66.77990	716.29937	117.56263	-543.46946	1
18201	O	81.09700	80.01880	67.19390	469.88919	-448.28960	430.34229	1
18202	N	82.89000	79.89280	65.78590	178.60863	742.30407	-373.20411	1
18203	H	83.69400	80.36680	65.43590	1905.14723	-541.57481	2432.25945	1
18204	C	82.59700	78.59880	65.20790	44.61787	777.20444	-489.23877	1
18205	H	81.57800	78.58580	64.84890	-1058.63008	2434.04493	1702.79436	1
18206	C	83.57500	78.33080	64.01290	587.18264	-678.89911	51.86181	1
18207	H	84.59400	78.72480	64.21390	-506.67878	2046.68760	-2348.09777	1
18208	C	83.59900	76.78780	63.77490	222.56906	-872.16790	-53.80558	1
18209	H	84.31500	76.28780	64.46290	237.29848	210.01570	-3134.58664	1
18210	H	83.98300	76.51480	62.76890	-2347.76777	290.43070	2081.95348	1
18211	H	82.64600	76.27180	64.01990	-2677.18266	270.47322	-1651.28823	1
18212	C	83.00400	79.04680	62.75690	-688.89411	267.30127	548.01628	1
18213	H	81.91100	78.88580	62.63890	3109.59648	-300.41890	-266.69542	1
18214	H	83.47200	78.73680	61.79890	-202.07650	3031.12063	-856.68925	1
18215	H	83.14800	80.14080	62.88390	1761.75991	-2401.73212	-976.90497	1
18216	C	82.54300	77.54080	66.30590	-640.20002	152.33778	638.21347	1
18217	O	81.51500	76.91780	66.54690	-139.00049	587.41302	515.67853	1
18218	N	83.59100	77.46180	67.16990	118.05853	-110.46016	822.31414	1
18219	H	84.39600	78.01380	66.96890	1947.99311	-1109.82332	-2199.69674	1

18220	C	83.61000	76.47880	68.21290	164.42156	-878.69462	-138.38041	1
18221	H	83.48300	75.48980	67.79590	1992.96545	-2184.51893	-1049.43428	1
18222	C	85.03500	76.38780	68.80890	-556.68581	-700.11344	-181.95602	1
18223	H	85.44800	77.41780	68.87090	-1712.21024	1687.22724	2037.63034	1
18224	C	85.07400	75.72080	70.18590	-547.45866	-533.84552	493.75497	1
18225	H	86.10000	75.62280	70.60190	-2619.49490	1746.09905	-225.49320	1
18226	H	84.55100	76.30080	70.97590	-504.51032	-1165.57100	2872.75286	1
18227	H	84.66100	74.69080	70.12890	2360.72387	-2050.74295	237.51182	1
18228	C	85.97700	75.72480	67.76590	-98.18311	-238.41847	868.29468	1
18229	H	85.69100	74.65480	67.67490	-1516.47071	2275.84290	-1579.19068	1
18230	H	85.74100	76.16480	66.77290	1462.57973	1874.99856	2055.33318	1
18231	C	87.47200	75.97180	67.95890	390.06594	406.60744	710.68259	1
18232	H	88.05300	75.45780	67.16290	1576.13022	-2592.13432	-798.95125	1
18233	H	87.73000	75.66880	68.99590	1400.72879	3.39213	2807.28553	1
18234	H	87.69600	77.04780	67.79490	1752.71508	-1723.16113	-1955.06933	1
18235	C	82.51700	76.61280	69.28290	-620.28303	86.79355	-675.01447	1
18236	O	81.96700	75.61980	69.76790	-708.37877	241.28089	274.05532	1
18237	N	82.13600	77.82380	69.67790	-405.37820	-492.03869	550.69439	1
18238	H	82.59400	78.62980	69.31090	643.48411	2523.32227	1767.65899	1
18239	C	81.05000	78.07380	70.56590	646.20240	-585.12291	-237.33088	1
18240	H	81.27600	77.50580	71.45590	-385.17836	-3111.51755	-210.90985	1
18241	C	81.05200	79.58980	71.00790	-122.45321	868.02473	269.13565	1
18242	H	80.98000	80.15680	70.05590	934.85597	-567.14802	-2948.55670	1
18243	H	82.02300	79.80180	71.50490	-1756.22962	661.79516	-2534.59089	1
18244	C	79.92200	80.03280	71.97990	444.64135	532.81259	587.62017	1
18245	C	79.38500	79.12780	72.88490	747.08396	204.11898	-473.48387	1
18246	H	79.82100	78.13980	72.84190	2337.29381	-2085.87072	175.96666	1
18247	C	78.46300	79.55580	73.85390	-200.60253	802.41742	-397.01121	1
18248	H	78.13700	78.88380	74.63390	502.81930	2846.76741	1244.38230	1
18249	C	77.98700	80.85580	73.88990	702.32145	193.96661	-541.05088	1
18250	O	76.96700	81.12580	74.81990	326.91092	-635.25500	-323.92512	1
18251	H	77.08100	82.02380	75.14090	1599.39933	-1707.94424	2094.54542	1
18252	C	79.47200	81.38480	72.01490	-512.08454	743.42893	175.91709	1
18253	H	79.94600	82.09480	71.35290	1997.37048	-795.13771	2286.85788	1
18254	C	78.48900	81.79280	72.93090	683.63573	409.78497	-435.38856	1
18255	H	78.06400	82.77980	73.03490	43.21796	761.38660	-3053.68203	1
18256	C	79.67300	77.54080	70.07190	-599.60519	-266.32678	-641.46102	1
18257	O	78.96500	76.79380	70.76590	472.86070	-467.85158	-414.18717	1
18258	N	79.39400	77.68380	68.75890	-750.56784	-396.55506	3.18549	1
18259	H	79.95300	78.19680	68.11190	-1161.45304	-979.47494	2753.69883	1
18260	C	78.20500	77.02080	68.19390	53.36784	801.68309	438.01833	1
18261	H	77.43900	76.92980	68.94890	2948.95071	317.17172	1024.98411	1
18262	C	77.48800	77.80880	67.07390	356.32206	-635.43654	-537.39957	1
18263	H	76.97700	77.12180	66.36490	1480.23108	-2369.63446	1424.18386	1
18264	O	78.48200	78.54080	66.33890	-438.91983	-396.49627	-528.04442	1
18265	H	77.96600	79.06380	65.71990	-583.51300	2171.64280	2207.61326	1
18266	C	76.51200	78.84980	67.67590	688.63003	564.42455	179.79774	1
18267	H	76.14500	79.53180	66.87990	2240.35661	-1711.13794	-1375.63757	1
18268	H	77.06600	79.47580	68.40790	2625.80217	-1595.41141	626.26001	1
18269	H	75.64300	78.39980	68.20290	-722.19249	1855.38658	2441.24259	1
18270	C	78.36700	75.56380	67.75190	-15.45537	-791.20725	439.20027	1
18271	O	77.49200	74.70580	67.73790	231.74486	731.95887	-200.53705	1
18272	N	79.64800	75.13880	67.41590	-417.04813	729.58663	146.55234	1
18273	H	80.37000	75.81880	67.31490	481.84237	-2724.87400	-1486.18360	1
18274	C	79.99100	73.68980	67.21490	88.61976	910.31216	-75.63605	1
18275	H	79.38000	73.32380	66.40290	1627.53249	86.60163	2681.67877	1
18276	C	81.38900	73.44280	66.61790	744.85556	-136.45899	488.45660	1
18277	H	82.10200	74.18380	67.03690	-7.17878	-3122.37513	321.67498	1
18278	C	81.96200	72.04380	66.97190	581.85838	170.24355	670.09217	1
18279	H	82.88300	71.83080	66.38890	1726.18988	-1900.91977	-1808.47207	1
18280	H	81.18600	71.31880	66.64490	2495.23235	-876.93291	-1693.93308	1
18281	H	82.34400	71.99180	68.01390	417.09881	-1852.17733	-2508.37003	1

18282	C	81.32400	73.80080	65.10990	462.85643	442.26735	643.13038	1
18283	H	80.97800	74.84980	64.98990	2737.92801	-1509.59695	-229.85742	1
18284	H	82.37400	73.66580	64.77390	-1760.96601	1443.80697	-2188.29896	1
18285	H	80.63300	73.08980	64.60990	673.90006	-2975.76099	724.53691	1
18286	C	79.75400	72.79980	68.47990	-619.47648	625.62151	-275.61530	1
18287	O	79.20000	71.70380	68.33390	532.05505	395.53368	419.73852	1
18288	N	80.08100	73.22380	69.70090	172.91307	-496.29476	649.76621	1
18289	H	80.50800	74.12280	69.76890	-630.92253	-2683.67019	-1513.74082	1
18290	C	79.61600	72.58280	70.91190	-765.40476	82.82988	-505.29216	1
18291	H	79.83700	71.53080	70.80090	-2395.78744	-662.87450	1930.26743	1
18292	C	80.32000	73.15880	72.15090	166.68697	890.87963	121.05007	1
18293	H	80.52000	74.24680	72.04990	-494.45600	2922.19678	-1076.19734	1
18294	H	81.33400	72.70680	72.18690	-1949.49855	-1099.58608	-2219.90203	1
18295	C	79.57500	73.06880	73.50490	-6.02462	-706.39997	567.06380	1
18296	O	78.59100	73.73680	73.79790	496.58987	-66.62512	-608.64221	1
18297	N	80.05400	72.13480	74.36090	390.92450	-699.02938	242.07280	1
18298	H	80.91400	71.64380	74.22290	2437.24680	1923.59509	-498.06818	1
18299	H	79.62900	72.06180	75.26290	-1609.93060	-1822.22870	1993.21624	1
18300	C	78.06400	72.62880	71.06090	-130.35900	906.99412	-51.15619	1
18301	O	77.44500	71.63380	71.38190	-394.11678	287.39302	622.90152	1
18302	N	77.42000	73.74480	70.75490	-514.51697	-662.82992	-102.80784	1
18303	H	77.98600	74.52280	70.49790	-2042.12336	-2302.99929	653.81551	1
18304	C	76.00300	73.97580	70.88590	-853.49326	104.48439	-328.17675	1
18305	H	75.75900	73.92180	71.93690	1775.83032	-2456.36118	812.57362	1
18306	C	75.56400	75.38480	70.54190	-260.84233	-866.59548	88.80442	1
18307	H	75.41200	75.53680	69.45190	2139.40063	1429.51646	1802.39704	1
18308	H	76.35700	76.10880	70.82590	2119.95453	-2284.69824	-363.89328	1
18309	C	74.25900	75.91580	71.28290	-532.63391	548.48908	507.24060	1
18310	H	73.50300	75.10180	71.26190	-1673.71938	-2296.31594	1350.56780	1
18311	C	74.54200	76.24980	72.74990	-625.08393	-481.67277	460.69830	1
18312	H	74.82100	75.38380	73.38690	-358.26018	2868.99237	-1252.75363	1
18313	H	73.69400	76.78080	73.23390	-1927.88942	2245.74079	1084.89629	1
18314	H	75.40100	76.95280	72.71390	-596.90663	-2944.67558	923.91443	1
18315	C	73.71700	77.15380	70.58690	-95.59545	485.33462	768.21288	1
18316	H	72.74800	77.35680	71.09090	-1284.05773	2229.85564	1819.58436	1
18317	H	73.66100	76.90080	69.50690	-2211.89881	939.00296	2040.21554	1
18318	H	74.31300	78.05480	70.84590	-1242.66947	-2559.58921	1340.34148	1
18319	C	75.09600	73.04480	70.08690	-830.67000	391.40814	-68.73387	1
18320	O	74.19500	72.43780	70.57690	519.18896	459.19864	-377.07439	1
18321	N	75.58000	72.79280	68.84390	436.15886	-707.58737	-89.98110	1
18322	H	76.37800	73.29880	68.52390	593.94315	1451.42222	-2732.23636	1
18323	C	75.03800	71.79380	67.92590	32.93483	-544.63417	-729.87678	1
18324	H	73.97500	71.68380	68.08490	-951.47697	2270.49321	1965.34726	1
18325	C	75.21300	72.27780	66.44590	-7.92597	-905.10498	-37.37704	1
18326	H	74.68000	71.57580	65.76990	-399.32974	2225.39817	2191.84349	1
18327	H	76.30400	72.25780	66.23490	1244.19765	1670.42319	-2361.98875	1
18328	C	74.58800	73.64280	66.30190	17.91820	867.05587	296.10125	1
18329	C	73.40500	74.05580	66.90090	-629.94929	172.76706	-648.54161	1
18330	H	72.87400	73.31580	67.48090	2137.53221	2092.16844	-971.97083	1
18331	C	72.89700	75.36980	66.79290	-866.40716	249.81499	-191.97272	1
18332	H	72.03100	75.61380	67.39190	1594.61666	2179.29777	1611.49213	1
18333	C	73.59500	76.30480	66.07290	-548.19151	458.28481	-581.56154	1
18334	O	73.11000	77.58880	66.04690	451.16441	-249.30900	587.55699	1
18335	H	73.77800	78.08480	65.56790	2097.73861	-2261.07488	562.46490	1
18336	C	75.25300	74.59480	65.48390	-693.82110	87.46767	-599.33160	1
18337	H	76.17700	74.26580	65.03190	43.90296	-2922.94761	1142.27067	1
18338	C	74.76400	75.91180	65.39090	326.51314	472.42453	706.07737	1
18339	H	75.26000	76.67480	64.80990	2038.03290	-728.82327	-2274.80383	1
18340	C	75.55000	70.36280	68.08790	-738.36483	231.49811	-500.99192	1
18341	O	74.98700	69.48580	67.47890	484.80912	-461.66460	-407.98912	1
18342	N	76.64500	70.10980	68.85690	324.60309	-569.45571	-526.45440	1
18343	H	77.20900	70.81580	69.27890	-339.70625	-1607.88736	2675.75720	1

18344	C	77.21400	68.74780	68.93090	-690.73412	-61.80774	-605.38966	1
18345	H	76.76200	68.11280	68.18290	-2607.33324	1615.93048	732.73339	1
18346	C	78.76800	68.59680	68.72990	596.02643	453.96324	510.22043	1
18347	H	78.91700	68.76980	67.64290	2138.28278	-2293.65718	60.69739	1
18348	H	79.12100	67.55780	68.90390	-2646.86455	-693.10762	1555.95790	1
18349	O	79.43400	69.45380	69.61290	753.72654	216.49744	7.30554	1
18350	H	79.36600	70.29480	69.15390	-3054.98067	-659.25907	404.56468	1
18351	C	76.83600	68.12980	70.21990	498.71611	598.64270	-478.33864	1
18352	O	76.31600	67.01880	70.22490	-312.07694	534.42851	-505.87461	1
18353	N	76.90800	68.88580	71.39690	76.33347	474.55010	-701.74167	1
18354	H	77.09200	69.86380	71.34290	-1873.04815	2138.99858	1358.29924	1
18355	C	76.65900	68.29280	72.72790	493.82183	466.96369	-611.47836	1
18356	H	77.37300	67.49480	72.86990	-357.76700	-43.84511	-3132.16884	1
18357	C	76.99100	69.27280	73.89690	719.73008	76.41368	-552.60761	1
18358	H	78.08900	69.43780	73.90890	361.06741	3126.67842	-106.55854	1
18359	H	76.72300	68.86880	74.89590	2924.45232	81.36901	1137.66210	1
18360	O	76.37400	70.60180	73.75590	273.61857	523.50887	-528.99627	1
18361	H	76.99100	71.20580	73.33690	528.11915	2600.07205	-1699.16572	1
18362	C	75.22200	67.71180	72.98090	196.28844	-546.19085	693.27251	1
18363	O	75.04700	66.54180	73.22690	538.98853	-305.48630	-486.85253	1
18364	N	74.23400	68.54880	72.77190	-758.33135	-378.09186	-40.27274	1
18365	H	74.49300	69.49780	72.60890	1261.70224	2610.83105	1217.32485	1
18366	C	72.81700	68.20780	72.84690	703.93705	-424.81460	-384.02028	1
18367	H	72.69700	67.79180	73.83690	-692.38117	-1497.57152	-2683.39721	1
18368	C	71.92400	69.42580	72.75590	202.77923	-32.89934	882.88937	1
18369	H	72.28100	70.22380	73.44090	-2091.53959	2287.16702	572.96627	1
18370	C	71.88500	70.06880	71.32090	493.00725	-488.95624	-585.77024	1
18371	H	72.95400	70.30580	71.12690	2772.48877	743.89161	1271.35317	1
18372	H	71.46800	69.35080	70.58190	1517.77981	-1884.46883	-2005.61431	1
18373	H	71.31100	71.01980	71.33190	2630.76383	-1626.74725	-534.69420	1
18374	C	70.59100	69.04780	73.37790	-378.88912	-732.89266	385.00383	1
18375	H	69.91400	69.92780	73.42990	1618.89530	2264.70550	1460.04092	1
18376	H	70.01500	68.20180	72.94690	-870.29212	-2004.25216	2259.40314	1
18377	H	70.85600	68.68180	74.39290	-475.23382	2022.86710	2361.68283	1
18378	C	72.36900	67.11980	71.85690	623.20020	362.10758	-558.81193	1
18379	O	71.52900	66.26080	72.13090	-595.74733	366.56695	-384.55340	1
18380	N	72.91100	67.09180	70.61690	-455.97143	172.27515	-699.66837	1
18381	H	73.50900	67.85780	70.39290	1958.03657	-650.46098	-2373.29850	1
18382	C	72.45400	66.06380	69.71790	461.99671	-457.81713	625.57484	1
18383	H	71.39000	65.90280	69.80790	2184.99381	1250.03941	-1887.47170	1
18384	C	72.66000	66.54280	68.23090	-177.42518	-608.43741	647.48733	1
18385	H	72.52100	65.61380	67.63890	-2069.03808	-952.19184	2169.35455	1
18386	H	73.68700	66.96680	68.24990	1998.35153	413.78573	-2394.70920	1
18387	C	71.72500	67.59780	67.72090	121.19142	-722.64103	529.47482	1
18388	C	71.74100	68.95780	67.92090	886.99513	-24.53604	170.31397	1
18389	H	72.58600	69.44280	68.38690	2022.75025	2063.16446	1237.10149	1
18390	N	70.70500	69.55680	67.31790	719.53588	426.09331	-84.48278	1
18391	H	70.35400	70.42880	67.57890	-1981.56115	-1646.90024	1806.18484	1
18392	C	69.94900	68.58180	66.73890	235.53366	-58.03303	-880.19701	1
18393	C	70.55000	67.30580	66.99790	-198.50399	178.07977	870.36562	1
18394	C	69.90800	66.17080	66.61990	-101.37054	-655.12410	616.99733	1
18395	H	70.39900	65.26380	66.93990	2041.65126	-2011.44243	1272.68526	1
18396	C	68.76100	66.27480	65.85090	-384.86010	-612.26075	550.34397	1
18397	H	68.26800	65.37480	65.51390	1723.02216	-2323.15690	1212.00617	1
18398	C	68.83000	68.69180	65.97190	722.53225	-298.96665	-456.21608	1
18399	H	68.33200	69.62280	65.74690	-2328.63348	1344.50900	1646.60985	1
18400	C	68.20200	67.49880	65.54590	-252.48188	-636.25672	596.14240	1
18401	H	67.29300	67.52580	64.96390	-1273.79055	2123.00722	-1956.12699	1
18402	C	73.19300	64.74780	69.88990	-489.30772	-406.56480	-661.24204	1
18403	O	72.67800	63.69780	69.58190	-233.60774	521.33148	-558.55381	1
18404	N	74.40600	64.73880	70.51790	300.33587	447.64090	-656.17288	1
18405	H	74.96100	65.55880	70.63090	534.99465	-2258.70916	-2123.53367	1

18406	C	74.94700	63.53980	71.09390	205.50117	672.67114	576.15143	1
18407	H	75.05800	62.74180	70.37490	1187.37735	-1522.03301	2471.27108	1
18408	C	76.44200	63.74480	71.56290	-170.28977	-873.13127	-192.98627	1
18409	H	76.37000	64.76080	72.00790	-1636.27212	2148.64190	1618.30073	1
18410	C	76.85300	62.73380	72.62490	-614.08486	-644.14417	194.61024	1
18411	H	77.96400	62.74180	72.63890	2690.82302	-1616.65571	-45.44834	1
18412	H	76.59800	61.68380	72.36590	1174.25606	2734.89555	1016.14241	1
18413	H	76.41300	62.97180	73.61690	-1483.48706	1608.29212	-2274.23664	1
18414	C	77.39100	63.63880	70.36590	2.02453	270.51159	864.67500	1
18415	H	76.79400	64.06380	69.53090	456.22267	-2929.35831	-1043.04055	1
18416	H	77.58600	62.57880	70.09590	-1522.33790	1473.88629	2324.72180	1
18417	C	78.55700	64.57680	70.48490	833.31547	-350.08014	-28.82711	1
18418	H	79.21500	64.35480	71.35190	-442.63608	-2981.14660	-897.69110	1
18419	H	78.21700	65.63480	70.49190	2169.61326	-1944.70136	1159.98261	1
18420	H	79.23400	64.48180	69.60890	-338.07991	2201.89939	2220.20129	1
18421	C	74.09700	62.96180	72.24090	643.98279	642.01619	39.32556	1
18422	O	73.82900	61.77480	72.30290	-143.84965	181.02449	-764.32075	1
18423	N	73.51000	63.84680	73.06590	350.91058	-533.48797	538.90566	1
18424	H	73.79600	64.80180	73.04790	598.83253	2819.82152	1259.03548	1
18425	C	72.53000	63.56280	74.09690	-372.74664	822.39106	150.88159	1
18426	H	72.92800	62.80480	74.75590	-2235.70465	-2201.25487	-260.62730	1
18427	C	72.31300	64.68880	75.09590	-718.61129	536.43211	-198.55836	1
18428	H	71.43000	64.41080	75.70990	733.09784	-1444.89752	2688.71754	1
18429	H	71.98400	65.56780	74.50090	982.98567	-2621.13423	1421.93926	1
18430	C	73.46500	64.97780	76.06990	310.77232	812.52691	-280.37822	1
18431	H	74.37300	65.14780	75.45290	-1412.77966	-146.27732	2803.47063	1
18432	C	73.19900	66.08480	77.11390	-690.87982	-495.35593	-342.32155	1
18433	H	74.07700	66.31080	77.75590	170.57592	-2542.35200	-1848.37104	1
18434	H	72.87400	67.00380	76.57990	-2614.76317	-1499.93874	906.71710	1
18435	H	72.38300	65.70780	77.76590	1611.42585	-2453.78058	-1127.49665	1
18436	C	73.79100	63.67480	76.88490	647.00214	175.89547	-620.46536	1
18437	H	74.66400	63.90280	77.53190	1925.89868	-2009.14973	1452.19707	1
18438	H	72.87900	63.35080	77.43090	-542.02898	2886.01368	1129.03557	1
18439	H	74.16100	62.87780	76.20390	839.19187	-2802.67704	-1155.33045	1
18440	C	71.22700	62.91880	73.51690	182.50807	-386.97716	-808.81667	1
18441	O	70.71800	61.98380	74.14690	572.32794	-40.76907	530.69074	1
18442	N	70.70300	63.40180	72.34790	122.58244	635.50850	538.66868	1
18443	H	71.10300	64.26580	72.05290	181.07960	101.74061	-3144.70988	1
18444	C	69.73400	62.58180	71.58590	648.34332	-575.12251	-268.42957	1
18445	H	68.87900	62.38480	72.21590	1292.68007	-2809.95447	-553.13786	1
18446	C	69.26800	63.38280	70.33890	-415.98133	458.27721	670.51897	1
18447	H	68.28800	62.96680	70.02090	2100.01921	-2274.49337	515.39410	1
18448	H	69.96100	63.29480	69.47590	-2169.74637	29.44790	-2289.89062	1
18449	H	69.03900	64.45180	70.53990	1001.19022	952.27062	-2830.56755	1
18450	C	70.21000	61.21680	71.12590	485.52598	601.92988	-488.54126	1
18451	O	69.50700	60.27980	71.39790	-538.20560	-399.96629	-427.50780	1
18452	N	71.39700	61.10080	70.48690	-231.10616	-772.99183	234.04033	1
18453	H	71.96500	61.91780	70.43290	2161.00328	696.11652	-2180.21176	1
18454	C	71.91600	59.80780	70.10590	-131.76248	580.05229	688.18706	1
18455	H	71.21400	59.26580	69.48990	-696.12998	-1785.35097	-2501.25870	1
18456	C	73.26300	60.01580	69.27590	218.20334	189.20292	-872.24376	1
18457	H	73.86400	59.08180	69.30890	-1625.27937	-2118.81823	-1671.43583	1
18458	H	73.85400	60.81780	69.76790	1907.54809	-1736.68707	-1797.76264	1
18459	C	73.07700	60.37180	67.86290	-628.60216	-258.40322	604.55473	1
18460	C	71.99300	61.12680	67.38390	-160.61150	-687.47958	-579.58518	1
18461	H	71.19200	61.52980	67.98490	-1058.16331	-1862.78307	2296.25158	1
18462	C	71.80300	61.37380	66.02090	-115.57533	-454.91596	-786.29457	1
18463	H	70.93800	61.91180	65.66190	-2704.05929	573.98030	-1523.91824	1
18464	C	72.70500	60.88880	65.10690	551.44707	-580.45346	411.01262	1
18465	H	72.48900	61.01780	64.05590	-1401.12217	1805.65015	-2179.77737	1
18466	C	73.97600	59.87980	66.90290	-675.00621	-286.58379	-555.12678	1
18467	H	74.74700	59.17780	67.18090	-526.20559	-1943.58855	-2422.71101	1

18468	C	73.75000	60.08480	65.52790	338.21879	-758.88555	348.12355	1
18469	H	74.35200	59.44180	64.90390	1609.41313	-2422.45396	1168.43439	1
18470	C	72.12500	58.72180	71.18490	-309.08295	859.87109	-88.78740	1
18471	O	71.74000	57.56280	70.96290	-450.74789	521.30109	-405.22988	1
18472	N	72.61100	59.07480	72.37390	619.37944	-38.21568	558.54478	1
18473	H	72.89000	60.02280	72.50490	-2039.37977	-299.12877	-2388.61338	1
18474	C	72.68100	58.14080	73.49390	708.97810	-430.88606	357.45936	1
18475	H	73.09600	57.19180	73.18990	-1638.31849	657.59144	-2616.76016	1
18476	C	73.64600	58.74880	74.51190	255.77426	-15.45086	865.29395	1
18477	H	74.62300	58.87080	73.99490	-2072.23954	-1940.68312	-1366.77572	1
18478	C	73.16700	60.07580	75.15390	435.61198	-540.05119	-593.80901	1
18479	H	72.36900	59.90880	75.90790	-1739.45405	-1836.82695	-1879.90486	1
18480	H	72.74200	60.71680	74.35090	2071.55604	1148.21861	-2075.11122	1
18481	H	73.98700	60.55380	75.73090	56.95115	-2000.80573	-2433.02826	1
18482	C	74.00800	57.66680	75.58290	-411.79847	567.39218	-597.19857	1
18483	H	74.22300	56.72280	75.03790	-1798.06929	1570.17343	-2064.29712	1
18484	H	73.10600	57.48480	76.20490	-1529.55720	1841.99986	-2054.55968	1
18485	C	75.17000	58.18180	76.40990	761.30637	232.02322	-448.62555	1
18486	H	76.07100	58.47080	75.82890	2382.84635	-200.87051	2030.30033	1
18487	H	74.83000	59.07680	76.97390	-1841.75455	2220.25220	-1273.48893	1
18488	H	75.49500	57.43180	77.16290	2555.24984	732.06459	1669.21487	1
18489	C	71.27200	57.86480	74.12990	-478.07483	548.98183	-563.71422	1
18490	O	71.00500	56.75880	74.66690	-273.65406	341.08985	652.05306	1
18491	N	70.33700	58.79980	73.99790	641.71210	537.06900	89.08113	1
18492	H	70.55600	59.61580	73.46790	776.24324	-2095.15863	-2217.82991	1
18493	C	68.93700	58.59380	74.35490	588.89804	570.71732	-402.55005	1
18494	H	68.88800	58.26980	75.38390	203.23721	2079.24169	-2361.03565	1
18495	C	68.03700	59.88580	74.21290	-222.12311	-814.89646	334.76139	1
18496	H	66.94500	59.71580	74.32590	-663.69994	-2533.94876	1735.14646	1
18497	H	68.26200	60.32580	73.21790	-1038.34843	-2153.58984	-2051.15742	1
18498	O	68.38100	60.83480	75.21390	-258.51343	747.89098	44.86106	1
18499	H	69.14200	61.29780	74.85590	798.65678	3023.22937	-361.03401	1
18500	C	68.26600	57.55280	73.49690	-34.64225	-623.44795	-669.78394	1
18501	O	67.62400	56.66180	74.00890	-151.56733	766.53488	-141.11515	1
18502	N	68.41900	57.71580	72.14690	-292.81708	-25.95530	-800.49424	1
18503	H	68.91000	58.48880	71.75390	1140.43721	-2419.80352	1640.31736	1
18504	C	68.00800	56.73880	71.10290	154.59126	-400.43724	-809.47162	1
18505	H	66.93000	56.69380	71.05990	-2634.46903	1719.21771	-207.97587	1
18506	C	68.42200	57.32980	69.74790	-565.77673	-684.20661	-217.27932	1
18507	H	68.40100	56.60980	68.90190	699.79321	2174.96144	-2173.20039	1
18508	H	69.46400	57.71380	69.75790	-2182.27260	983.25788	2042.04955	1
18509	C	67.53700	58.48480	69.21390	-509.04354	81.57893	749.55058	1
18510	H	67.35400	59.16180	70.07590	1497.21856	-2759.38451	62.57491	1
18511	C	68.30300	59.44180	68.21290	-895.61475	92.00868	-187.77756	1
18512	H	67.50000	60.12880	67.86990	-473.68580	2720.45063	-1524.11903	1
18513	H	68.58400	58.83980	67.32290	3132.79836	-194.67120	-69.94405	1
18514	H	69.13000	60.00380	68.69590	-2156.15281	630.44582	-2216.70720	1
18515	C	66.27600	58.00980	68.50990	-861.56866	272.50213	-172.18448	1
18516	H	66.46300	57.26280	67.70990	-2988.03930	-565.76506	818.08468	1
18517	H	65.65900	58.82780	68.07890	796.64720	-1276.57705	-2765.46102	1
18518	H	65.59800	57.65380	69.31590	1204.62388	2489.99411	-1507.39327	1
18519	C	68.65300	55.42080	71.41890	386.38309	-377.78527	-738.50772	1
18520	O	67.96100	54.39280	71.36790	450.99383	548.47046	-353.16586	1
18521	N	69.99700	55.34680	71.65690	346.71945	566.61872	512.77007	1
18522	H	70.50300	56.19780	71.54090	-1984.42164	-2337.97912	696.34487	1
18523	C	70.66600	54.11680	71.95390	431.14343	177.04636	-791.38270	1
18524	H	70.37400	53.43580	71.16790	858.97596	2362.43786	-1903.96474	1
18525	C	72.21100	54.42880	71.99990	386.65291	680.85764	-478.46943	1
18526	H	72.41300	55.16980	72.80390	347.39631	-483.57060	-3097.72771	1
18527	H	72.52700	54.79380	70.99990	-2879.08386	-486.36130	-1191.42693	1
18528	C	72.99600	53.16680	72.28990	-162.36433	901.00101	23.58668	1
18529	O	73.09800	52.74080	73.45190	-323.81024	-33.74805	710.50385	1

18530	O	73.42800	52.48280	71.30890	17.19265	-568.35196	532.86874	1
18531	C	70.16900	53.41580	73.19190	742.77876	14.57817	513.42717	1
18532	O	70.09800	52.19680	73.28190	-326.03462	-298.40892	645.09130	1
18533	N	69.80300	54.19280	74.24790	-538.52781	-441.30656	470.39086	1
18534	H	69.85400	55.18780	74.23790	-102.52100	2182.23573	2257.74734	1
18535	C	69.17300	53.66180	75.45390	485.67326	636.36060	426.27044	1
18536	H	69.73600	52.83980	75.86990	-2532.61294	-1778.37191	-585.60540	1
18537	C	69.09800	54.71380	76.61790	-511.92869	605.20728	-465.13399	1
18538	H	69.19700	55.75280	76.23590	-2709.95308	521.74877	-1526.03547	1
18539	H	68.12200	54.60580	77.13890	1666.07427	1345.95866	-2311.39773	1
18540	C	70.26100	54.47080	77.66490	625.76425	-234.80350	607.57599	1
18541	H	70.11000	55.20080	78.48890	-1949.05624	1914.79601	1555.66742	1
18542	H	70.18700	53.40880	77.98390	-1772.06706	-2204.40894	1370.24183	1
18543	C	71.68300	54.73580	77.10590	319.95907	729.92053	433.92246	1
18544	H	72.30700	54.92680	78.00490	1722.79218	1880.79349	1830.99462	1
18545	H	71.52300	55.67780	76.53890	1227.31225	-704.41588	2798.91778	1
18546	N	72.29500	53.58780	76.26790	-649.48269	-479.90054	240.73562	1
18547	H	72.33300	53.71780	75.27790	-2300.91377	1213.15076	-1786.09770	1
18548	C	72.51900	52.36480	76.67390	658.79524	239.81014	569.80737	1
18549	N	72.45100	51.90980	77.92390	520.40839	588.43220	296.66953	1
18550	H	72.43900	52.51280	78.72190	-1789.89220	2470.46668	767.75309	1
18551	H	72.53400	50.92280	78.06190	616.86770	37.44322	3073.25972	1
18552	N	72.86300	51.48580	75.77490	-502.92684	367.77036	562.87129	1
18553	H	72.93300	51.87680	74.85690	425.10840	-2756.69158	-1460.24775	1
18554	H	73.24600	50.61580	76.08390	2885.34443	27.61262	-1258.51722	1
18555	C	67.78400	53.02580	75.23090	415.89836	-700.06882	394.58431	1
18556	O	67.57600	51.90080	75.66890	736.34238	-6.12107	-286.14530	1
18557	N	66.94800	53.66880	74.42790	268.38440	-524.78883	-609.45730	1
18558	H	67.26800	54.51680	74.01190	-118.71029	572.50983	3083.56521	1
18559	C	65.70600	53.17180	73.94890	798.57576	-340.13837	-273.85681	1
18560	H	65.24000	52.91680	74.88890	-777.19848	2936.86036	818.69882	1
18561	C	65.01600	54.39180	73.21590	-518.41563	-571.16632	-495.91629	1
18562	H	65.75700	55.08780	72.76690	581.60943	-1169.21922	-2868.10925	1
18563	H	64.48300	54.96280	74.00590	-1922.49656	-1948.20523	-1561.50398	1
18564	C	63.96000	54.00580	72.20890	585.02317	-648.56867	-252.85794	1
18565	C	62.81500	53.27380	72.56890	77.90767	-899.83397	97.58132	1
18566	H	62.64500	52.99980	73.59990	-1371.72827	-1994.38578	2002.98816	1
18567	C	61.86200	53.00680	71.55590	-404.11114	297.81288	757.07708	1
18568	H	60.98800	52.51080	71.95090	-297.05407	-3087.18672	-525.41814	1
18569	C	62.07000	53.38380	70.23690	-278.41132	82.26813	858.85904	1
18570	O	61.17200	53.02380	69.23190	490.50998	-71.58155	-617.49853	1
18571	H	61.57000	53.06280	68.35890	846.26218	-2243.81213	2022.91976	1
18572	C	64.22300	54.25280	70.86090	645.44227	-302.93341	-568.85148	1
18573	H	65.19200	54.70680	70.71490	1344.70304	2776.59144	-628.17127	1
18574	C	63.28000	53.95980	69.85490	-282.88346	538.36387	676.59364	1
18575	H	63.50300	54.29180	68.85190	1269.87847	-1225.09801	-2607.79956	1
18576	C	65.83400	51.91380	73.11590	570.09357	144.67543	-702.98137	1
18577	O	65.14200	50.94680	73.39390	548.59067	522.52322	-227.76100	1
18578	N	66.72600	51.85580	72.13990	417.84106	577.38608	-461.39207	1
18579	H	67.18100	52.70080	71.86790	1198.78391	-1027.58146	2709.18606	1
18580	C	67.06100	50.73780	71.34590	785.97495	427.23626	-174.59115	1
18581	H	66.18800	50.37980	70.82090	-2266.40685	-448.14061	-2149.12831	1
18582	C	68.18900	50.95680	70.27890	608.44143	649.53353	186.62614	1
18583	H	68.49600	49.97580	69.85790	1443.40853	1578.25930	2296.81528	1
18584	H	69.07300	51.42780	70.75990	-526.79684	3104.55861	89.92415	1
18585	C	67.74500	51.90280	69.18490	-396.14694	-811.61088	104.76430	1
18586	H	67.22000	52.78380	69.61290	-1781.41989	1365.21645	2202.18508	1
18587	C	68.90400	52.46280	68.26490	504.95426	644.93313	-410.88927	1
18588	H	69.21300	51.65180	67.57190	-820.20035	2424.67766	1828.26751	1
18589	H	69.81900	52.69180	68.85290	2302.05945	-1571.81411	-1455.44090	1
18590	H	68.67000	53.44480	67.79890	-518.40019	2264.39172	2119.08616	1
18591	C	66.79800	51.18780	68.16290	108.46188	249.95829	-880.23372	1

18592	H	67.28100	50.33580	67.63890	-1966.22193	-2095.88910	-1290.70459	1
18593	H	66.50300	51.92080	67.38290	-1871.88238	482.04052	-2496.44150	1
18594	H	65.90400	50.68680	68.59190	-1254.86745	1248.48020	-2614.70789	1
18595	C	67.57100	49.59980	72.22890	-514.05196	-752.71970	2.31411	1
18596	O	67.16500	48.45580	72.05690	166.26395	-392.52137	-672.66968	1
18597	N	68.39700	49.92080	73.24090	640.73237	411.91259	-370.88811	1
18598	H	68.72700	50.85680	73.34190	1475.57266	-44.98565	2766.14541	1
18599	C	69.08400	48.91580	74.02090	-274.21480	-764.85011	400.53276	1
18600	H	69.46000	48.13080	73.38090	1794.28436	437.75446	2533.73362	1
18601	C	70.26000	49.50580	74.88190	465.07817	-768.30340	124.75253	1
18602	H	69.96200	50.21280	75.68490	2051.24820	1368.97422	1941.07548	1
18603	H	70.89000	50.10780	74.19090	-2150.13984	1285.24650	-1920.06528	1
18604	H	70.83600	48.64580	75.28590	1456.55190	2742.13972	-522.23648	1
18605	C	68.12500	48.26380	75.04290	753.21694	507.98283	-70.86154	1
18606	O	68.45400	47.23480	75.64590	293.57383	-701.59669	191.54468	1
18607	N	66.89700	48.82080	75.37790	94.64898	401.19529	726.83615	1
18608	H	66.81100	49.74780	75.01990	-1514.42229	30.16907	-2769.26699	1
18609	C	65.93700	48.35880	76.39690	-627.14102	502.16741	-446.60511	1
18610	H	66.38800	47.45080	76.76890	-1513.50443	-1839.57855	2045.13431	1
18611	C	65.75500	49.42180	77.42890	-344.14157	-695.69183	469.41871	1
18612	H	65.76800	50.45180	77.01090	-1465.47371	1154.16753	2525.96007	1
18613	C	64.37800	49.29580	78.19190	-251.04184	762.97568	-442.89049	1
18614	H	64.35700	50.15180	78.89890	1470.24948	2763.43617	296.69239	1
18615	H	63.54600	49.42280	77.46690	1385.14424	-2562.76816	-1193.71654	1
18616	H	64.34900	48.32980	78.73890	2103.66702	-2040.30616	1130.96503	1
18617	C	66.94300	49.36980	78.37390	599.71160	-537.10553	414.22148	1
18618	H	67.87300	49.13980	77.81290	1555.79173	2342.06569	-1420.94173	1
18619	H	66.93800	48.50780	79.07490	1412.68826	694.68681	-2733.56706	1
18620	C	67.20200	50.71380	79.14890	-597.67340	367.43867	575.03284	1
18621	H	68.24400	50.65780	79.52990	-1749.71494	853.07562	-2483.22628	1
18622	H	66.39500	50.70680	79.91290	1659.23905	-1989.56077	1773.96148	1
18623	H	67.23000	51.56080	78.43090	2690.47753	-1447.46889	731.92960	1
18624	C	64.68400	47.94480	75.66090	9.81646	-907.09297	68.63304	1
18625	O	64.12400	46.89680	75.93190	-371.73781	-538.55501	-453.22230	1
18626	N	64.12500	48.67480	74.69190	85.34776	128.86434	820.13647	1
18627	H	64.58500	49.51780	74.42290	1218.80747	2315.48748	-1756.27576	1
18628	C	62.87300	48.23880	73.93890	697.46491	576.46033	-109.99669	1
18629	H	62.32800	47.76380	74.74190	1623.45023	-734.73399	2581.04448	1
18630	C	62.19700	49.49980	73.38790	-829.28761	66.25522	372.49021	1
18631	H	62.95800	50.04680	72.79190	26.82580	2228.65577	2213.69601	1
18632	C	61.03600	49.08980	72.50190	-502.56488	-241.24068	-732.22460	1
18633	H	61.35600	48.76480	71.48890	-2530.07179	1856.54130	-290.26858	1
18634	H	60.40500	48.31080	72.98290	-2246.08123	-1793.82772	1273.75598	1
18635	H	60.31000	49.90180	72.28490	2309.59696	-1445.39379	-1573.83196	1
18636	C	61.82500	50.37880	74.60090	-594.71770	-660.66756	200.20246	1
18637	H	61.06500	51.09380	74.21890	1952.00322	-430.70463	2418.44399	1
18638	H	62.72800	50.86480	75.02890	1186.82737	-2492.58644	1495.72972	1
18639	H	61.21500	49.71080	75.24590	-2262.35212	2111.20102	-592.28096	1
18640	C	63.20100	47.23580	72.87290	414.41401	309.52256	739.92325	1
18641	O	62.38700	46.38080	72.49590	-496.09719	597.62076	-172.21620	1
18642	N	64.47400	47.13380	72.43890	-197.18453	675.10461	-482.28510	1
18643	H	65.23300	47.65180	72.82590	467.54532	-1157.14390	-2896.88759	1
18644	C	64.77200	46.31680	71.22390	-613.62625	217.85179	-653.63917	1
18645	H	64.08400	45.51580	70.99690	-2483.82574	1234.52887	-1504.29886	1
18646	C	64.96500	47.11680	69.95990	-651.03536	643.52027	47.00296	1
18647	H	65.19000	46.42980	69.11690	785.79507	-2383.23414	-1901.89063	1
18648	H	65.80000	47.84180	70.06290	-2000.84926	-1790.43591	-1651.63719	1
18649	N	62.80000	47.30780	68.67190	243.65230	-156.86633	-800.63788	1
18650	H	62.85700	46.39880	68.25890	-1776.63609	2279.77499	1245.90447	1
18651	C	63.74700	47.92880	69.43990	-682.11039	608.36415	69.41078	1
18652	C	61.90700	48.23880	68.29190	393.99747	-518.63584	622.88364	1
18653	H	61.02100	47.93880	67.73390	-690.00605	490.98112	-3040.89364	1

18654	N	62.23400	49.43580	68.75890	409.66570	-664.77070	-315.91329	1
18655	C	63.35500	49.21480	69.53490	-534.13582	701.63540	-261.19813	1
18656	H	63.91700	50.02480	69.98390	-1324.76358	1004.83821	2665.20732	1
18657	C	66.09300	45.60480	71.41390	744.75796	-199.38263	-491.48612	1
18658	O	67.00800	45.60980	70.60490	546.19526	-562.54509	16.14102	1
18659	N	66.26200	44.96680	72.58690	-405.10445	-338.90929	647.45977	1
18660	H	65.54000	44.88280	73.26990	-1653.59558	1010.28629	2469.92102	1
18661	C	67.55100	44.53680	72.97490	-447.40240	539.27468	-600.41090	1
18662	H	68.36100	45.24380	72.87890	2745.12062	-1447.39523	480.12539	1
18663	C	67.54100	44.11380	74.52790	681.89240	132.54495	-600.55265	1
18664	H	67.20500	45.01580	75.08290	1849.54689	-1065.76317	-2320.26434	1
18665	H	66.79700	43.31280	74.72290	2407.82067	597.48768	-1944.91855	1
18666	H	68.52800	43.74880	74.88590	-1385.48577	-909.36494	-2687.57381	1
18667	C	68.08100	43.25480	72.25790	-401.21713	103.56178	801.29027	1
18668	O	69.24900	42.90780	72.37290	633.50709	-460.24013	-75.39025	1
18669	N	67.23100	42.50780	71.53190	1.17026	601.62127	582.50236	1
18670	H	66.32800	42.91980	71.44090	2909.38184	-472.00592	1078.07351	1
18671	C	67.54800	41.26580	70.93090	-338.44930	262.00579	794.11714	1
18672	H	68.32300	40.86780	71.56890	-2013.24624	1755.77455	-1682.79321	1
18673	C	66.43900	40.21380	70.95290	655.32282	516.87371	-379.97912	1
18674	H	66.01200	40.24680	71.97790	-1855.66420	1358.63043	-2164.37354	1
18675	O	66.96200	38.92080	70.87490	548.00677	85.71075	545.65181	1
18676	H	67.72100	38.72880	71.43090	-1579.23912	-1207.89929	2423.94821	1
18677	C	65.34400	40.37980	69.88590	746.57363	-32.05747	-530.74692	1
18678	H	64.40400	39.92280	70.26290	1712.84568	2073.29222	-1646.69109	1
18679	H	65.72800	39.97280	68.92590	-222.11109	-3063.65086	650.10859	1
18680	H	65.10900	41.45680	69.74290	1930.58464	1989.37299	-1500.71192	1
18681	C	68.04700	41.39180	69.50990	-682.22827	-594.28687	99.84075	1
18682	O	68.49600	40.41480	68.88190	289.42357	-339.70757	-661.64733	1
18683	N	67.97800	42.58880	68.90590	-102.57670	-222.98859	793.97315	1
18684	H	67.40400	43.31080	69.28390	1227.16811	1521.91003	2452.90968	1
18685	C	68.25700	42.84080	67.50690	-686.22325	477.14325	365.48814	1
18686	H	69.24300	42.47480	67.26390	1559.56426	-1926.96112	-1942.17554	1
18687	C	67.21300	42.10680	66.52190	752.89058	501.05338	96.04710	1
18688	H	67.50300	42.52180	65.53290	-2127.67054	372.28641	2279.83436	1
18689	H	67.39400	41.01280	66.44490	1700.38691	-128.77776	-2654.38843	1
18690	C	65.73100	42.38580	66.82990	-611.01660	-666.37811	-126.74558	1
18691	O	65.28300	43.17080	67.69590	696.32674	205.17871	292.00715	1
18692	N	64.85100	41.84280	65.95390	-475.25658	149.03727	673.32057	1
18693	H	65.23300	41.18080	65.30890	1893.29674	-1549.48730	-1982.33454	1
18694	H	63.87600	42.02380	66.07990	-980.91644	-1774.67666	-2416.00243	1
18695	C	68.28700	44.37280	67.28890	599.02635	256.65407	622.99842	1
18696	O	67.32600	45.05080	66.84790	-287.83890	76.28086	-745.68891	1
18697	N	69.42800	45.01480	67.51390	-514.37875	444.22513	497.16592	1
18698	H	70.29900	44.54280	67.62790	3068.96976	101.45686	652.67547	1
18699	C	69.59800	46.39680	67.30590	-255.33356	-745.87011	-464.56225	1
18700	H	69.34300	46.64780	66.28690	2375.14555	533.17972	1976.64375	1
18701	C	68.81800	47.28080	68.35890	-755.86137	373.39015	-373.47589	1
18702	H	67.74200	47.08880	68.15690	-1139.96449	1167.34942	2682.60577	1
18703	H	68.95200	48.36380	68.15390	2616.99703	1603.60439	672.81059	1
18704	O	69.09100	46.87480	69.72790	78.78937	581.43306	-544.07698	1
18705	H	68.34100	46.30280	69.90690	-998.35527	-1705.25099	2435.37657	1
18706	C	71.05900	46.81080	67.33990	-603.39884	-241.06350	-654.52919	1
18707	O	71.31200	47.99080	67.04890	-124.93277	-411.25865	648.15512	1
18708	N	72.08300	46.00080	67.59690	-240.12044	192.00784	-801.75217	1
18709	H	71.88000	45.04780	67.80590	-1945.99244	372.17189	2435.09883	1
18710	C	73.48600	46.44780	67.59790	-122.01471	813.53038	392.76429	1
18711	H	73.52400	47.26880	68.29890	-98.77291	560.75476	-3108.03626	1
18712	C	74.37500	45.29980	68.15590	344.83797	-689.17323	462.82236	1
18713	H	74.02300	44.33880	67.72490	2183.16678	1739.96521	-1464.64439	1
18714	H	74.17000	45.24680	69.24690	-466.31978	-670.60991	3024.09815	1
18715	C	75.92100	45.26480	67.94090	-692.79726	-182.89493	-581.70156	1

18716	H	76.30900	44.56380	68.70990	896.48900	2488.63148	1694.43600	1
18717	H	76.31100	46.28280	68.15790	2718.26765	922.81864	1268.03305	1
18718	C	76.47700	44.90180	66.52690	-699.18889	68.25363	573.26474	1
18719	O	77.48800	45.40880	66.06490	-588.36333	-396.41601	-362.25008	1
18720	N	75.84000	43.91380	65.89590	672.99079	-408.03938	-300.08580	1
18721	H	75.05300	43.46880	66.32490	1596.68199	2246.03387	1507.48763	1
18722	H	76.20200	43.57880	65.02690	1903.00392	-174.10758	-2509.86880	1
18723	C	74.06300	47.03080	66.32090	516.96651	-569.60057	-490.01852	1
18724	O	74.69700	48.06380	66.27790	239.25143	-340.95713	653.09351	1
18725	N	73.75600	46.55480	65.10790	-762.97200	150.92084	-356.39819	1
18726	H	73.25200	45.70380	64.98290	-489.56238	494.52513	3056.80764	1
18727	C	74.08400	47.23980	63.86290	-167.33684	-743.48236	479.22659	1
18728	H	75.12800	47.51180	63.92690	-1070.95554	-2925.27309	393.28814	1
18729	C	74.06800	46.20880	62.72890	-737.26254	-462.33586	262.44693	1
18730	H	73.13500	45.60880	62.79690	-2014.95128	-1591.83512	1804.63613	1
18731	H	74.85700	45.42680	62.72790	-422.45800	-521.30722	3059.46218	1
18732	C	74.06200	46.76480	61.27790	-783.39815	-428.49391	180.08899	1
18733	H	73.11700	47.30680	61.06290	1410.75592	2745.79577	-639.75603	1
18734	H	74.90400	47.46680	61.10090	-1653.65977	876.11261	-2549.17887	1
18735	C	74.25100	45.71380	60.15490	781.08808	-423.87682	-168.94738	1
18736	H	75.13100	45.04580	60.27290	-2347.46345	1042.99132	1815.65100	1
18737	H	73.41700	44.99080	60.02890	-282.91913	2911.76533	1166.15965	1
18738	N	74.37500	46.45680	58.85890	-549.00922	-475.50562	416.01853	1
18739	H	73.83000	47.27780	58.68890	432.48442	2685.84398	1580.50816	1
18740	C	74.66200	45.80580	57.73890	405.23041	612.07520	-559.53666	1
18741	N	75.21300	44.60980	57.67290	336.16035	-474.57223	586.23416	1
18742	H	75.14000	43.94180	58.41390	1059.80701	1711.21555	-2435.92192	1
18743	H	75.29600	44.15880	56.78390	-2748.92980	601.32314	-1439.84142	1
18744	N	74.43800	46.41980	56.59390	-660.42550	451.27371	-316.01628	1
18745	H	74.35200	47.41580	56.55990	-373.93637	-824.26229	-3024.33804	1
18746	H	74.81700	46.00380	55.76690	-2097.32999	-2341.91090	-25.13575	1
18747	C	73.45900	48.66280	63.65890	361.32950	-642.02644	512.49571	1
18748	O	74.22500	49.62080	63.25590	585.44956	-298.37823	-436.45338	1
18749	N	72.19600	48.93680	63.88290	-575.89993	564.60104	-288.63468	1
18750	C	71.15200	47.91380	63.64390	548.94581	321.19184	639.73344	1
18751	H	71.01200	47.26380	64.53490	-413.84573	-2501.49060	1843.33151	1
18752	H	71.30300	47.24080	62.77290	2308.10647	-2078.90596	425.61972	1
18753	C	71.58800	50.28980	63.86990	217.23388	-565.55243	662.80544	1
18754	H	71.84300	50.86080	62.98890	2437.44045	-1871.98459	617.37501	1
18755	C	70.07700	50.06480	63.96190	-445.95951	-565.58922	546.76390	1
18756	H	69.46100	50.84980	63.47390	-2711.42939	798.66443	1387.32466	1
18757	H	69.73700	49.93580	65.01190	-1622.03770	-405.29586	-2678.51147	1
18758	C	69.87000	48.68880	63.34890	-613.21563	-673.42588	10.38788	1
18759	H	69.82900	48.81780	62.24590	1995.17600	2198.29174	-1055.23047	1
18760	H	68.94600	48.19980	63.72390	-1186.91566	-2500.82987	1478.01520	1
18761	C	72.06400	51.10980	65.08690	412.53173	-609.17385	-537.78032	1
18762	O	72.36800	52.25980	64.91690	-317.02332	-681.59418	221.31612	1
18763	N	72.14200	50.58980	66.34490	-294.89778	-590.75016	511.50242	1
18764	H	71.85400	49.64680	66.48990	1358.25410	2598.70764	-1158.03879	1
18765	C	72.81900	51.31980	67.35990	351.91091	633.91148	544.68531	1
18766	H	72.31400	52.25080	67.56990	2497.19955	1403.22538	1285.89274	1
18767	C	72.89600	50.49980	68.67390	-262.44793	-477.52780	-740.98348	1
18768	H	73.60400	51.00680	69.36290	-2488.28117	1677.30182	954.74163	1
18769	H	73.30500	49.50780	68.38590	-1682.51852	2352.04220	1243.44402	1
18770	C	71.62900	50.31280	69.43890	-168.37168	-586.08073	-686.27707	1
18771	H	70.76200	49.92680	68.86190	-559.65797	2994.19767	-818.97110	1
18772	H	71.29200	51.26680	69.89990	476.39114	-1471.94550	-2746.97423	1
18773	C	71.72500	49.24180	70.58390	442.49825	-770.19268	-191.37206	1
18774	H	70.75000	48.93880	71.02290	1482.53120	-1567.26582	2273.32451	1
18775	H	72.23500	48.32680	70.21490	-1812.15875	1957.55504	1665.61453	1
18776	N	72.53600	49.96180	71.58390	-297.14036	790.41810	-101.18643	1
18777	H	72.73100	50.93480	71.46790	-1198.30436	2652.10244	-1219.21024	1

18778	C	73.24800	49.36280	72.44790	806.90231	-413.38071	7.94799	1
18779	N	73.02000	48.12780	72.87290	-790.92055	-156.60550	246.63520	1
18780	H	72.19900	47.67380	72.52690	-2517.18007	-423.28480	1831.04580	1
18781	H	73.73800	47.68480	73.40890	1841.69352	1765.33507	1828.36066	1
18782	N	74.05500	50.13280	73.16390	-15.04288	845.36897	48.60781	1
18783	H	74.03900	51.12880	73.07790	-994.43650	-2633.28870	1390.20117	1
18784	H	74.58500	49.72780	73.90890	-1580.20108	1004.53104	2519.55615	1
18785	C	74.26400	51.75680	67.03390	485.27188	-82.81479	-774.61144	1
18786	O	74.70400	52.87880	67.34290	-103.24079	-776.13933	42.07046	1
18787	N	74.99000	50.84080	66.43790	385.87259	-410.16592	-633.22636	1
18788	H	74.53700	50.00780	66.12990	-2440.43973	1269.25506	-1552.81444	1
18789	C	76.32900	51.05180	65.91890	750.00473	431.44780	270.18258	1
18790	H	76.92000	51.30980	66.78590	2377.60066	981.56217	1795.48304	1
18791	C	76.94900	49.70280	65.47390	-132.79331	456.55058	-795.66158	1
18792	H	76.30500	49.24080	64.69590	-1467.85942	-770.05688	2662.50296	1
18793	H	76.96900	49.10280	66.40990	2345.99452	2045.00219	-474.78415	1
18794	C	78.38400	49.85180	64.90690	501.27405	436.58084	611.26410	1
18795	H	78.99800	50.42380	65.63490	1533.51034	2184.92047	-1681.92621	1
18796	H	78.48000	50.46080	63.98190	491.62756	1593.39586	-2684.06982	1
18797	C	79.08600	48.50880	64.76090	-471.22170	-572.24939	-541.93719	1
18798	H	80.13800	48.65880	64.43590	-1804.39904	2105.93179	-1517.35324	1
18799	H	79.13800	48.00180	65.74790	-1717.84197	2023.05771	1689.18624	1
18800	C	78.42400	47.54480	63.73590	-282.71738	-453.98516	722.09007	1
18801	H	77.43900	47.19580	64.11290	2057.04869	-893.43939	2184.30410	1
18802	H	78.43800	48.07180	62.75690	-587.98097	-1288.61506	2793.13125	1
18803	N	79.19100	46.31480	63.58490	663.03911	-41.16655	498.17751	1
18804	H	79.15700	45.54480	64.28290	-1460.83311	2741.40663	-567.74920	1
18805	H	78.84600	45.88880	62.70090	2796.33516	704.04280	-1264.11311	1
18806	H	80.20700	46.41180	63.38790	-1400.97448	175.46195	-2829.79287	1
18807	C	76.45600	52.09780	64.76190	-346.83726	385.92933	-767.86486	1
18808	O	77.33400	53.00380	64.73790	474.52158	281.17854	-574.87307	1
18809	N	75.49900	52.07180	63.80890	468.21756	170.61529	-690.17931	1
18810	H	74.82500	51.33980	63.87890	-1350.05438	-1821.86440	-2190.50158	1
18811	C	75.37200	53.05880	62.72290	498.99985	-637.04090	-411.13316	1
18812	H	76.24900	53.07880	62.09390	1989.27152	-1787.29559	1628.91077	1
18813	C	74.08200	52.69580	61.93290	459.99495	-628.05981	-468.20702	1
18814	H	73.19500	52.54980	62.58490	2985.21577	-690.76197	666.48193	1
18815	H	74.18000	51.73280	61.38690	-2650.71923	-1370.19298	993.79664	1
18816	C	73.59900	53.60380	60.75090	738.94847	-140.03042	492.00150	1
18817	H	73.51200	54.61580	61.20090	-2267.06883	2008.63595	878.54273	1
18818	C	74.75200	53.70080	59.70190	385.10775	826.78280	-98.44269	1
18819	H	75.73100	53.99880	60.13390	966.29002	-2222.42708	-2003.84499	1
18820	H	74.40100	54.35980	58.87990	-2815.63690	-601.89582	-1291.99105	1
18821	H	74.77600	52.72380	59.17190	453.24426	-2957.84310	929.50604	1
18822	C	72.26900	52.99980	60.24790	138.30100	-603.52171	-670.64694	1
18823	H	72.31900	51.91280	60.01990	-2685.30396	725.39069	-1498.25548	1
18824	H	71.53100	53.17380	61.05890	2803.73150	724.06968	-1227.75871	1
18825	H	71.90400	53.53280	59.34390	-589.89200	1823.06455	-2513.22049	1
18826	C	75.26700	54.48680	63.29190	857.46373	-203.01132	-210.72295	1
18827	O	75.99400	55.39780	62.81990	-730.11267	-57.51772	-321.30755	1
18828	N	74.42500	54.77980	64.32690	49.60680	668.92250	-530.84638	1
18829	H	73.71000	54.13580	64.58490	1475.19613	2730.42400	-542.84923	1
18830	C	74.40000	55.99780	65.09690	128.71191	895.37080	142.24922	1
18831	H	74.15100	56.75380	64.36690	1809.47997	-1652.55803	1951.69755	1
18832	C	73.31000	55.86980	66.17990	141.09321	808.97746	-415.52063	1
18833	H	73.30000	56.73880	66.87090	-1885.75583	563.97614	2451.36681	1
18834	H	73.61800	54.94780	66.71790	-130.39787	1128.27826	2926.58921	1
18835	C	71.87600	55.65080	65.62390	-298.99488	-453.06640	-740.65503	1
18836	H	71.83700	54.60480	65.25090	847.23306	-45.83255	-3037.20758	1
18837	C	70.97400	55.48080	66.86590	-268.31261	281.79241	-837.38622	1
18838	H	71.23100	54.55980	67.43290	-41.66374	1344.65351	-2855.93313	1
18839	H	71.08600	56.36480	67.52890	684.15038	-2296.87017	2021.74742	1

18840	H	69.94100	55.32880	66.48690	782.90579	-2493.64858	1732.03370	1
18841	C	71.25800	56.61480	64.56090	500.24046	567.01962	-518.45106	1
18842	H	70.17700	56.37880	64.46190	-1753.33254	-1854.42977	1831.68873	1
18843	H	71.83700	56.72880	63.61990	1428.70709	2806.10593	8.29230	1
18844	H	71.32500	57.64680	64.96790	-609.20163	-2181.51549	-2187.55219	1
18845	C	75.73500	56.27280	65.77590	442.77175	697.00924	-400.76698	1
18846	O	76.34600	57.33580	65.63190	91.38162	-730.89108	-274.59935	1
18847	N	76.31200	55.24680	66.49890	467.86672	701.95531	52.50885	1
18848	H	75.88100	54.35180	66.58390	-2134.34327	2175.76858	802.37847	1
18849	C	77.48200	55.40080	67.33590	-194.85262	690.52994	-582.81457	1
18850	H	77.32600	56.29280	67.92390	-2254.29297	1530.60254	-1597.16347	1
18851	C	77.62100	54.17580	68.29490	651.18316	-245.72227	569.25506	1
18852	H	78.49700	54.34580	68.95590	-1360.61252	2562.72275	1222.50909	1
18853	H	76.75900	54.12480	68.99390	-191.70204	-694.55094	-3072.66743	1
18854	H	77.70900	53.20180	67.76690	758.40050	-1521.56714	2630.59552	1
18855	C	78.78300	55.65680	66.64290	-510.71876	524.13799	544.80839	1
18856	O	79.62000	56.37780	67.15490	-526.47782	-549.71917	197.75963	1
18857	N	78.96700	55.15180	65.41590	-176.63391	790.11408	-276.58616	1
18858	H	78.26300	54.58880	64.98890	-2836.84021	302.58266	-1352.82670	1
18859	C	80.24300	55.01480	64.81890	-749.27072	-312.40969	-433.00281	1
18860	H	80.93500	55.54480	65.45490	-1290.53626	1413.88268	2492.52386	1
18861	C	80.74100	53.60680	64.68090	363.21828	-782.78577	-277.39084	1
18862	H	81.54200	53.50280	63.91790	1360.46863	2837.76882	-157.94459	1
18863	H	79.93900	52.99380	64.21490	-1237.18088	-440.35238	-2872.88940	1
18864	C	81.19200	53.07180	66.00590	-445.80418	438.14582	659.81821	1
18865	H	80.21400	52.97080	66.52290	816.48576	-2070.56846	2202.74617	1
18866	H	81.98500	53.67880	66.49090	2419.78114	1972.54137	-400.75966	1
18867	C	81.80000	51.67080	65.81990	-200.72994	649.06205	-630.96281	1
18868	O	82.54700	51.38680	64.86090	484.43785	518.88131	335.20637	1
18869	O	81.46400	50.77080	66.62690	581.34300	104.41494	505.76077	1
18870	C	80.24800	55.64180	63.46990	-400.60600	-291.88705	754.54583	1
18871	O	81.28400	56.18180	63.05390	178.28896	-755.60998	-87.90331	1
18872	N	79.10300	55.73680	62.73990	-6.02370	628.30108	-583.69403	1
18873	H	78.21300	55.39680	63.03490	-2998.36955	-315.60248	908.76507	1
18874	C	79.08500	56.37380	61.44790	449.18781	-543.41871	553.23660	1
18875	H	80.07800	56.57180	61.07090	2073.18563	-149.35995	2343.34040	1
18876	C	78.41800	55.43180	60.43790	587.60089	-254.02333	-649.63633	1
18877	H	77.80000	55.86380	59.62190	-1209.28454	1925.82846	-2197.24391	1
18878	H	77.61800	54.90880	61.00490	-2347.29435	2088.79092	-321.19380	1
18879	C	79.39200	54.30580	59.96390	516.14872	559.38488	-515.81585	1
18880	H	80.20100	54.78780	59.37390	1624.40086	621.50424	2607.25318	1
18881	H	79.81400	53.79280	60.85490	3074.89944	-621.35754	-23.82686	1
18882	C	78.69400	53.25980	59.05890	527.44625	-544.60194	-499.72818	1
18883	H	78.18300	53.69880	58.17490	-2904.62717	-1218.45469	-34.80698	1
18884	H	77.89200	52.86580	59.71890	567.14931	-3059.47331	-401.96550	1
18885	C	79.52300	52.08780	58.64990	112.08407	-207.76697	-889.93133	1
18886	H	78.88900	51.18480	58.52290	1543.22358	-127.34759	2721.13691	1
18887	H	80.17100	51.87080	59.52690	-1843.37379	85.47762	-2566.67083	1
18888	N	80.41500	52.29680	57.45590	-348.93292	-228.42309	721.88373	1
18889	H	81.01600	53.14280	57.39090	2069.20691	1720.94978	1617.13397	1
18890	H	80.99800	51.45480	57.27390	2028.83707	-1669.01547	-1724.54868	1
18891	H	79.79000	52.30380	56.62490	-145.24844	-2222.30847	2199.78620	1
18892	C	78.36900	57.66680	61.44790	-443.85329	503.46723	-639.59044	1
18893	O	78.89200	58.71780	61.08490	-95.56371	-603.51848	481.31239	1
18894	N	77.09500	57.58980	61.86190	599.82624	535.38486	-265.87578	1
18895	H	76.77100	56.72180	62.22990	1451.04393	-1989.28140	-1954.82403	1
18896	C	76.09900	58.66480	61.66090	125.40718	-776.41859	436.18634	1
18897	H	76.35500	59.15680	60.73390	-2983.52435	-984.63203	234.76565	1
18898	C	74.63500	58.10880	61.42090	-243.53900	694.76222	-560.48350	1
18899	H	74.40700	57.32080	62.17090	-2600.34443	293.95016	-1768.08687	1
18900	C	73.63900	59.25180	61.53490	404.56248	75.43875	802.11199	1
18901	H	73.66300	59.64980	62.57190	1116.90884	1038.27498	-2759.57414	1

18902	H	72.61900	58.85480	61.34290	-2450.60433	-1677.98237	1036.03466	1
18903	H	73.85800	60.07080	60.81690	1047.57058	-1523.09928	2529.50736	1
18904	C	74.54200	57.54180	59.97590	-330.85686	394.38267	751.39924	1
18905	H	75.40900	56.88280	59.75790	1212.42514	-2094.84714	1986.27471	1
18906	H	73.71200	56.81880	59.81990	2006.98204	1375.03937	1983.28321	1
18907	H	74.61300	58.32480	59.19190	292.93704	-2506.89357	1856.27013	1
18908	C	76.21100	59.84480	62.65990	-20.19817	14.46279	-920.43837	1
18909	O	75.93300	60.98580	62.30390	568.43492	220.81106	-504.14863	1
18910	N	76.85000	59.71980	63.88290	-402.51819	467.08611	-596.43216	1
18911	H	76.85700	58.81880	64.30890	-1752.78236	-2608.11605	-116.81619	1
18912	C	77.20900	60.88380	64.76190	675.24898	-359.06390	472.58917	1
18913	H	76.28000	61.42980	64.83790	-1976.32822	1643.79874	1819.96294	1
18914	C	77.73400	60.39280	66.08790	-534.94606	-101.37022	-744.42155	1
18915	H	77.00500	59.71580	66.58190	2067.39703	1549.87069	1783.72348	1
18916	C	79.03700	59.53180	65.95890	-165.90729	-553.14012	-711.45673	1
18917	H	79.91700	60.21080	65.96790	3074.96229	-7.27957	622.91396	1
18918	H	79.30200	58.94780	65.05190	-1126.62849	-2545.24816	-1469.26867	1
18919	H	79.18400	58.75480	66.73890	-2405.44286	592.49887	-1959.28981	1
18920	C	77.96200	61.63780	66.98490	230.87880	-722.08789	485.91949	1
18921	H	78.82900	62.29580	66.75890	2523.65181	1761.93189	-650.71781	1
18922	H	78.00300	61.31880	68.04790	-1572.75740	1841.02619	2010.59348	1
18923	H	77.05900	62.28480	66.98290	-1202.01580	2428.19398	-1621.59416	1
18924	C	78.17500	61.78680	63.99590	583.78685	304.43068	-635.74563	1
18925	O	78.09900	62.98780	64.12390	-687.77655	408.88809	-10.25757	1
18926	N	79.04000	61.27880	63.15690	453.72176	230.57172	-679.78649	1
18927	H	79.21600	60.30180	63.07090	-359.18443	1960.50849	2432.39110	1
18928	C	79.83300	62.16880	62.23990	-751.46667	-443.26194	265.15522	1
18929	H	80.38500	62.91080	62.79690	-575.58032	2265.57573	2108.01287	1
18930	C	80.87800	61.35180	61.53590	239.37329	885.59131	-44.18072	1
18931	H	81.46900	62.00780	60.86190	1659.63450	-2653.30173	156.23329	1
18932	H	80.48200	60.49880	60.94490	3023.96529	329.25121	765.58974	1
18933	C	81.78800	60.76180	62.55890	-550.21739	460.85781	-586.63005	1
18934	C	81.47900	59.48980	63.13990	602.84787	88.41092	-682.85346	1
18935	H	80.54500	58.99280	62.92390	2086.51558	-2299.50166	-443.53573	1
18936	C	82.33100	58.99680	64.14690	-635.09973	-277.82176	585.66247	1
18937	H	82.11600	58.00880	64.52490	1281.83923	-2491.63988	-1421.73036	1
18938	C	83.50600	59.67180	64.52090	590.08671	566.42652	-414.11907	1
18939	O	84.34300	59.10380	65.48790	777.92006	-8.50792	-97.28425	1
18940	H	85.16400	59.59980	65.50190	1982.35277	2347.75954	-693.28586	1
18941	C	82.96400	61.42180	62.94590	-751.60863	-219.21431	-485.84314	1
18942	H	83.22800	62.37680	62.51590	-1609.56871	-1945.08154	-1884.88264	1
18943	C	83.79600	60.81880	63.85490	-654.16529	651.01902	-22.72083	1
18944	H	84.68400	61.36680	64.13590	-1085.03970	1769.54483	2363.40748	1
18945	C	79.07200	63.01480	61.18490	747.41413	-495.49191	68.05880	1
18946	O	79.35300	64.19780	61.05590	296.52150	541.63349	488.49945	1
18947	N	78.11400	62.42880	60.51990	-339.15127	761.69630	-199.30970	1
18948	H	77.89300	61.46280	60.63090	-1809.25602	-2409.61269	-907.14035	1
18949	C	77.45200	63.00280	59.37490	-180.07709	896.37031	114.34817	1
18950	H	77.88600	63.93180	59.03590	1736.02504	-283.85762	-2608.81330	1
18951	C	77.51400	62.02580	58.15990	487.04969	433.28826	-645.09008	1
18952	H	78.58700	61.74980	58.07590	-1996.81996	1603.89019	1837.01622	1
18953	C	76.64800	60.74380	58.20490	-847.15506	68.48776	345.88648	1
18954	H	76.89000	60.04880	57.37290	1940.83473	-923.95083	-2294.36115	1
18955	H	75.57900	61.03780	58.26890	-1404.42562	2697.07929	844.51504	1
18956	H	76.88300	60.24480	59.16990	-864.46497	693.05221	2940.52911	1
18957	C	77.07000	62.83080	56.90790	-580.46090	-599.63346	358.32039	1
18958	H	77.53500	63.83980	56.88090	466.82891	-673.48808	3026.23040	1
18959	H	77.24600	62.12980	56.06390	-2198.97686	-1800.79180	1343.07341	1
18960	H	75.98500	63.07180	56.90790	-1340.37592	-1408.04660	2465.87345	1
18961	C	75.96700	63.43180	59.71690	-281.24034	-583.33562	-645.05832	1
18962	O	75.23100	63.95280	58.88690	-92.80887	419.57774	-676.26520	1
18963	N	75.55600	63.14580	60.96990	-159.21374	833.73552	85.19709	1

18964	H	76.07500	62.48980	61.51290	495.75025	2423.88883	1943.74229	1
18965	C	74.24300	63.52480	61.53090	-532.45093	369.55641	-659.57635	1
18966	H	73.64800	62.66780	61.80990	-1290.94369	2678.37987	1051.58848	1
18967	H	73.74100	64.17580	60.82990	-2172.98733	-661.90614	-2189.45440	1
18968	C	74.39400	64.47380	62.76890	659.07886	-586.40855	-189.23257	1
18969	O	73.38900	65.08080	63.16490	205.13911	500.01744	572.93663	1
18970	N	75.62000	64.65580	63.34290	399.56257	-520.73957	510.51012	1
18971	H	76.40600	64.05980	63.19790	-1573.61474	-717.40465	2623.82629	1
18972	C	75.80700	65.65780	64.37690	240.49383	567.21993	668.73841	1
18973	H	74.96800	66.32780	64.49790	-143.08701	2862.38767	-1319.58968	1
18974	C	76.01200	64.93380	65.67590	271.00381	-364.05890	778.45565	1
18975	H	76.89500	64.26080	65.65490	2086.07268	-2297.06148	-463.35788	1
18976	C	76.30800	65.94080	66.83790	652.38309	-147.19577	-616.82951	1
18977	H	77.32300	66.35880	66.66890	2596.77436	1424.28181	-1057.80538	1
18978	H	76.23100	65.35680	67.77990	1835.78682	1281.32310	2201.29192	1
18979	H	75.48500	66.68680	66.80890	2549.49239	-1822.59998	-132.55930	1
18980	C	74.73100	64.15080	66.04990	-268.25646	596.39359	-650.94474	1
18981	H	73.85200	64.82480	66.13390	-1567.36498	-2584.04256	-875.87048	1
18982	H	74.86500	63.63880	67.02690	-1590.28974	896.18077	-2575.75427	1
18983	H	74.49800	63.28680	65.39090	-1485.33817	-1557.27222	-2302.37301	1
18984	C	76.98200	66.54980	64.00090	-319.62905	-656.65072	535.58414	1
18985	O	76.81300	67.75280	63.82890	484.62355	-560.74831	234.53268	1
18986	N	78.17500	65.95380	63.88490	661.23506	330.10514	-407.42313	1
18987	H	78.34800	64.98480	64.04090	-1960.31912	-1894.52189	1564.12119	1
18988	C	79.38000	66.79380	63.80390	266.98529	277.29598	-833.31883	1
18989	H	79.33300	67.52180	64.60090	427.35846	-1558.06577	-2700.69354	1
18990	C	80.72500	65.95580	63.88190	775.73837	-400.65193	-231.25890	1
18991	H	81.57500	66.47980	63.39390	944.14519	2553.79953	1576.74243	1
18992	H	80.62700	65.05980	63.23190	-943.89031	-1353.39837	-2685.48031	1
18993	C	81.07600	65.46380	65.23690	748.79857	-494.74360	-91.17663	1
18994	C	81.17800	64.13780	65.68490	-800.26077	-344.33405	-290.24381	1
18995	H	81.15400	63.23580	65.09090	401.89647	1628.37139	-2673.89716	1
18996	N	81.54500	64.11680	67.03990	-635.21560	256.01380	-514.51776	1
18997	H	81.89000	63.41080	67.61890	-806.42737	1859.05762	-2422.82009	1
18998	C	81.67300	65.44380	67.41590	792.62484	-392.56919	-188.04299	1
18999	C	81.36600	66.28480	66.35090	-269.13274	-596.15425	624.27452	1
19000	C	81.43800	67.69780	66.49390	442.17669	-618.22955	-495.22018	1
19001	H	81.35400	68.36680	65.64990	2129.29498	1833.70266	1405.18937	1
19002	C	81.95200	68.19480	67.67890	788.14822	-395.96127	183.75422	1
19003	H	82.20600	69.23880	67.78590	-1107.60105	2901.37586	548.19788	1
19004	C	81.95100	65.96580	68.65390	-483.74781	770.68565	132.03154	1
19005	H	82.12500	65.34080	69.51690	2145.51891	779.86574	2152.19918	1
19006	C	82.16800	67.36880	68.71590	105.15084	-685.59158	-590.83826	1
19007	H	82.68500	67.67280	69.61390	-1258.30837	-1413.83318	2505.82014	1
19008	C	79.54100	67.60780	62.56990	-670.83785	-390.62879	-490.51508	1
19009	O	79.68900	68.83180	62.62190	-81.63037	691.29861	383.18344	1
19010	N	79.43900	66.98780	61.39490	225.08745	-467.31575	-663.66519	1
19011	H	79.52900	65.99580	61.36090	-1667.41157	-135.09976	2662.36747	1
19012	C	79.40100	67.72880	60.09790	655.25659	-578.23167	204.79411	1
19013	H	80.27400	68.36380	60.06790	807.40031	610.16136	-2984.75803	1
19014	C	79.57800	66.71580	58.97690	-99.15614	139.28121	891.10475	1
19015	H	79.06400	65.76680	59.23990	1511.07981	1989.27557	1907.48586	1
19016	C	79.02300	67.18080	57.59490	-576.33391	596.49450	401.70896	1
19017	H	79.08700	66.33780	56.87390	-755.60676	-1558.36590	2616.33608	1
19018	H	77.97200	67.53780	57.64990	2918.22463	1094.17986	-390.03962	1
19019	H	79.57700	68.09680	57.29790	2033.50425	-2074.78549	-1178.76925	1
19020	C	81.08100	66.50980	58.92390	378.81266	704.92986	436.65804	1
19021	H	81.56100	66.51280	59.92590	2712.55304	-1224.27163	975.98595	1
19022	H	81.53800	67.31980	58.31590	1789.47265	2411.54523	937.78298	1
19023	C	81.48100	65.22680	58.17990	544.95429	-304.88049	-659.74369	1
19024	H	82.58100	65.23080	58.01990	-558.70171	-2323.65979	-2045.43343	1
19025	H	81.14600	64.38880	58.82690	-1072.10281	1855.55210	2307.27899	1

19026	H	81.07500	65.34680	57.15190	-2536.71703	-1834.85846	-337.60796	1
19027	C	78.20300	68.68480	59.97390	-178.68822	518.11313	731.42557	1
19028	O	78.39300	69.81780	59.50690	-740.86036	-154.03873	244.86235	1
19029	N	76.94300	68.38580	60.25590	372.83429	-441.77333	597.30598	1
19030	C	76.40600	67.04980	60.23790	92.20920	48.26332	-911.32467	1
19031	H	76.84500	66.50280	61.09990	-44.30372	-2356.41240	-2081.16667	1
19032	H	76.61900	66.55080	59.26890	-2225.02899	1840.83087	-1284.66671	1
19033	C	75.89100	69.36780	60.47890	-513.29334	-374.50043	-661.55612	1
19034	H	75.63800	69.83980	59.54090	2400.43543	1727.70564	-1069.60121	1
19035	C	74.79500	68.58480	61.07990	313.33841	-414.71185	735.65127	1
19036	H	74.84900	68.53780	62.18890	-1049.71664	-1893.96860	-2285.14776	1
19037	H	73.81200	69.09380	60.98690	2232.63141	-2140.04970	-511.85871	1
19038	C	74.91000	67.23780	60.38990	-334.73327	-647.86420	-548.61103	1
19039	H	74.48000	66.36180	60.92190	2396.04926	206.03947	2012.75875	1
19040	H	74.36300	67.34880	59.42990	-66.09527	854.67675	3024.37293	1
19041	C	76.27700	70.60180	61.32290	693.50925	-38.42021	-583.46927	1
19042	O	75.93900	71.65980	60.85690	-733.48608	-193.64087	-247.19952	1
19043	N	76.98300	70.49280	62.53090	432.56564	359.12845	622.92414	1
19044	H	77.22900	69.59880	62.89790	-1007.53313	-2119.55950	2086.55158	1
19045	C	77.34300	71.60280	63.34590	42.68293	715.22039	-577.25576	1
19046	H	76.43300	72.10680	63.63490	2889.05142	-1164.87975	-357.57866	1
19047	C	78.07100	71.11780	64.56590	-261.82031	666.29798	-581.96253	1
19048	H	77.40400	70.42680	65.12390	-1419.62469	-2307.54121	-1601.95493	1
19049	H	78.32800	71.98480	65.21090	-2718.39690	374.82847	1551.02186	1
19050	H	79.06500	70.67980	64.33290	-3075.84667	144.86915	-692.39826	1
19051	C	78.26200	72.58380	62.57290	673.06652	455.16243	402.60916	1
19052	O	77.99600	73.79480	62.52490	-487.85868	558.35324	299.36893	1
19053	N	79.28600	72.04380	61.88190	-199.61111	-622.86003	-532.24627	1
19054	H	79.45000	71.06180	61.82190	1704.70720	1957.20149	-1783.57001	1
19055	C	80.16600	72.83480	60.97290	-491.35076	-358.93419	676.62999	1
19056	H	80.56600	73.62780	61.58790	-7.90732	3150.20417	-174.53145	1
19057	C	81.26100	71.99780	60.26490	-652.21970	-591.55684	235.40881	1
19058	H	80.87300	71.21680	59.57690	1243.84230	-2868.22342	-217.61628	1
19059	H	81.86300	72.79880	59.78490	1341.72893	-2400.91828	-1508.75716	1
19060	C	82.21600	71.17680	61.14290	27.57144	707.86204	578.53810	1
19061	H	81.67600	70.33280	61.62390	-1345.08475	-1070.71383	-2642.25981	1
19062	C	83.30900	70.67280	60.22790	-657.48643	-283.50665	564.55440	1
19063	H	82.82200	70.02180	59.46990	-344.33767	1921.21255	2469.81018	1
19064	H	83.81700	71.51980	59.71990	-1104.56714	2160.81211	2011.93571	1
19065	H	84.03400	70.09680	60.84190	2159.85173	-2222.86834	-463.94355	1
19066	C	82.83200	72.00880	62.34890	-743.72962	-21.00980	-545.64023	1
19067	H	81.97800	72.18080	63.03890	1609.20860	2650.04229	542.06596	1
19068	H	83.61500	71.40980	62.85990	1025.72647	1227.48140	-2715.80249	1
19069	H	83.28400	72.93580	61.93590	894.41993	2728.43596	1292.38142	1
19070	C	79.39800	73.56380	59.85490	-423.18297	820.77333	-51.76486	1
19071	O	79.60700	74.74080	59.58190	-275.78072	696.10315	281.59806	1
19072	N	78.44400	72.86480	59.19490	620.08219	465.31907	-331.82323	1
19073	H	78.25100	71.91980	59.44990	-2238.48934	1247.22921	1839.25719	1
19074	C	77.51900	73.42580	58.26290	455.83227	-592.20465	497.82511	1
19075	H	78.15500	73.93980	57.55690	1326.29671	-2712.76738	-838.88686	1
19076	C	76.60000	72.37380	57.56490	299.20902	440.60336	-745.45259	1
19077	H	75.90000	72.97980	56.94990	331.41798	-2236.12979	2172.76913	1
19078	H	76.05600	71.96080	58.44090	1074.20211	938.16104	-2807.43600	1
19079	C	77.41200	71.39580	56.68990	855.61287	262.90448	124.86789	1
19080	H	78.23700	70.92380	57.26490	-1880.98495	-1582.98942	1960.26724	1
19081	C	76.51500	70.32580	56.03890	-590.39960	-514.86965	464.11298	1
19082	H	75.79800	70.79480	55.33190	1937.84676	-2439.93705	304.53988	1
19083	H	77.06300	69.52180	55.50390	924.90167	-2825.90107	983.28528	1
19084	H	76.02800	69.82180	56.90090	-2214.64161	1007.78362	-2015.97120	1
19085	C	78.08700	72.20080	55.55590	-559.93978	-205.27941	691.03286	1
19086	H	78.93000	72.84180	55.89090	2435.28200	-879.84844	-1770.78919	1
19087	H	77.35600	72.90380	55.10290	-30.90421	-3069.61804	-643.98096	1

19088	H	78.47800	71.55980	54.73690	-1983.70216	-1439.32854	1971.20232	1
19089	C	76.65800	74.51080	58.81890	221.29771	571.52990	-682.53442	1
19090	O	76.44500	75.53780	58.13990	703.06541	-30.75151	-337.65438	1
19091	N	76.13800	74.39180	60.04090	607.02510	295.28631	-502.53976	1
19092	H	76.10800	73.55980	60.58990	2155.50746	-1845.03157	-1335.01778	1
19093	C	75.18900	75.41980	60.53390	690.78667	-516.69752	250.82729	1
19094	H	74.52600	75.63580	59.70990	932.19047	-2935.52705	582.20902	1
19095	C	74.32700	74.98880	61.72290	-459.75931	-335.68086	-717.41210	1
19096	H	73.68700	75.85480	61.99690	2625.00466	195.92129	1706.69283	1
19097	H	75.08200	74.73680	62.49790	-2845.95063	1129.51046	768.86118	1
19098	C	73.43400	73.79580	61.37990	-410.20594	374.71992	729.85548	1
19099	H	73.87200	73.05280	60.67990	-2491.98032	-1104.49096	1578.09738	1
19100	C	73.20600	72.96180	62.64590	515.10632	380.91286	-648.43760	1
19101	H	72.47500	72.15780	62.41390	-144.61805	1456.87451	-2792.05397	1
19102	H	72.89900	73.58880	63.51090	-228.98401	-1194.04164	2896.99241	1
19103	H	74.09900	72.35780	62.91390	1555.56595	1588.09768	-2228.36189	1
19104	C	72.04600	74.18280	60.80190	-283.80572	423.88915	761.69400	1
19105	H	71.38500	73.30880	60.62390	739.94229	-2798.41693	1206.30418	1
19106	H	71.56400	75.00680	61.36990	1616.80317	-1965.59983	-1834.22272	1
19107	H	72.15400	74.59180	59.77490	-2167.82668	-588.68824	-2212.80742	1
19108	C	75.85100	76.71480	60.91390	411.64184	-380.48005	-710.84916	1
19109	O	75.24100	77.76980	61.06290	-546.80566	155.80816	558.90441	1
19110	N	77.17700	76.61080	61.06990	424.90511	434.81303	-586.89528	1
19111	H	77.61500	75.74080	60.85690	3066.35354	-164.76678	631.29385	1
19112	C	78.06900	77.62580	61.56690	-395.66455	631.77743	-544.95499	1
19113	H	77.44900	78.34180	62.08490	1208.89925	2261.74677	1823.53816	1
19114	C	79.05700	77.17280	62.62790	-219.67119	-668.53281	571.31625	1
19115	H	79.78300	77.96780	62.90290	-2056.90350	799.17527	2251.69792	1
19116	O	79.81600	75.99880	62.30490	-547.24314	495.65730	-315.63501	1
19117	H	79.18000	75.28680	62.20490	1716.32183	-1698.00638	1998.15508	1
19118	C	78.13500	76.76780	63.83490	234.66870	-852.99271	174.25984	1
19119	H	77.36500	77.55080	64.00490	-1796.53536	-1425.96404	-2158.93782	1
19120	H	78.74600	76.71880	64.76190	-1228.01056	2034.14866	2071.79134	1
19121	H	77.51500	75.84680	63.79690	-476.23723	-685.34452	3030.24867	1
19122	C	78.80100	78.28280	60.43990	-676.59126	465.67604	-425.97191	1
19123	O	79.82000	78.91780	60.65690	-563.04016	566.47697	85.51670	1
19124	N	78.35900	78.17880	59.20190	-173.33991	-565.20626	594.59712	1
19125	H	77.57900	77.59780	58.98190	-378.56668	-1892.55032	-2481.50634	1
19126	C	78.86300	79.05080	58.16390	-25.49605	-438.00347	-796.34859	1
19127	H	79.93700	78.96980	58.24790	-2004.09576	-1599.98681	1824.00637	1
19128	C	78.55500	78.55580	56.73090	644.18188	-519.17384	-349.94297	1
19129	H	77.45400	78.54380	56.58590	-2227.23334	2238.01908	-165.36703	1
19130	C	79.23400	79.47680	55.69190	-171.65359	513.14394	741.96704	1
19131	H	79.23300	79.06580	54.66090	2866.76385	-1255.69529	60.15515	1
19132	H	78.67300	80.41380	55.48890	3120.36933	-44.57245	-286.63545	1
19133	H	80.26600	79.78080	55.97290	-378.34591	-1145.79812	-2905.07384	1
19134	C	79.06900	77.10780	56.54390	-405.85815	631.47601	-541.68589	1
19135	H	79.00500	76.45980	57.44390	-2510.66162	-1540.86089	1113.19532	1
19136	H	80.15200	77.14780	56.29690	688.92150	2273.32972	-2073.80635	1
19137	C	78.26600	76.33080	55.51690	-577.77835	-622.99635	-334.07641	1
19138	H	78.23500	76.94280	54.59090	-1813.04525	-2234.03311	-1273.48904	1
19139	H	77.16900	76.27180	55.68190	2406.97194	-1953.39123	434.63609	1
19140	H	78.74700	75.33680	55.39290	655.53009	-2138.08350	2195.45950	1
19141	C	78.55300	80.52180	58.35990	629.90991	-3.45889	-649.37358	1
19142	O	79.45400	81.34280	58.28290	418.24404	-381.35659	-536.00691	1
19143	N	77.30800	80.94280	58.79090	-713.42213	119.54194	454.92666	1
19144	C	76.06600	80.31780	58.47990	-469.78434	453.44999	-652.15478	1
19145	H	75.80500	79.49080	59.17390	1823.25331	2553.98545	234.81074	1
19146	H	76.09400	79.92480	57.44090	-2300.77681	1690.10603	1353.45014	1
19147	C	77.11200	82.34380	59.28390	673.82307	597.16398	125.42642	1
19148	H	77.25900	83.06080	58.48990	-2815.54335	-1122.20710	-870.33359	1
19149	C	75.62100	82.35380	59.68890	253.60509	818.23424	-325.41372	1

19150	H	75.54600	82.00980	60.74290	-1981.99377	2012.65591	-1413.12877	1
19151	H	75.08500	83.32580	59.65190	-1987.15054	255.53046	2436.59504	1
19152	C	75.00600	81.34580	58.64290	-741.14373	520.31913	-194.76731	1
19153	H	74.62200	81.75380	57.68290	15.45380	2687.22712	1651.25763	1
19154	H	74.09500	80.94680	59.13790	-1453.85275	-2478.30331	-1277.72462	1
19155	C	78.03700	82.78180	60.40490	-299.72846	-855.83958	-27.40984	1
19156	O	78.48700	83.90380	60.44290	59.77811	-678.56130	-382.36546	1
19157	N	78.30300	81.91980	61.40090	187.74278	750.96759	348.15147	1
19158	H	77.87300	81.02280	61.32790	-2910.33825	1098.48771	549.29266	1
19159	C	79.25100	82.16380	62.47790	-733.68360	425.54731	-367.80906	1
19160	H	78.89200	83.09180	62.89790	1617.39444	-2315.57867	-1360.30646	1
19161	C	79.28600	81.04580	63.50590	809.27887	350.70485	203.86501	1
19162	H	80.16800	81.03780	64.18090	-2681.51260	1121.65418	-1234.87323	1
19163	H	79.41000	80.13580	62.87990	-1631.15399	-1174.18381	2421.68131	1
19164	C	78.00000	80.97680	64.30490	472.19911	644.29030	-440.60752	1
19165	O	77.75200	81.96580	65.02190	-557.31693	570.73410	78.28402	1
19166	O	77.25500	79.98480	64.24790	461.94657	-365.96450	510.21618	1
19167	C	80.65900	82.48880	61.91190	-617.26384	-452.08860	500.27815	1
19168	O	81.35100	83.42380	62.34390	415.14157	-531.52148	386.85445	1
19169	N	81.09300	81.65880	60.95190	211.36359	237.69372	779.85955	1
19170	H	80.60900	80.81980	60.71590	867.16627	-195.41891	-3016.10288	1
19171	C	82.35100	81.84880	60.18090	-77.06504	-898.92975	43.06637	1
19172	H	83.14500	81.81080	60.91190	949.26265	-2224.07508	-1999.29721	1
19173	C	82.61200	80.57680	59.36790	644.91732	-401.24233	-484.08751	1
19174	H	81.68500	80.38480	58.78690	2126.37805	265.94545	-2296.34994	1
19175	H	82.65500	79.66680	60.00390	1800.34278	2268.32361	1227.92084	1
19176	C	83.86900	80.51280	58.43890	580.55069	-537.01999	-428.72967	1
19177	C	85.11900	81.10280	58.74990	447.25002	-624.89947	-469.33615	1
19178	H	85.29600	81.67880	59.64590	-1980.58035	-1693.49139	1763.11402	1
19179	C	86.16200	81.10780	57.83790	-589.16118	-694.92187	-11.62482	1
19180	H	87.06200	81.63480	58.11890	905.39309	2220.76512	-2046.15688	1
19181	C	85.98200	80.43580	56.65890	-895.32717	219.29523	85.65220	1
19182	H	86.69700	80.46980	55.84990	-1077.47895	-973.01051	-2795.46777	1
19183	C	83.79600	79.72480	57.31990	451.11837	632.82890	-482.91563	1
19184	H	82.86100	79.25980	57.04390	-899.98930	1712.31678	-2495.85290	1
19185	C	84.80600	79.76980	56.36290	519.75540	-476.44951	-561.00796	1
19186	H	84.81800	79.17080	55.46490	-2254.09432	-1128.37504	-1893.84342	1
19187	C	82.49700	83.11280	59.39990	-16.22563	-664.20386	-615.75940	1
19188	O	83.51000	83.80280	59.50090	277.55415	-597.40090	412.23448	1
19189	N	81.49500	83.40680	58.56490	-495.86895	-623.10980	-279.97650	1
19190	H	80.75700	82.74780	58.43890	-2105.55753	-1996.84538	1218.49334	1
19191	C	81.46900	84.64280	57.71890	439.17989	-774.16144	110.39379	1
19192	H	82.41100	84.77380	57.20590	-1830.53945	-1519.83786	-2062.62189	1
19193	C	80.38000	84.70980	56.67890	578.84199	-251.72890	-642.96563	1
19194	H	79.41800	84.79380	57.22890	-1946.28735	-1004.26525	-2264.91847	1
19195	C	80.45145	85.95136	55.72399	-313.80469	-795.64793	730.48868	1
19196	H	80.36975	86.88843	56.29716	-967.14708	-123.62424	3104.04852	1
19197	H	79.58865	85.98491	54.99404	88.56156	1958.88884	-74.61835	1
19198	H	81.39982	86.03778	55.12108	-56.82881	-1155.36573	-962.66506	1
19199	C	80.27800	83.41680	55.77490	58.56899	-719.44325	540.53171	1
19200	H	80.08400	82.53880	56.42690	1868.93798	2013.48913	-1533.16754	1
19201	H	81.26700	83.29280	55.28390	573.91809	2104.30621	2273.18621	1
19202	C	79.15000	83.46480	54.79990	508.44956	-365.49591	-646.93054	1
19203	H	79.31000	82.70080	54.00990	-870.57016	1969.28971	2307.68831	1
19204	H	79.14200	84.43280	54.25390	1792.03248	-563.30942	-2511.98078	1
19205	H	78.13300	83.27280	55.20590	1486.23023	-2742.52218	-266.04005	1
19206	C	81.43162	85.80453	58.90876	1326.81635	-837.44069	-282.09575	1
19207	O	82.20743	86.71869	58.74245	-294.45750	684.73305	-78.82367	1
19208	N	80.49185	85.60172	59.82656	47.66469	15.26297	-342.26023	1
19209	H	80.01266	84.62550	59.81362	-759.11078	314.58046	-862.51522	1
19210	C	79.94267	86.70489	60.50067	122.01129	792.01683	1288.02345	1
19211	H	80.45133	87.55201	59.98463	3966.10799	-2400.61080	277.85921	1

19212	C	78.34099	86.63951	60.63034	-337.59966	196.27130	560.22733	1
19213	H	78.00663	85.80721	61.28084	176.24394	1769.84020	3325.04415	1
19214	H	78.05889	87.62595	61.18559	-892.79870	-2956.33023	-433.42727	1
19215	C	77.62436	86.58520	59.23348	-535.64993	-15.32406	133.97790	1
19216	C	77.82797	87.68876	58.35356	306.51012	-83.37272	361.34695	1
19217	H	78.30855	88.60254	58.68456	-1147.98880	-1394.80220	2201.18952	1
19218	C	77.17049	87.65068	57.08535	-1206.63950	-499.64873	-244.40780	1
19219	H	77.20285	88.62227	56.44143	234.20499	-1791.44656	1910.26198	1
19220	C	76.27090	86.60353	56.80044	200.12999	967.32229	192.72399	1
19221	H	75.66584	86.65113	55.94089	-913.66361	1753.55336	1512.78296	1
19222	C	77.00622	85.39002	58.80890	-556.13579	99.47718	1060.47155	1
19223	H	76.72596	84.56250	59.45149	-341.62217	-682.15109	3361.20543	1
19224	C	76.20193	85.51605	57.66210	55.09274	157.40276	-950.31133	1
19225	H	75.46461	84.68799	57.35883	2731.10929	2065.95481	-1926.28517	1
19226	C	80.57822	86.75892	62.06969	1279.33445	-609.31409	-951.03534	1
19227	O	79.80871	87.12915	62.94023	387.89013	179.13899	-28.70507	1
19228	N	81.79993	86.30315	62.18145	-116.13746	-368.43262	933.57610	1
19229	H	82.20339	86.04287	61.30378	-358.94859	-240.27964	-1127.43012	1
19230	C	82.53539	86.77232	63.32353	-599.77562	-461.48622	-191.50172	1
19231	H	81.71356	87.24088	63.94643	-1122.14017	-1488.91100	-918.66781	1
19232	C	83.25557	85.41886	63.77104	384.86423	-483.23638	264.64790	1
19233	H	84.08932	85.61310	64.54784	65.34021	610.68347	-1707.96706	1
19234	H	83.68000	84.87680	62.92990	-2808.11188	-1164.93592	833.61193	1
19235	H	82.44800	84.78880	64.16490	730.59968	1466.66037	-2688.08976	1
19236	C	83.72152	87.65165	62.65200	-149.67006	-163.67911	182.70019	1
19237	O	84.33767	87.31136	61.60078	-335.10554	154.40632	587.54103	1
19238	N	84.02764	88.60999	63.45788	-409.45575	481.47790	323.84537	1
19239	H	83.49069	88.71175	64.33860	-2223.12910	1072.90237	3075.35337	1
19240	C	84.99177	89.57070	63.09868	-116.63019	-774.70896	-646.20402	1
19241	H	85.72575	89.00815	62.49734	-1800.70074	-899.43041	-1947.03725	1
19242	C	84.33410	90.66860	62.21344	-1052.17370	-1038.86025	12.88850	1
19243	H	84.07450	90.25614	61.20166	2524.11441	-301.30684	-1550.24540	1
19244	H	85.10282	91.38214	61.93716	-2333.95961	-385.02911	-1441.75363	1
19245	C	83.03877	91.42961	62.83931	50.28658	433.06136	-536.67876	1
19246	O	81.96042	91.31577	62.28657	-509.81158	313.20592	348.25378	1
19247	N	83.38556	92.28723	63.81282	-130.11064	-1013.66191	222.88996	1
19248	H	84.27100	92.44900	64.28621	1226.39438	-1115.85631	1809.40497	1
19249	H	82.58515	92.90156	64.12488	-200.34157	-212.88036	151.76674	1
19250	C	85.55695	90.07143	64.60311	-574.08931	379.67109	-309.47145	1
19251	O	85.14340	89.50664	65.61121	413.27605	77.87923	703.68624	1
19252	N	86.51733	90.96307	64.45159	326.40973	116.11904	-136.92971	1
19253	H	86.61552	91.38415	63.53998	-356.27307	809.61170	-1374.52684	1
19254	C	86.77973	91.70132	65.64924	763.09346	351.11667	-224.77107	1
19255	H	86.26103	91.22441	66.51680	-3306.16733	-1690.20112	-608.70506	1
19256	C	88.35184	91.81116	65.72423	-997.09082	-642.96573	276.53867	1
19257	H	88.75207	92.27137	64.81329	383.94613	-1376.35127	3648.84676	1
19258	C	88.67026	92.68341	66.97217	-251.60266	-359.00156	-889.79276	1
19259	H	88.26772	92.15414	67.96270	1006.65263	2998.77062	1003.68502	1
19260	H	88.19678	93.71498	66.90401	-1609.94832	482.09131	2447.12788	1
19261	H	89.76620	92.78844	67.11885	1643.98059	-444.49253	1255.33094	1
19262	C	89.01768	90.44183	66.06797	181.87788	-398.15025	77.46257	1
19263	H	90.16583	90.45820	66.12145	-1149.40152	1287.61963	1222.20579	1
19264	H	88.62019	90.13950	67.06128	1510.46813	2401.27247	-637.91199	1
19265	H	88.82167	89.65816	65.27254	-32.60689	-271.33419	-441.90137	1
19266	C	86.32878	93.28417	65.54669	-176.40029	-1016.79078	-172.60485	1
19267	O	86.35345	93.85084	64.47569	46.14701	101.70127	-551.08872	1
19268	N	85.98839	93.77706	66.71898	582.08267	879.01496	228.70266	1
19269	H	86.03704	93.18328	67.59913	1530.19630	107.78516	-124.83629	1
19270	C	85.29808	95.07063	66.80649	221.72237	247.45700	1187.28008	1
19271	H	85.61156	95.55384	65.81375	1006.31839	-704.67618	239.70229	1
19272	C	83.75554	94.85904	66.86216	439.17977	560.20623	138.62768	1
19273	H	83.40166	94.39456	67.84713	1406.12075	-324.63577	699.20267	1

19274	H	83.59716	94.21694	65.95215	-2085.74471	1194.03554	1459.11513	1
19275	O	82.85547	96.01761	66.67846	289.61713	-173.73050	57.70077	1
19276	H	82.26623	95.90548	67.50618	-4312.47755	413.28369	-2889.96736	1
19277	C	85.99966	95.82834	68.03598	419.49138	-458.36602	317.52689	1
19278	O	87.13212	95.58834	68.40456	1102.34268	-210.85619	-52.25566	1
19279	N	85.14818	96.63987	68.64491	-244.95068	-105.20694	126.69639	1
19280	H	84.19726	96.78736	68.28393	391.96124	2476.53458	-901.94263	1
19281	C	85.53884	97.54164	69.65792	-864.85109	-285.89849	-1277.80362	1
19282	H	86.43500	97.20108	70.15365	4024.95702	-2700.99937	3579.85657	1
19283	C	85.87757	98.97129	68.94561	-73.48378	-188.47613	474.26616	1
19284	H	85.96210	99.80632	69.69495	658.68111	73.83953	-4953.54824	1
19285	H	85.13192	99.29793	68.28143	567.91870	-2692.92539	-1085.30535	1
19286	C	87.11583	98.90223	68.08217	-902.41412	934.78247	-683.89986	1
19287	H	87.85569	99.63003	68.43289	-2401.18554	721.00136	3224.51268	1
19288	H	87.63446	97.93118	68.06333	-2380.03384	1282.96672	-627.75075	1
19289	C	86.37326	99.22471	66.55581	177.03268	-221.79988	55.70290	1
19290	O	85.85247	98.35140	65.87003	-1059.48033	630.34132	630.37529	1
19291	O	86.46844	100.37639	66.16511	496.60781	142.96899	790.08495	1
19292	C	84.20938	97.76942	70.61663	-657.95963	101.57876	636.14654	1
19293	O	83.36077	98.53861	70.22143	-243.30563	-205.53501	260.97502	1
19294	N	84.21681	96.97536	71.67387	-219.17387	-338.53747	-639.63633	1
19295	H	84.95988	96.30290	71.70660	-2199.74230	931.86590	1474.68872	1
19296	C	83.18867	97.00451	72.69454	-575.95374	-206.85746	-51.74779	1
19297	H	82.59634	97.82312	72.22276	1773.40169	-2239.13113	-1869.27611	1
19298	C	82.45049	95.58516	72.65969	-357.58056	-180.42349	1125.97241	1
19299	H	83.04228	94.73965	73.04297	401.51958	4103.15765	-1199.61266	1
19300	H	82.11103	95.22543	71.66834	938.92636	-206.53186	-1379.38121	1
19301	H	81.49147	95.67036	73.24334	1572.89016	1164.21516	1448.42472	1
19302	C	83.76268	97.21449	74.17045	702.58132	-353.02546	-959.58106	1
19303	O	84.45290	96.37297	74.69478	-372.66281	-113.68728	1018.28249	1
19304	N	83.02275	98.17292	74.84077	9.46358	24.83220	390.20228	1
19305	H	82.32263	98.67561	74.22427	-719.54082	1489.80857	1250.60157	1
19306	C	83.58235	99.00563	75.89534	366.27710	-230.50759	284.96082	1
19307	H	82.85411	99.83139	76.06656	-545.36525	-1933.73173	320.12096	1
19308	C	84.17687	98.14778	77.06389	-1126.28838	-495.90301	745.01121	1
19309	H	84.52602	97.20822	76.58840	1053.41805	292.70797	-2575.67013	1
19310	H	85.06500	98.69737	77.46005	595.20028	-422.59728	-647.77814	1
19311	C	83.12874	97.95838	78.21693	-560.90390	22.06621	780.47190	1
19312	O	82.39650	98.84876	78.61336	413.08715	-156.32122	-143.89337	1
19313	O	83.14836	96.69955	78.78990	-197.36119	211.15209	549.42685	1
19314	C	84.89225	99.76271	75.21358	378.62040	516.61336	212.35023	1
19315	O	85.75695	100.15812	75.94609	363.78775	839.06535	507.83787	1
19316	N	84.81265	99.76997	73.86672	-243.31444	151.93520	-478.93176	1
19317	H	83.86872	99.50636	73.58988	382.94525	-2805.35330	2094.87512	1
19318	C	85.64794	100.66854	73.12346	115.53297	-478.90974	-936.92478	1
19319	H	84.92560	100.86366	72.35132	-3283.08912	-2767.68952	-484.91267	1
19320	C	85.96784	102.02142	73.81087	-115.45927	1319.87927	-673.27307	1
19321	H	86.81690	102.46922	73.27679	-2931.50804	-1164.42497	-1349.39856	1
19322	H	86.18318	101.88069	74.91015	3059.01738	-1378.14602	-2056.59152	1
19323	C	84.51685	102.83784	73.74938	34.54280	-345.99891	302.76568	1
19324	O	84.17638	103.52399	74.71409	-394.96250	719.75660	173.14243	1
19325	O	83.95815	102.63824	72.67217	341.24476	-768.18772	7.60742	1
19326	C	86.99716	100.02307	72.40896	-904.46889	41.51552	900.26840	1
19327	O	87.85272	100.75920	71.95741	225.65530	747.59625	-321.85319	1
19328	N	86.92375	98.70838	72.14039	-404.17937	-15.76933	-500.58597	1
19329	H	86.10194	98.34142	72.67536	1889.16380	-502.01511	-80.16761	1
19330	C	88.21578	98.04694	72.37371	-266.00139	698.50150	-439.01910	1
19331	H	88.98210	98.66839	71.81330	4.26696	-1365.07216	-2687.66862	1
19332	C	88.43086	97.91057	73.94471	1004.10732	-680.66450	-114.88311	1
19333	H	89.41662	97.39287	74.16451	-1315.44851	187.28639	-918.10526	1
19334	H	88.31243	98.97086	74.37913	262.98001	176.80911	-416.79305	1
19335	C	87.28849	97.07688	74.61431	709.22699	649.77937	-181.30773	1

19336	H	86.73950	96.37948	73.84378	-773.60256	1138.68639	-1523.71251	1
19337	H	86.50695	97.75958	74.99841	-1404.68059	395.44482	-1684.66264	1
19338	C	87.90468	96.30755	75.82744	-94.31002	23.81508	265.61865	1
19339	H	87.10564	96.21342	76.67642	-1031.05778	-1261.55971	-1324.27140	1
19340	H	88.90323	96.65412	76.22015	-438.81002	-1873.82796	1337.46272	1
19341	N	88.13534	95.16256	75.02691	175.88190	-193.46939	-372.16150	1
19342	H	88.74717	95.20646	74.23097	-446.97337	-403.80684	1418.52083	1
19343	C	87.65092	94.00286	75.32622	-52.17754	203.46481	-983.99773	1
19344	N	88.06919	92.95726	74.52522	-1574.56160	71.65278	89.30253	1
19345	H	88.49019	93.00126	73.52651	300.22935	-75.99800	220.45999	1
19346	H	87.95536	91.95845	74.74854	-2247.09109	85.41403	2561.48089	1
19347	N	86.81825	93.75114	76.46785	380.42153	-77.33650	-329.87409	1
19348	H	86.98385	94.30328	77.32979	-858.57728	247.46635	-4093.18142	1
19349	H	86.39573	92.83765	76.76883	-1102.36279	732.85474	275.51003	1
19350	C	88.01679	96.58103	71.77391	-17.66527	-10.38496	134.38288	1
19351	O	86.94180	95.95380	71.65692	-184.83503	-311.93770	125.65338	1
19352	N	89.20520	96.11828	71.45406	84.46737	56.81346	-178.23726	1
19353	H	89.94139	96.78370	71.71997	-589.05560	2221.45577	-402.49431	1
19354	C	89.39114	95.15644	70.38088	517.56786	68.05355	1503.34134	1
19355	H	88.81628	95.51755	69.57867	3057.65502	-2054.06371	-2234.57984	1
19356	C	90.96347	95.23700	70.22792	-271.08410	146.15156	899.92237	1
19357	H	91.27225	94.87159	71.27589	1668.20220	187.12519	-1922.49047	1
19358	H	91.37193	96.22473	70.06667	-2559.16056	3200.59746	418.98903	1
19359	C	91.41394	94.31170	69.09159	-439.69149	259.92582	-713.75530	1
19360	C	91.74395	92.96914	69.36633	-515.93878	-140.37897	249.15774	1
19361	H	91.77287	92.49397	70.37990	-693.34723	-1080.66252	2113.70226	1
19362	C	92.22374	92.19227	68.27141	-781.14626	762.72164	253.32944	1
19363	H	92.66493	91.22554	68.60891	2238.27092	-1381.04349	-612.48830	1
19364	C	92.31928	92.63276	66.90710	394.56384	-241.70936	638.58827	1
19365	O	92.86828	91.73222	65.90945	157.38211	-461.89132	291.14840	1
19366	H	93.18455	91.02765	66.46712	-2379.45279	-2382.38085	1156.25376	1
19367	C	91.49854	94.81140	67.73943	185.49948	439.40145	113.48882	1
19368	H	91.10633	95.80609	67.53942	1055.78083	1501.90361	3543.78167	1
19369	C	91.94085	93.98837	66.67119	-70.92795	64.28008	-872.00527	1
19370	H	91.92572	94.46717	65.64808	-491.29855	2050.52852	95.88616	1
19371	C	88.75569	93.80315	70.94135	583.54532	200.51347	427.67084	1
19372	O	89.26609	93.13954	71.87620	-195.75010	483.26639	625.32030	1
19373	N	87.56893	93.58617	70.38059	-60.31777	318.68003	206.22074	1
19374	H	87.23245	94.13499	69.66603	1447.04878	-552.16904	-688.64106	1
19375	C	86.82844	92.46992	70.91627	-1386.40873	103.01639	809.24746	1
19376	H	87.60995	92.07168	71.68586	-1086.13905	-44.12157	-1513.58397	1
19377	C	85.58753	93.16003	71.55135	142.01899	459.78775	237.02711	1
19378	H	85.90666	94.12738	72.08301	1913.85145	1848.95557	3158.04847	1
19379	C	84.54101	93.31048	70.35630	1628.98981	212.32109	-297.37032	1
19380	H	83.64036	93.82113	70.72356	-1438.20613	537.44134	-1170.06453	1
19381	H	84.98894	93.88348	69.48666	-338.46830	-1306.26956	1254.61050	1
19382	H	84.26541	92.29757	69.87711	38.12850	-362.77642	1328.25803	1
19383	C	84.78523	92.14460	72.49890	-78.09829	124.93655	-671.05694	1
19384	H	84.96630	91.05638	72.14945	-814.54010	484.58832	-564.59536	1
19385	H	83.72009	92.37083	72.36896	568.58119	2202.31812	2254.37908	1
19386	C	85.04709	92.34577	74.01907	-732.47883	632.08153	730.40480	1
19387	H	85.01844	93.45970	74.32658	-2304.44783	-1865.53455	814.55219	1
19388	H	84.31113	91.72140	74.51815	-1502.58916	-132.00591	635.29705	1
19389	H	86.02275	91.93402	74.36797	1030.44628	-1443.58215	62.51597	1
19390	C	86.48652	91.41306	69.68409	-74.69995	-672.78012	721.57706	1
19391	O	86.24001	91.88536	68.56082	244.19435	-406.74222	-39.09961	1
19392	N	86.31614	90.22061	70.13318	-630.08624	288.07106	-886.57760	1
19393	H	86.53158	89.98482	71.09685	-645.89063	-732.50064	-1321.33180	1
19394	C	85.65350	89.20859	69.32686	-866.42334	-394.87180	-682.34969	1
19395	H	86.24573	89.18618	68.34527	-2675.93056	679.11773	2629.31080	1
19396	C	85.68083	87.83912	70.11357	-358.16333	313.12281	925.34128	1
19397	H	86.23474	87.95868	71.13447	-16.24114	-103.25532	376.39771	1

19398	H	84.68576	87.54794	70.38962	1718.82246	1326.38695	-630.55678	1
19399	S	86.61023	86.64469	69.06215	-50.82005	101.37724	108.52684	1
19400	C	84.10099	89.64817	69.19973	250.28225	421.86916	421.67475	1
19401	O	83.47844	90.06724	70.14782	518.43160	658.49807	501.25809	1
19402	N	83.62418	89.26721	68.01808	388.36428	-593.77937	3.36559	1
19403	H	84.30889	88.90981	67.27880	7.99775	-517.41069	3082.36441	1
19404	C	82.40033	89.86957	67.54325	33.04059	395.74339	696.30494	1
19405	H	81.92367	90.20402	68.45631	-1695.75470	-1279.06619	1519.24325	1
19406	C	82.98938	91.06734	66.80358	-97.03444	643.41197	462.01586	1
19407	H	83.06227	90.71667	65.73300	301.39525	667.39860	1197.64732	1
19408	H	84.01056	91.32885	67.20216	-2717.24498	1403.26406	4554.72692	1
19409	C	81.86241	92.33144	66.83931	-100.51346	-355.94163	451.35959	1
19410	O	81.26444	92.49629	67.88133	-123.49448	836.49012	-423.84977	1
19411	O	81.73824	92.90212	65.73953	505.87243	-49.16202	-136.67580	1
19412	C	81.44699	88.95273	66.49321	-697.74549	-128.14395	-396.21222	1
19413	O	81.94340	88.22000	65.64855	-135.62184	-202.50531	111.11008	1
19414	N	80.18566	89.19185	66.68201	822.78239	517.46133	19.22785	1
19415	H	79.99725	89.95430	67.34157	-4216.95115	-491.14391	2841.03205	1
19416	C	79.25950	88.39655	65.93604	443.32225	-274.70689	-250.75267	1
19417	H	79.84541	87.77789	65.22792	-2063.19944	100.63986	-2432.86572	1
19418	C	78.37578	87.50275	66.91723	331.70625	97.08802	18.52404	1
19419	H	77.46021	88.04328	67.20138	-1853.06432	-296.24531	303.25194	1
19420	H	79.08735	87.36853	67.75147	218.81671	395.32797	3882.92164	1
19421	C	77.86445	86.09505	66.48082	-861.66110	-393.03663	324.19958	1
19422	H	77.49317	86.19663	65.42070	-609.89146	-1110.45287	2388.08102	1
19423	H	77.06464	85.75577	67.14655	734.71172	1230.63013	1383.57171	1
19424	C	79.23914	85.17589	66.55653	13.54552	-176.86676	601.56429	1
19425	H	79.81563	85.43332	65.65973	-1742.89265	-1996.79897	-783.33539	1
19426	H	79.75020	85.58081	67.48286	1259.57953	-1783.00874	-775.02640	1
19427	N	78.71300	83.93980	66.64390	129.68470	638.74798	541.49376	1
19428	H	78.51800	83.39480	65.82790	1536.04414	1718.37737	-2140.13364	1
19429	C	78.40500	83.36480	67.75690	-669.71685	382.72445	-503.93154	1
19430	N	78.10900	83.97080	68.86490	775.37864	311.89971	-57.01942	1
19431	H	78.26600	84.95480	68.95690	-1726.74713	1644.23690	-2064.52110	1
19432	H	77.74400	83.35480	69.56290	-1361.87435	1940.68538	-2079.11843	1
19433	N	78.05200	82.10080	67.70790	-574.68861	534.41367	-338.04985	1
19434	H	78.04200	81.66580	66.80690	-1278.12271	2590.29701	1268.70153	1
19435	H	77.44800	81.87880	68.47390	-1860.96389	1828.68648	-1774.12020	1
19436	C	78.18749	89.41033	65.27618	54.23989	450.25796	-398.77136	1
19437	O	77.58516	90.09318	66.06454	97.39588	327.97479	-462.24407	1
19438	N	77.97230	89.27335	63.89942	444.24809	-848.81051	200.21653	1
19439	H	78.56204	88.63627	63.36686	1491.72204	-1070.38255	-1131.95692	1
19440	C	77.34463	90.46538	63.33059	-186.11373	719.37517	621.55804	1
19441	H	76.52031	90.54675	64.07759	2479.72502	-492.10809	-247.93904	1
19442	C	78.10418	91.83296	63.36213	432.13280	40.09186	-661.77841	1
19443	H	78.80808	91.96760	64.23468	249.16135	2339.24070	1689.01571	1
19444	H	78.59313	92.08194	62.39732	-804.69176	984.95620	2451.58074	1
19445	C	76.93771	92.84413	63.51903	883.70022	108.99035	-499.42560	1
19446	C	76.31184	93.11507	64.77101	375.62821	260.13413	-265.29274	1
19447	H	76.67070	92.50892	65.62093	251.28372	2272.05111	3646.81408	1
19448	C	75.06274	93.77305	64.78640	-1039.80341	-483.95541	-223.09308	1
19449	H	74.61781	93.92579	65.74902	609.06427	1627.16102	-2294.24544	1
19450	C	74.56445	94.32082	63.63323	-555.85474	1173.19664	410.61196	1
19451	H	73.66404	94.96001	63.74251	-1892.15202	-99.15710	1651.25894	1
19452	C	76.50489	93.48598	62.29256	-800.23239	277.58418	367.48673	1
19453	H	77.02959	93.34363	61.40474	3888.79891	-74.90274	634.54392	1
19454	C	75.32764	94.23569	62.41796	-811.87674	648.73363	430.02642	1
19455	H	74.94333	94.74129	61.50952	-189.21388	4005.88840	1716.38096	1
19456	C	76.91122	90.07453	61.80850	692.81359	-767.31540	160.29140	1
19457	O	77.77899	89.68264	61.04103	-250.47585	-1381.68350	965.45360	1
19458	N	75.69633	90.44671	61.56273	873.02674	911.77347	128.26745	1
19459	H	74.95642	90.76769	62.24674	-1268.02416	695.74117	307.31918	1

19460	C	75.10684	89.79408	60.41496	682.48534	-581.01073	755.49108	1
19461	H	75.83452	89.08477	59.95318	717.71158	-726.57847	-1445.89999	1
19462	C	73.80415	89.19404	61.07405	-253.54974	-200.23671	-231.60822	1
19463	H	73.18449	88.69099	60.32478	-1816.42715	1932.31430	-979.80437	1
19464	H	73.16839	89.97070	61.56040	-224.31734	-1193.32647	-1173.96055	1
19465	C	74.22058	88.09670	62.09458	590.00212	-315.84469	-396.72286	1
19466	C	74.78829	86.83020	61.74759	-39.72636	-103.32033	-147.74330	1
19467	H	74.80502	86.53663	60.70991	532.73761	835.94774	2012.99728	1
19468	C	75.21693	85.94472	62.76974	-143.70030	-7.92584	239.23695	1
19469	H	75.63354	84.95101	62.48320	2280.84454	1517.01068	1295.85349	1
19470	C	75.13551	86.32585	64.08954	-98.95772	362.30450	-582.98103	1
19471	O	75.51380	85.64882	65.28416	-244.90161	799.44028	-643.66805	1
19472	H	75.54600	84.77580	64.99090	1.54280	-1167.25246	2919.82418	1
19473	C	74.42402	88.56586	63.42849	330.60110	21.29089	361.51161	1
19474	H	74.35145	89.66635	63.69364	1224.44501	-355.79845	-2316.81213	1
19475	C	74.74296	87.65016	64.41151	-71.88011	-510.35767	-1189.66379	1
19476	H	74.71045	87.96104	65.46387	49.44394	1046.49665	-3997.91403	1
19477	C	74.63764	90.99784	59.41960	645.43937	-1004.78933	-113.83676	1
19478	O	74.67270	92.13446	59.82094	-516.89844	79.70442	401.04258	1
19479	N	74.17189	90.53887	58.23478	239.12225	235.41362	365.71322	1
19480	C	74.61516	89.27536	57.67748	-49.97044	1188.40902	-1032.71165	1
19481	H	75.71704	89.27899	57.72980	1150.78506	-1173.49198	2040.99089	1
19482	H	74.16980	88.49123	58.36129	1143.08029	-2543.09585	4438.59231	1
19483	C	73.84743	91.54492	57.26137	104.34994	312.86407	1050.61331	1
19484	H	74.61909	92.35368	57.27031	-1890.81394	-1101.27740	-24.23334	1
19485	C	73.87500	90.81323	55.86168	67.06406	644.13764	511.97468	1
19486	H	72.94154	91.10455	55.24846	-966.27173	1398.15772	35.46250	1
19487	H	74.74307	91.07685	55.29465	-1763.64934	964.48530	1942.12307	1
19488	C	73.96588	89.30941	56.23797	327.92219	313.24712	-498.31240	1
19489	H	72.97938	88.89459	56.31087	-526.57899	295.26440	-1281.11507	1
19490	H	74.57310	88.65982	55.49075	-11.57043	-1822.42607	3233.41165	1
19491	C	72.35163	92.17950	57.41610	505.73855	374.30391	-62.04388	1
19492	O	71.98225	92.99767	56.62479	293.35885	450.17397	54.92198	1
19493	N	71.70800	91.47762	58.38820	200.44096	446.68373	455.38199	1
19494	H	72.13406	90.85945	59.13805	1490.53185	-644.50962	983.16267	1
19495	C	70.58810	92.23568	58.96953	27.44304	502.04342	504.65477	1
19496	H	70.88398	93.37104	58.98650	1111.88311	-1426.50171	389.36462	1
19497	C	69.40421	91.85527	58.07281	210.71359	98.46252	1016.05619	1
19498	H	69.70020	91.91930	57.00498	-354.72891	1558.27058	1310.42428	1
19499	H	69.17260	90.73274	58.09640	2927.13254	-122.69263	2293.88617	1
19500	C	68.00740	92.60354	58.42037	857.97505	-793.36211	-50.13130	1
19501	O	67.75071	93.40153	59.33187	-768.25882	338.90199	326.31268	1
19502	N	67.13480	91.95400	57.66172	41.74500	-1044.78947	197.69479	1
19503	H	67.60729	91.15650	57.17868	506.08343	-2008.76223	-3107.63087	1
19504	H	66.06408	91.99785	57.61407	-654.91593	-104.90745	-1477.71600	1
19505	C	70.55654	91.44675	60.39288	-786.90017	528.45783	476.52803	1
19506	O	71.20668	90.47442	60.72535	-822.97524	-681.85117	-363.83931	1
19507	N	69.64252	92.10117	61.10124	-289.94309	-19.27188	277.28540	1
19508	H	69.02845	92.80890	60.56961	-1659.39008	-465.80113	-1704.12861	1
19509	C	69.27308	91.63346	62.39704	497.86010	-51.47180	491.51164	1
19510	H	69.97693	90.82876	62.49897	335.24338	-2706.43653	360.15508	1
19511	C	69.61885	92.81130	63.39761	-674.55896	1512.09179	-75.46493	1
19512	H	69.54210	93.84160	62.92548	3770.27092	996.51408	447.25720	1
19513	H	68.85775	92.82902	64.22208	1464.76837	612.48018	2711.27262	1
19514	C	71.12694	92.75759	63.94777	-324.37189	-232.22168	-505.57142	1
19515	O	71.44407	91.90625	64.82324	-330.28277	261.22540	-226.53969	1
19516	O	71.84414	93.65248	63.49228	-33.12240	-581.16667	326.81597	1
19517	C	67.72907	91.15092	62.46447	-346.60001	-517.92104	-243.32046	1
19518	O	67.22326	90.83276	63.51633	-230.93422	403.88923	794.64703	1
19519	N	67.11517	91.02385	61.30238	654.46879	-429.34320	1036.77696	1
19520	H	67.68776	91.33533	60.49225	-1144.45368	-1402.34028	729.62035	1
19521	C	66.13250	90.03481	61.02655	-82.27284	116.27101	-111.90561	1

19522	H	65.59929	89.83524	61.96129	914.91672	-2638.18675	-1216.17878	1
19523	C	64.99391	90.53647	60.00452	796.05292	319.07999	-79.33213	1
19524	H	64.77657	91.60281	60.26300	1190.50969	2327.08943	-534.85023	1
19525	H	65.48384	90.79404	59.00012	1764.52536	-1948.57536	-1056.93357	1
19526	C	63.75366	89.73468	59.86033	-167.34428	301.73079	-235.14835	1
19527	H	64.03495	88.68055	59.68411	686.43430	271.06019	-61.81419	1
19528	C	62.80505	89.84587	61.06504	613.39313	-80.02355	-345.99187	1
19529	H	61.86609	89.23605	60.90709	-855.48305	1754.55356	-723.40860	1
19530	H	62.31412	90.87194	61.35183	-466.79812	2530.40366	-435.45808	1
19531	H	63.26468	89.55406	62.01586	927.69308	-1055.95336	-1442.32973	1
19532	C	62.88471	90.19797	58.74330	871.61383	606.67437	388.64466	1
19533	H	63.46063	90.49862	57.82481	2651.64316	74.68060	1634.49088	1
19534	H	62.02559	89.48491	58.48438	-1085.49424	-1115.61647	-911.74082	1
19535	H	62.35680	91.08480	59.14873	1810.63726	3641.62336	441.12054	1
19536	C	66.93284	88.75161	60.47991	-602.53598	226.85941	-982.83794	1
19537	O	66.42202	87.63191	60.66416	-365.04610	-105.76908	-269.99700	1
19538	N	68.00865	88.97952	59.69989	775.16080	85.15073	-761.48662	1
19539	H	68.36824	89.90230	59.78319	5643.73079	700.32236	-3079.55840	1
19540	C	68.89919	87.87667	59.54001	14.87435	287.61631	-442.15552	1
19541	H	68.28057	87.17717	58.97790	893.09574	734.01386	621.02204	1
19542	C	70.15894	88.39082	58.73071	487.80086	-516.18902	-57.46484	1
19543	H	70.86944	87.72850	59.23047	-1160.17836	1893.40235	261.10157	1
19544	H	70.50019	89.44857	58.91634	-1420.54571	-1965.88950	-11.84655	1
19545	C	69.90239	88.23424	57.24604	809.92307	-434.56535	362.30267	1
19546	C	69.67396	89.09544	56.18202	-148.47082	164.39923	-253.11859	1
19547	H	69.71822	90.21811	56.12992	1636.60832	-3986.68704	-1704.50931	1
19548	N	69.34838	88.36538	55.10742	-377.83795	252.91748	-760.28776	1
19549	H	69.22169	88.79172	54.18761	35.32705	-1321.45633	-483.92943	1
19550	C	69.38045	87.02142	55.34425	298.23918	400.84461	-716.85798	1
19551	C	69.76084	86.85032	56.76805	-100.10357	533.86625	374.16985	1
19552	C	69.74657	85.57794	57.38896	-513.48771	380.59575	-150.16837	1
19553	H	70.08934	85.44094	58.47661	2863.10293	-195.14269	-853.70822	1
19554	C	69.68000	84.43180	56.55090	-261.75673	529.31251	708.63711	1
19555	H	69.73600	83.43380	56.95890	1497.44626	472.94824	2722.92890	1
19556	C	69.18754	85.81288	54.55624	-40.94057	-686.72534	613.40267	1
19557	H	68.61766	85.75357	53.62452	59.80149	575.99326	751.89077	1
19558	C	69.46400	84.55980	55.13790	-738.99889	-507.25343	195.19978	1
19559	H	69.43900	83.61780	54.60990	-1250.26919	2891.48783	254.33855	1
19560	C	69.44910	87.18086	60.94681	-1170.34469	90.36302	642.18919	1
19561	O	69.88141	86.04319	60.95530	406.05595	-351.89187	9.21031	1
19562	N	69.57229	88.14888	61.83459	-18.73821	458.82937	-104.76858	1
19563	H	69.16400	89.06385	61.56010	-763.05138	-90.10880	-1261.58454	1
19564	C	69.84095	87.77082	63.22262	338.49306	-670.37104	289.21627	1
19565	H	70.38442	86.82924	63.08864	-1055.85625	2329.75192	833.14103	1
19566	C	70.56310	88.96396	63.97860	-169.13952	104.20929	54.94118	1
19567	H	71.09183	89.77673	63.35304	88.75086	-2.38056	488.71165	1
19568	C	69.58448	89.66496	64.97482	529.10244	-206.63019	189.23429	1
19569	H	69.39341	88.93959	65.82638	-3257.81036	133.47510	-1547.95172	1
19570	H	68.63442	89.99187	64.40871	2773.38087	230.36602	-1421.35943	1
19571	H	70.03147	90.61421	65.40769	1350.46725	1840.00804	119.43503	1
19572	C	71.71769	88.29011	64.79727	-1069.34355	-458.70308	-24.95146	1
19573	H	72.38203	89.10235	65.18101	1393.56829	935.90725	-899.19632	1
19574	H	71.29081	87.66824	65.60288	144.02910	-1121.88419	2204.69673	1
19575	H	72.37987	87.55710	64.22189	2131.39101	-889.69757	887.63281	1
19576	C	68.52421	87.34661	64.05306	-331.85411	-547.41812	612.97996	1
19577	O	68.69639	86.71690	65.09476	-186.14819	434.09962	-334.45584	1
19578	N	67.33713	87.68877	63.50892	369.77257	-158.59307	498.41048	1
19579	H	67.43863	87.95768	62.50980	3642.11307	330.12935	-2965.52310	1
19580	C	66.22124	86.89700	63.95606	-262.30506	-713.05130	-246.12800	1
19581	H	66.52292	87.00553	65.03684	-845.25102	2706.19875	-1716.22839	1
19582	C	64.83624	87.61677	63.54502	-67.53124	-241.04251	-385.25436	1
19583	H	65.03826	88.69492	63.37315	-2058.72128	-133.48622	466.97123	1

19584	C	63.98962	87.03997	62.35574	469.22553	-101.07522	-147.96311	1
19585	H	63.81657	85.88961	62.48976	1769.81522	117.32704	491.13250	1
19586	H	62.95572	87.54141	62.30421	69.90659	3727.86753	-1310.36539	1
19587	H	64.45609	87.09748	61.37849	210.78386	-3399.97836	-3870.94070	1
19588	C	63.82093	87.53987	64.76007	224.65255	-350.36708	-640.28890	1
19589	H	62.84968	87.93923	64.43239	1731.28621	-176.10338	1874.11508	1
19590	H	63.66077	86.47533	65.05344	-3395.60855	-2172.79601	-1018.22669	1
19591	H	64.14573	88.21737	65.56670	1405.64664	2055.88077	2712.95669	1
19592	C	66.40608	85.38646	63.45800	394.70721	190.41470	-112.23742	1
19593	O	66.19800	84.42780	64.14390	-493.11914	598.47032	202.09267	1
19594	N	66.97967	85.36540	62.20224	-338.75811	-197.64111	780.10877	1
19595	H	66.93528	86.19950	61.61556	62.77103	-2480.36867	-242.26833	1
19596	C	67.17300	83.92780	61.67790	674.54896	328.55623	510.61167	1
19597	H	66.24200	83.39480	61.79890	1638.57860	2263.41028	1446.62985	1
19598	C	67.57000	83.97580	60.15290	593.55725	-404.78203	546.19152	1
19599	H	68.48300	84.59580	60.02690	2092.95810	2025.78972	-1178.76287	1
19600	C	67.61400	82.57980	59.52390	-555.46018	461.17386	576.70484	1
19601	H	66.79600	81.88480	59.80990	1850.95937	-1436.48296	-2082.21162	1
19602	H	68.52000	82.02080	59.84090	2853.10552	1308.51358	-28.99859	1
19603	H	67.66500	82.68580	58.41990	-2623.79696	-1730.10003	-230.85054	1
19604	C	66.50700	84.79580	59.46790	822.57960	356.96003	-111.35045	1
19605	H	66.63300	84.77480	58.36390	-2518.88562	-463.89648	-1838.32479	1
19606	H	66.54812	85.88824	59.74779	-363.92100	-610.36256	-1065.48989	1
19607	H	65.54000	84.29880	59.69790	-1709.77409	-2187.65009	-1478.61206	1
19608	C	68.20200	83.10680	62.39890	539.66221	596.06844	-423.27764	1
19609	O	68.02100	81.91380	62.76490	254.46358	-638.90999	-367.88389	1
19610	N	69.35700	83.66280	62.70190	600.68696	-446.16128	-363.29158	1
19611	H	69.64500	84.55180	62.35490	-1794.89989	-1009.30813	-2381.52954	1
19612	C	70.38900	83.01780	63.55090	-427.52719	400.57925	710.40315	1
19613	H	70.48900	81.98180	63.26390	-1082.04763	2674.05858	-1277.50920	1
19614	C	71.76000	83.63580	63.31290	-495.13612	714.33280	311.70241	1
19615	H	72.58800	82.97480	63.64590	-2649.12598	1678.41681	377.38975	1
19616	H	71.82400	84.63980	63.78390	-809.58490	3047.25306	123.96293	1
19617	C	72.03300	83.72280	61.79390	-226.37882	-514.53022	717.45198	1
19618	C	71.81600	82.59080	60.95990	268.69434	-710.11494	-486.53216	1
19619	H	71.47000	81.69580	61.45590	-2327.39246	1917.39177	941.36044	1
19620	C	72.08100	82.67680	59.54890	595.09723	107.47225	674.57000	1
19621	H	71.79200	81.91980	58.83390	-2140.52028	1676.37226	-1606.78140	1
19622	C	72.48800	83.89180	59.02390	184.09325	862.65264	-250.80159	1
19623	H	72.66000	83.92580	57.95890	-2550.20373	1504.79887	1105.49257	1
19624	C	72.42300	84.92880	61.19290	-61.69377	134.37953	-899.76818	1
19625	H	72.60212	85.79382	61.83553	286.60225	1115.18370	3011.02290	1
19626	C	72.64557	85.06358	59.78246	-514.01070	-363.62584	-333.81257	1
19627	H	72.90056	86.07285	59.41189	-1916.18500	1137.40556	-4053.63405	1
19628	C	70.05300	82.90880	64.99590	-713.76563	573.76150	119.90452	1
19629	O	70.29400	81.84380	65.59190	572.39985	-252.02142	-465.85988	1
19630	N	69.42700	83.89580	65.60790	-680.07231	-222.55687	-457.85248	1
19631	H	69.17200	84.72080	65.10890	-2608.54160	1221.67570	1294.60872	1
19632	C	68.97800	83.85380	67.00790	-793.53447	-174.45386	432.25232	1
19633	H	69.89000	83.70380	67.56490	336.69557	-2272.71660	-2140.46556	1
19634	C	68.19327	85.20238	67.38052	20.96052	396.91929	320.18631	1
19635	H	67.15103	85.17565	66.88814	-2200.24288	-1309.18315	-1205.69578	1
19636	H	68.76227	86.12614	67.01445	1316.29897	-2602.75607	-963.48885	1
19637	C	67.94777	85.26782	68.92136	-939.38271	-300.42884	-433.51516	1
19638	H	67.37700	84.47980	69.36990	-260.93854	459.34235	-3099.80111	1
19639	H	67.25253	86.15706	69.13509	3670.77444	485.60289	-1509.75950	1
19640	C	69.32120	85.46765	69.61893	-543.00283	73.27686	911.21640	1
19641	O	69.82172	86.61465	69.64047	-327.08045	-494.93437	-375.20095	1
19642	N	70.01700	84.39780	70.10590	421.94438	-470.16065	-547.39151	1
19643	H	69.81800	83.47480	69.77790	1622.55556	1466.17372	-2256.12547	1
19644	H	70.95200	84.61280	70.38790	-1626.88291	-2631.03011	582.28280	1
19645	C	68.01400	82.64180	67.17590	-691.47896	-70.35297	-598.42540	1

19646	O	68.15500	81.79780	68.04290	494.45132	295.38965	536.06006	1
19647	N	67.09000	82.50080	66.23490	-551.73207	104.93306	-637.14924	1
19648	H	67.03700	83.21580	65.54290	-1837.25908	1532.87338	2058.40188	1
19649	C	66.19800	81.42780	66.04390	-658.87063	636.21011	110.13260	1
19650	H	65.61500	81.36480	66.95090	-759.21271	2996.09497	624.74465	1
19651	C	65.20800	81.57280	64.87290	366.33712	-420.55116	-710.52024	1
19652	H	64.70000	82.55680	64.95890	702.59930	-2273.50156	-2045.72539	1
19653	H	65.78400	81.60080	63.92390	-2791.58441	1459.92500	-216.71896	1
19654	C	64.14300	80.54880	64.85190	187.84801	-873.43987	144.54341	1
19655	C	64.10100	79.51580	63.85590	-299.93141	-537.13496	674.88244	1
19656	H	64.80100	79.56380	63.03490	2737.37139	337.63242	1498.19734	1
19657	C	63.15900	78.47080	63.93090	606.96738	327.26839	591.34489	1
19658	H	63.17600	77.65880	63.21990	2075.93021	1599.28753	-1732.86698	1
19659	C	62.29400	78.35380	65.04990	324.67526	-801.51592	265.39230	1
19660	H	61.65200	77.48780	65.10490	-1204.67534	-2702.79375	1068.70587	1
19661	C	63.23200	80.41480	65.92290	645.76086	-202.91495	601.66398	1
19662	H	63.26300	81.05080	66.79490	-1816.94921	942.85338	2400.80517	1
19663	C	62.34100	79.34080	66.02690	-647.29577	632.72424	-170.73402	1
19664	H	61.57100	79.40480	66.78190	-2437.31887	825.01055	1827.11800	1
19665	C	66.93500	80.04880	65.78090	185.51737	-787.23867	-405.11360	1
19666	O	66.63200	79.06580	66.49690	43.02157	685.26939	-396.46884	1
19667	N	67.94200	79.96780	64.95690	-157.12304	-819.41831	101.50161	1
19668	H	68.28900	80.79880	64.52890	631.81715	-2943.34618	889.07764	1
19669	C	68.76200	78.73780	64.76490	-293.23029	419.11986	762.23257	1
19670	H	68.18600	77.88280	64.44390	883.51482	-325.42108	-2998.15999	1
19671	C	69.92700	79.06480	63.73590	-29.97833	743.23518	-536.57555	1
19672	H	70.79800	79.64880	64.10390	710.23353	-279.83598	-3048.93808	1
19673	H	69.47600	79.59580	62.87090	-1776.60285	2484.17863	800.90759	1
19674	C	70.63800	77.74080	63.25190	-577.75789	-688.99587	-158.42621	1
19675	H	69.81100	77.09780	62.88090	1459.71849	2646.72906	-877.34153	1
19676	H	71.15600	77.18480	64.06190	1320.76984	2329.68180	1651.82632	1
19677	C	71.61500	77.98280	62.06390	-183.57874	683.34146	-587.44140	1
19678	O	71.30400	77.62580	60.88590	242.65659	755.72354	-3.70144	1
19679	N	72.76000	78.65180	62.30290	-767.02497	255.55323	279.40772	1
19680	H	73.02500	78.74080	63.26290	-86.07817	1769.30667	2604.48148	1
19681	H	73.53400	78.74680	61.67590	-1140.38143	2031.38641	-2128.31023	1
19682	C	69.42700	78.31480	66.03490	-560.53207	-306.17687	656.15684	1
19683	O	69.49300	77.10380	66.30090	598.34213	158.15066	480.70878	1
19684	N	69.91900	79.24580	66.90290	435.18209	-379.81905	-605.43855	1
19685	H	69.86900	80.20080	66.61990	2586.19785	41.11701	-1776.96585	1
19686	C	70.55000	78.86580	68.12590	-792.89712	-47.72209	462.42339	1
19687	H	71.32000	78.13480	67.92590	-470.84950	-2694.18667	1548.35292	1
19688	C	71.25000	80.09480	68.80590	188.39862	894.86349	14.70330	1
19689	H	71.58700	79.73080	69.79990	2737.90395	307.94611	-1504.50617	1
19690	H	70.61000	80.97980	69.01290	-3106.40486	-542.35814	-61.66605	1
19691	N	73.40700	81.20880	68.59690	-218.00415	627.20489	531.09856	1
19692	H	73.43300	81.28880	69.59390	-2049.35763	1016.00048	2170.68230	1
19693	C	72.35200	80.62980	68.01290	-257.13638	569.33224	-671.77808	1
19694	C	74.26900	81.55580	67.58590	-164.56622	-892.94456	-4.45513	1
19695	H	75.19500	82.08080	67.81790	964.36751	-214.85061	2983.57918	1
19696	N	73.76200	81.31280	66.40590	153.90073	-146.19086	814.23736	1
19697	C	72.56300	80.67780	66.66290	675.42861	306.15047	-521.55498	1
19698	H	72.02400	80.25780	65.82290	1189.81656	-2020.43699	-2086.34960	1
19699	C	69.64000	78.25780	69.17190	-755.56318	359.94509	383.12254	1
19700	O	70.02400	77.39280	69.98090	-542.31828	-575.57332	46.31880	1
19701	N	68.39300	78.68480	69.17490	37.03482	-838.75477	6.91137	1
19702	H	68.03400	79.38880	68.56790	-2092.28871	1362.26491	-1926.01792	1
19703	C	67.34400	78.10680	69.99190	-494.55348	362.81404	683.20302	1
19704	H	67.88300	77.80780	70.87890	1815.76342	-2245.06283	-1231.15866	1
19705	C	66.26800	79.14380	70.38190	346.21217	-751.55797	-367.22305	1
19706	H	65.65100	79.44880	69.50990	-1693.58618	2212.05637	1478.65630	1
19707	C	65.27500	78.49980	71.45990	810.35051	372.83942	160.12749	1

19708	H	65.85400	78.09680	72.31790	-712.13120	2361.19444	1960.37271	1
19709	H	64.71300	77.63880	71.03790	-1930.22039	1063.31385	-2252.38262	1
19710	H	64.49100	79.19980	71.82090	958.24805	2014.32142	2219.50651	1
19711	C	66.88300	80.46080	70.88990	570.23939	-635.35497	299.77828	1
19712	H	67.63100	80.93980	70.22190	1952.82010	-583.24383	-2387.35068	1
19713	H	67.49200	80.42380	71.81890	-2319.38512	1816.46620	1127.13144	1
19714	C	65.83800	81.51180	71.27090	-837.47420	-341.87966	-155.34711	1
19715	H	65.02200	81.53180	70.51890	1138.12320	792.83102	-2818.84247	1
19716	H	65.46700	81.24480	72.28390	421.88059	-2162.87154	-2239.13990	1
19717	H	66.38100	82.47880	71.20490	-2339.64765	-1869.38214	-975.77161	1
19718	C	66.76900	76.84280	69.45490	-348.32388	614.17860	-585.60059	1
19719	O	66.63400	75.81380	70.12590	94.07323	-619.24440	474.58570	1
19720	N	66.31500	76.98580	68.18590	150.49793	832.75558	32.96124	1
19721	H	66.41500	77.87280	67.74190	-2625.27939	-320.82662	-1715.64358	1
19722	C	65.74200	75.94280	67.37790	143.03148	-218.12590	-870.92860	1
19723	H	64.79300	75.72480	67.84490	324.30234	2449.14976	1952.28320	1
19724	C	65.55500	76.47180	65.99690	507.46353	749.68793	101.41441	1
19725	H	65.01800	77.43680	65.87590	-2318.51205	-1644.79931	1358.65944	1
19726	H	66.57200	76.68280	65.60290	-2388.01253	1330.52391	1576.04284	1
19727	C	64.89500	75.49180	64.95890	689.88165	-81.96528	579.19872	1
19728	H	65.50600	74.59380	64.72490	1867.85014	-2493.78257	358.60383	1
19729	H	64.58300	76.09980	64.08290	-1223.06154	2904.21073	154.55697	1
19730	S	63.30800	74.83580	65.62490	407.32895	-312.54930	193.31094	1
19731	C	62.41500	74.52080	64.05090	-732.40188	539.76075	152.14615	1
19732	H	61.57500	73.84080	64.30990	1885.30766	-1394.65765	-2085.09637	1
19733	H	63.09600	74.03980	63.31690	1010.02979	2213.89121	1995.94345	1
19734	H	62.01300	75.46580	63.62590	-1991.76569	1155.70527	2156.46978	1
19735	C	66.62700	74.71180	67.33690	566.02024	-547.63433	-443.69196	1
19736	O	66.22400	73.62780	67.63590	480.69322	-603.67269	120.57797	1
19737	N	67.94400	74.80680	67.04190	404.31455	222.55930	702.67172	1
19738	H	68.38100	75.69680	66.93390	-1575.41415	1039.49512	2523.97734	1
19739	C	68.78100	73.65580	66.86890	-605.26123	88.09302	682.88605	1
19740	H	68.16600	72.78480	66.69290	1488.80437	731.21489	2668.47951	1
19741	C	69.72500	73.87980	65.70990	-184.38339	-815.74160	-356.41889	1
19742	H	70.51200	74.64080	65.89490	2162.54580	2261.53862	-309.31514	1
19743	C	70.49500	72.60180	65.37190	369.83477	57.93103	-830.26144	1
19744	H	71.16400	72.77680	64.50290	-1839.35718	-1920.56684	1681.26462	1
19745	H	71.16100	72.19280	66.16290	-1703.04796	-1030.51563	-2442.48400	1
19746	H	69.76400	71.82480	65.06090	1331.36376	2675.36942	-990.69164	1
19747	C	69.01400	74.34080	64.41390	-823.17850	-203.85299	-354.48575	1
19748	H	68.75000	75.40280	64.60590	-2516.38675	1881.30151	308.46887	1
19749	H	69.68600	74.31480	63.52990	-1954.85134	-2283.72458	-933.28185	1
19750	H	68.06000	73.80680	64.21390	2318.63136	2122.17780	38.83395	1
19751	C	69.60800	73.28180	68.10590	724.50327	-353.17356	406.48092	1
19752	O	69.97600	72.13480	68.30190	-6.48210	-546.09172	-568.24874	1
19753	N	69.88600	74.25980	68.99390	355.11130	-727.16783	212.01169	1
19754	H	69.62600	75.21180	68.84890	1747.25429	-2604.01094	-114.20069	1
19755	C	70.53000	73.95480	70.25190	890.15267	-98.99091	-124.15531	1
19756	H	70.92300	74.92080	70.53490	-44.29553	-2566.58964	-1815.10344	1
19757	H	71.34000	73.25280	70.12490	2699.65002	1506.22475	557.66958	1
19758	C	69.62700	73.38380	71.24690	-462.30739	567.03467	552.12983	1
19759	O	70.00600	72.62580	72.09890	-193.25623	-684.95282	337.23549	1
19760	N	68.35400	73.82580	71.22490	303.84146	607.84358	499.25097	1
19761	H	67.99000	74.44980	70.53890	1518.53857	633.74333	-2679.06692	1
19762	C	67.42000	73.44580	72.28490	481.95988	-659.95935	-392.42077	1
19763	H	67.91200	72.76780	72.96590	-209.37439	-173.82877	-3136.21574	1
19764	C	66.91300	74.68680	73.11490	277.41407	640.07114	586.05873	1
19765	H	66.12200	75.16780	72.50090	629.04919	1544.09082	-2668.03940	1
19766	H	67.73000	75.39380	73.37290	-1159.77067	-1007.18160	-2748.18601	1
19767	C	66.30000	74.35180	74.45690	522.88303	600.40511	-439.91228	1
19768	H	65.60900	73.48980	74.34190	-1410.89194	1895.47200	2082.55559	1
19769	C	67.30900	73.99080	75.58390	-362.58732	193.49428	-817.99640	1

19770	H	67.94500	74.88180	75.77790	-2892.61340	-571.10531	1112.20412	1
19771	H	67.87700	73.11080	75.21290	1548.61834	1909.14294	1958.98023	1
19772	H	66.84500	73.70680	76.55190	1694.49616	-1756.73421	1978.16583	1
19773	C	65.46100	75.57580	74.92890	-563.35646	-707.59131	135.68800	1
19774	H	66.10500	76.45080	75.16190	2758.03685	963.74418	1153.38843	1
19775	H	64.93300	75.42080	75.89390	-653.88616	-1901.84253	-2419.93456	1
19776	H	64.70300	75.83080	74.15790	-733.05921	964.69196	-2905.33347	1
19777	C	66.18200	72.68480	71.76890	-558.52970	148.18115	-712.57725	1
19778	O	65.92800	71.57280	72.17990	653.95009	-85.13834	422.08078	1
19779	N	65.43300	73.25880	70.81490	343.55608	-92.58705	-762.55901	1
19780	H	65.71600	74.14280	70.44990	-1163.42503	2422.63582	1645.51100	1
19781	C	64.18200	72.72380	70.30190	-374.46427	-586.85441	589.75481	1
19782	H	63.58800	72.69080	71.20390	-2352.18933	1347.05807	-1610.37968	1
19783	C	63.33000	73.64380	69.47090	-889.17524	-144.75981	-180.35622	1
19784	H	63.72500	73.82480	68.44790	-1271.23091	-2859.32624	-323.53179	1
19785	C	61.92300	73.14780	69.18390	-170.71055	892.82657	-116.98351	1
19786	H	61.36800	72.94880	70.12590	1861.32511	2276.00479	1113.35569	1
19787	H	61.30500	73.85280	68.58890	-2070.89136	1102.10971	-2105.49589	1
19788	H	61.96700	72.21880	68.57590	2155.72512	-1228.19024	-1923.78266	1
19789	C	63.22400	75.10980	70.05690	-718.62982	-198.66685	534.75858	1
19790	H	62.72800	74.93580	71.03590	-1730.32376	-2217.93762	-1413.04642	1
19791	H	64.20300	75.58080	70.29190	66.74507	-2988.46981	-970.29498	1
19792	C	62.38800	76.05980	69.16990	-910.04492	-86.37760	-98.35264	1
19793	H	62.69600	75.86280	68.12090	-2203.35371	-1315.82713	-1826.20805	1
19794	H	62.61200	77.12580	69.38790	-2967.06608	946.92023	504.47801	1
19795	H	61.29600	75.86780	69.23290	607.52105	231.86098	-3075.47318	1
19796	C	64.17900	71.32780	69.69790	608.41724	-497.19667	447.90782	1
19797	O	63.61300	70.39280	70.22690	665.77352	413.69124	-49.84050	1
19798	N	64.84000	71.21580	68.46890	23.26596	-686.29764	-486.31440	1
19799	H	65.25800	71.95580	67.94690	2826.50967	-1121.17158	771.95129	1
19800	C	64.86800	69.95580	67.69390	591.19307	-660.26052	174.57177	1
19801	H	63.81200	69.72680	67.68790	-2273.18201	-1201.80999	1818.09324	1
19802	C	65.36600	70.19380	66.22890	-483.83997	754.89336	204.77972	1
19803	H	66.39600	70.60980	66.18990	1939.75970	-2072.16207	1335.46095	1
19804	H	65.22500	69.21180	65.72890	-1111.15153	-1699.49992	2401.12144	1
19805	C	64.53200	71.18780	65.44590	637.31819	-520.43286	-373.01987	1
19806	H	64.74800	72.23680	65.73890	1025.98501	-427.56025	-2940.46084	1
19807	C	64.82900	71.16480	63.94490	-202.32466	501.12193	739.32363	1
19808	H	64.37600	72.06480	63.47790	1021.29033	-2824.30811	-910.15096	1
19809	H	64.51100	70.21780	63.45690	-1796.97869	1877.96864	-1789.41669	1
19810	H	65.92000	71.13280	63.73590	-2328.62841	435.95955	2079.76066	1
19811	C	63.01800	70.99680	65.50990	328.84530	468.07369	-710.26629	1
19812	H	62.67500	69.94880	65.36790	-2178.15872	-2094.92540	882.41572	1
19813	H	62.52000	71.27080	66.46390	1278.89592	-1968.60660	2084.62357	1
19814	H	62.58300	71.55980	64.65590	924.31313	2313.69340	-1923.70129	1
19815	C	65.59900	68.81180	68.33190	-494.70155	410.04553	-657.61829	1
19816	O	65.01500	67.77580	68.08990	44.43369	757.13622	-235.04732	1
19817	N	66.67700	68.82680	69.08290	709.14638	-412.54576	158.52437	1
19818	C	67.51000	69.99280	69.37990	-321.02388	-694.84543	492.07167	1
19819	H	67.00000	70.92280	69.70990	-1125.30740	2944.24355	44.27198	1
19820	H	68.07300	70.27080	68.46290	336.48408	2910.91108	-1156.77297	1
19821	C	67.20100	67.63480	69.73590	-541.32715	713.59851	201.67861	1
19822	H	67.07000	66.78880	69.07690	-864.49203	3027.86277	135.81839	1
19823	C	68.66500	68.04580	70.17490	474.53261	395.09626	664.78028	1
19824	H	69.12400	67.49880	71.02590	-2147.45487	-1999.86567	1136.60055	1
19825	H	69.38400	67.82280	69.35690	665.81493	2145.02501	2201.29420	1
19826	C	68.55100	69.51580	70.42490	-703.07688	-403.16392	-428.72291	1
19827	H	69.49600	70.06980	70.24090	-969.60565	2612.90599	1468.35788	1
19828	H	68.18300	69.79180	71.43690	-2268.10015	-1923.87449	-1037.29430	1
19829	C	66.39300	67.26680	71.00390	-460.22454	742.80488	277.12409	1
19830	O	66.32900	66.10480	71.31490	-143.79429	642.64690	438.70699	1
19831	N	65.84600	68.26680	71.68190	518.76376	647.47320	-148.97223	1

19832	H	65.99600	69.19580	71.35290	2323.79627	686.95939	-2002.31293	1
19833	C	64.95700	68.17180	72.79490	393.67741	-675.38736	458.18254	1
19834	H	64.63100	69.17880	73.00590	2050.39186	1122.31898	2098.92922	1
19835	H	65.55800	67.86280	73.63690	1727.63420	97.06101	-2626.58938	1
19836	C	63.76000	67.32980	72.57190	-16.15531	-836.72768	-359.42025	1
19837	O	63.42600	66.47880	73.44190	-442.74268	-215.22819	-623.63315	1
19838	N	63.06200	67.53680	71.42990	760.01015	163.12671	313.22686	1
19839	H	63.28600	68.31780	70.85290	-1868.34063	1372.32815	2132.69438	1
19840	C	61.89500	66.79280	71.11990	127.61219	-580.96582	685.46881	1
19841	H	61.24900	66.80980	71.98490	-1369.68121	-2720.16075	-794.36821	1
19842	C	61.08100	67.31480	69.93990	586.47292	-685.33796	-77.70395	1
19843	H	60.31700	66.55780	69.66190	1187.72408	2580.89911	-1353.08395	1
19844	C	60.20100	68.50380	70.43690	-68.98729	-705.54588	569.86940	1
19845	H	59.64400	68.05180	71.28490	1657.94306	1186.21215	2391.77831	1
19846	H	59.37700	68.71880	69.72290	-672.71707	3057.52386	-352.73998	1
19847	H	60.89200	69.32080	70.73390	1489.79135	-1900.50530	-2010.09223	1
19848	C	61.97000	67.64580	68.73790	-11.14916	824.00639	-399.73436	1
19849	H	62.59600	68.53580	68.96190	-12.33331	-233.10734	3135.47366	1
19850	H	62.67200	66.81080	68.52690	1504.73905	-444.53988	2720.01118	1
19851	C	61.18200	67.81180	67.43490	-836.13465	-316.02936	-207.71407	1
19852	H	61.83300	68.03080	66.56190	2978.93554	-733.17551	-660.43712	1
19853	H	60.42100	68.61980	67.48290	1463.84887	618.99150	2710.79834	1
19854	H	60.54100	66.91780	67.27590	1961.95166	-2309.78589	814.63559	1
19855	C	62.10100	65.27780	70.85890	536.24226	-408.84263	603.55484	1
19856	O	61.32600	64.41780	71.31790	-96.29828	-193.75489	-762.56759	1
19857	N	63.17400	64.90480	70.18990	-123.83526	378.17960	743.85218	1
19858	H	63.73500	65.66780	69.88090	727.85591	-2820.32900	-1180.35995	1
19859	C	63.66700	63.56780	70.06490	-596.17947	642.64117	-277.08099	1
19860	H	62.88200	62.91180	69.71890	1861.93921	2190.53873	-1278.30066	1
19861	C	64.85000	63.46980	69.11790	66.72759	-743.90270	512.52703	1
19862	H	65.76400	63.92480	69.55590	-67.35601	-1126.57123	-2939.82582	1
19863	C	65.11100	61.98380	68.79790	581.89830	-564.81118	-407.31289	1
19864	H	65.53400	61.39180	69.63790	2123.40360	1690.94945	1581.09418	1
19865	H	65.93800	61.98080	68.05590	862.69286	-2719.99370	1306.64822	1
19866	H	64.16200	61.56580	68.39990	-1390.04854	-1783.68373	-2193.03110	1
19867	C	64.66600	64.18280	67.82090	-518.92918	749.95530	110.93793	1
19868	H	64.71900	65.29080	67.87690	1580.94029	-184.48722	-2712.95926	1
19869	H	65.40800	63.84580	67.06590	1793.57735	-1931.01503	1701.33638	1
19870	H	63.66800	64.06080	67.34590	1340.76477	2036.46805	-1991.66304	1
19871	C	64.06000	63.02280	71.47490	-7.51084	754.87586	-519.77062	1
19872	O	63.68600	61.86980	71.71690	709.25250	-90.97897	-326.85921	1
19873	N	64.69800	63.81880	72.35490	545.63686	-395.88356	495.90340	1
19874	H	64.92200	64.75380	72.09190	1059.52783	2434.15084	-1692.27898	1
19875	C	64.99500	63.39580	73.70990	78.96657	857.57817	-308.32330	1
19876	H	65.58600	62.49180	73.72390	-1383.71628	-2171.90976	-1813.55464	1
19877	C	65.90700	64.41680	74.47290	-553.93910	-721.74333	77.72866	1
19878	H	65.40800	65.40280	74.35890	-804.24724	-3002.02377	482.90058	1
19879	C	65.96600	64.10380	75.97690	116.78843	469.48150	768.62941	1
19880	H	64.99500	64.04380	76.51390	1060.08381	1359.22657	-2634.66321	1
19881	H	66.52400	63.15380	76.11390	723.70093	-2506.91396	1749.17447	1
19882	H	66.62700	64.80880	76.52590	-2162.51048	217.29979	2275.06557	1
19883	C	67.28900	64.30380	73.77390	744.16528	-455.10374	-250.48438	1
19884	H	67.15200	64.24880	72.67190	-425.77974	-1906.07702	-2470.01860	1
19885	H	67.80800	63.36280	74.05590	1286.96860	-2511.08408	-1387.76591	1
19886	C	68.16400	65.49680	74.02690	-399.93473	465.53731	-683.56255	1
19887	H	67.70100	66.33980	73.47090	2080.81159	1739.17207	-1594.10860	1
19888	H	68.23500	65.67980	75.11990	2817.57021	-546.86014	1272.04864	1
19889	H	69.22100	65.29580	73.74790	1920.60780	-1483.18315	1990.46288	1
19890	C	63.73700	63.05580	74.48490	488.45607	-497.74511	-586.06088	1
19891	O	63.59500	61.94380	75.01890	-737.02026	92.16497	276.73800	1
19892	N	62.71100	63.97680	74.42690	-393.51217	-499.39871	-561.16694	1
19893	H	62.97700	64.85880	74.04390	1945.60809	-1150.36670	-2186.10609	1

19894	C	61.40000	63.89880	75.00690	-70.70251	688.68512	592.05453	1
19895	H	61.51400	63.67880	76.05790	-1955.87549	1538.79440	-1933.39315	1
19896	C	60.66100	65.21180	74.74190	517.43717	727.48888	-177.47926	1
19897	H	60.92700	65.60280	73.73690	-1880.25493	1773.58447	-1803.34982	1
19898	H	59.56300	65.07380	74.83190	-3112.41882	304.02274	-391.29498	1
19899	C	61.13800	66.33980	75.75290	-531.48320	-297.16207	680.15232	1
19900	H	62.24600	66.39680	75.69090	-1301.40630	1076.75184	-2659.62240	1
19901	C	60.60400	67.72780	75.32790	554.27240	572.37731	-439.24426	1
19902	H	60.92600	68.06380	74.31990	2171.18571	890.42568	2088.68801	1
19903	H	59.49500	67.79180	75.33190	-1723.26691	-2186.53689	-1471.95069	1
19904	H	60.93400	68.51280	76.04190	933.77526	2087.95228	-2159.88955	1
19905	C	60.79400	66.15080	77.20290	788.84956	-219.39317	-394.05462	1
19906	H	61.31900	65.24480	77.57390	-585.63575	1168.86331	-2865.25287	1
19907	H	60.95400	67.10180	77.75390	-2959.25444	506.47122	953.12281	1
19908	H	59.72800	65.90580	77.39990	1748.25453	232.66494	2600.24733	1
19909	C	60.68300	62.63780	74.55090	-427.75404	681.62713	431.98247	1
19910	O	60.15800	61.87580	75.38690	503.14428	598.19819	-97.94068	1
19911	N	60.66600	62.35580	73.27790	-577.70782	391.22150	479.29382	1
19912	H	61.20100	62.96480	72.69590	1744.47096	-2012.26006	-1670.52476	1
19913	C	60.10100	61.11180	72.65490	140.90697	301.04026	-852.75534	1
19914	H	59.04500	61.08180	72.87990	773.42778	-2128.58558	2176.82642	1
19915	C	60.12500	61.11180	71.07890	-87.20908	643.23334	639.62247	1
19916	H	59.92400	60.10280	70.65790	2235.18739	-2095.63068	684.66122	1
19917	H	61.15700	61.42380	70.81190	1729.03814	-2484.60271	-842.09458	1
19918	O	59.30200	62.05380	70.45490	-360.32839	-46.00652	700.71962	1
19919	H	58.40200	61.85880	70.72590	-977.88441	2987.43297	-209.18439	1
19920	C	60.70300	59.78680	73.11590	591.33585	-629.86168	272.96314	1
19921	O	59.91400	58.83680	73.29290	-342.32257	-9.17415	709.12639	1
19922	N	62.04400	59.67780	73.24190	210.26956	-353.23633	-740.02479	1
19923	H	62.55400	60.48180	72.94690	-1118.55459	-2281.51299	-1860.58936	1
19924	C	62.74300	58.45280	73.65390	-417.34587	-247.34127	768.36831	1
19925	H	62.41300	57.69680	72.95690	-622.77630	2900.95223	-1060.43901	1
19926	C	64.26900	58.73380	73.87290	-733.56851	261.43838	476.45738	1
19927	H	64.76100	57.78280	74.17290	897.14896	933.18841	-2873.12404	1
19928	H	64.35500	59.49580	74.67690	-1456.98083	-2620.25625	950.61363	1
19929	S	64.98900	59.21680	72.26490	-199.23621	-73.74322	511.45803	1
19930	H	64.69800	60.50780	72.31790	-686.62890	-1450.37428	2700.74460	1
19931	C	62.19100	57.92080	74.99590	112.65185	740.67851	-526.19692	1
19932	O	61.86400	56.75380	75.16990	178.67799	594.22236	482.25813	1
19933	N	62.14600	58.80680	76.01990	41.66216	805.73763	-255.60349	1
19934	H	62.48500	59.73680	75.89890	-679.08358	-2326.64101	-2011.41013	1
19935	C	61.69700	58.38880	77.38590	-744.60959	-479.04057	-234.94274	1
19936	H	62.07100	57.41880	77.67990	-2649.38099	1517.77581	764.80955	1
19937	C	62.30100	59.29480	78.44190	754.05497	468.38295	-200.48667	1
19938	H	61.96400	58.85080	79.40290	2402.98963	1320.73956	-1542.48239	1
19939	H	61.85500	60.29480	78.25690	2779.28262	1101.91177	964.42472	1
19940	C	63.83700	59.35180	78.28390	-806.64473	141.13776	402.51307	1
19941	C	64.38900	60.56680	77.83490	566.12223	536.25287	-473.78064	1
19942	H	63.80300	61.43580	77.57490	897.30392	2307.92115	1934.64121	1
19943	C	65.78200	60.60780	77.65190	-41.60776	-596.86470	-693.38240	1
19944	H	66.16600	61.51380	77.20790	-908.95382	1354.21544	2686.79991	1
19945	C	66.60500	59.53580	77.92290	-820.78401	-16.32267	-410.49309	1
19946	O	67.97300	59.58680	77.66090	-657.14196	-390.63375	201.56302	1
19947	H	68.15200	60.22280	76.96390	1756.12133	-2575.75318	-405.88925	1
19948	C	64.61200	58.27280	78.57190	-389.04374	437.27601	694.91365	1
19949	H	64.11800	57.43480	79.04090	2257.40182	-996.58226	1941.85223	1
19950	C	66.01500	58.33080	78.34490	-480.10183	-367.84540	677.96337	1
19951	H	66.62900	57.44280	78.37690	955.45519	-2912.16914	-711.08916	1
19952	C	60.22600	58.36380	77.44290	37.05971	834.47293	-370.28863	1
19953	O	59.63100	57.65280	78.25890	-325.84923	525.89385	-497.64653	1
19954	N	59.50100	59.13780	76.59090	184.80035	-563.00154	-604.34886	1
19955	H	59.91300	59.78880	75.95890	-2207.73499	1692.09611	1472.51889	1

19956	C	58.09000	58.99580	76.38390	-905.51445	-95.86793	93.04053	1
19957	H	57.66200	59.15280	77.36290	1909.48368	-2197.36945	1183.75963	1
19958	C	57.49900	60.00280	75.39790	-8.27331	-815.80633	402.82954	1
19959	H	57.89000	60.99280	75.71490	-1937.22446	-1895.93125	-1605.40177	1
19960	H	57.90100	59.81880	74.37790	726.15011	-3019.77396	486.06933	1
19961	S	55.72300	60.08580	75.22290	-13.04035	-298.18373	468.12165	1
19962	H	55.62900	59.09380	74.34990	-2342.28634	1913.77637	875.60362	1
19963	C	57.68600	57.57480	75.97290	-729.71906	212.29388	-514.16553	1
19964	O	56.79800	56.98380	76.56690	-679.06989	-371.53951	-176.30881	1
19965	N	58.36000	56.95880	75.04090	8.09640	-814.43915	-224.38680	1
19966	H	58.91300	57.53180	74.44090	-732.18158	2446.19823	1836.04905	1
19967	C	58.10400	55.59180	74.61790	-594.94755	131.40572	676.57127	1
19968	H	57.05600	55.50580	74.37190	1975.86784	-2440.28998	-144.62029	1
19969	C	58.88400	55.19280	73.32890	621.96808	-582.46387	-319.45686	1
19970	H	59.96700	55.39580	73.47690	-2097.39931	1787.72556	-1531.28666	1
19971	C	58.75700	53.70380	73.07890	-709.09967	109.95400	561.75738	1
19972	H	59.12800	53.48880	72.05390	2477.75423	1406.57395	-1334.67679	1
19973	H	59.29400	53.04680	73.79590	2779.83153	-1394.44616	-455.20003	1
19974	H	57.68400	53.41180	73.07590	2815.54171	1396.73836	15.96069	1
19975	C	58.35700	55.95380	72.10590	620.58163	-62.81054	-665.90660	1
19976	H	57.42400	55.51380	71.69390	1378.61682	2826.82428	-66.91023	1
19977	H	58.03500	56.99480	72.32590	2387.24290	2044.85179	36.63227	1
19978	C	59.39500	56.11680	70.97890	692.04483	-525.24606	-264.77266	1
19979	H	59.93700	55.16780	70.78090	1904.86729	-1421.95594	2048.55396	1
19980	H	59.03200	56.60880	70.05190	1915.49614	180.77640	2479.99205	1
19981	H	60.04100	56.97780	71.25290	2521.12411	1582.07890	1004.92652	1
19982	C	58.48800	54.59080	75.69290	-676.48537	35.99850	-620.26861	1
19983	O	57.74000	53.60180	75.90990	-481.87803	-400.26944	-490.12836	1
19984	N	59.64700	54.78980	76.37390	-598.07996	-518.47477	-306.02065	1
19985	H	59.99800	55.71780	76.27190	-2804.99307	-1160.15125	832.74280	1
19986	C	60.34200	53.84080	77.29690	-468.98440	-631.94864	-470.32158	1
19987	H	60.57700	52.90980	76.80290	2101.58109	-1398.49546	-1881.20471	1
19988	C	61.81500	54.30380	77.78890	560.75104	-478.72040	526.35275	1
19989	H	61.72400	55.38780	78.01790	-183.68794	2661.78188	-1673.95999	1
19990	C	62.20200	53.43880	79.01190	-738.27168	495.20263	203.78036	1
19991	H	62.13300	52.35980	78.75490	1742.20933	1919.14072	1772.74128	1
19992	H	63.25500	53.63080	79.30990	-2457.50379	-1863.42726	-640.01204	1
19993	H	61.54700	53.49980	79.90690	-3076.46603	509.65076	-439.93271	1
19994	C	62.82100	54.15980	76.66190	-538.83804	393.54338	-631.96227	1
19995	H	62.32800	54.42880	75.70290	2531.60287	-1815.59591	-421.05835	1
19996	H	63.23200	53.13380	76.55490	634.79353	-2995.48303	-724.70037	1
19997	C	64.08400	54.91880	76.90390	-184.13807	853.32626	260.59174	1
19998	H	63.83200	55.97580	77.13390	-2166.32618	-237.19619	-2279.15350	1
19999	H	64.72100	54.56480	77.74290	-684.98562	-2936.49469	-906.20132	1
20000	H	64.80100	54.81880	76.06190	-106.40325	-379.24058	-3128.92930	1
20001	C	59.39500	53.38480	78.45890	362.73728	-772.25232	313.20819	1
20002	O	59.23700	52.19880	78.85690	-133.38834	-582.76836	-524.39172	1
20003	N	58.74100	54.39080	79.02790	-582.71053	-498.63172	352.20370	1
20004	H	58.82900	55.33080	78.70690	-2468.04052	1949.32524	131.01141	1
20005	C	57.95400	54.24980	80.20890	550.60524	-540.01590	479.40228	1
20006	H	58.55600	53.66780	80.89190	-1938.31132	1680.24537	1815.99635	1
20007	C	57.67700	55.58980	80.88790	-547.28339	522.86882	-514.62002	1
20008	H	57.07200	55.33580	81.78590	2314.41723	-1889.26436	-990.52187	1
20009	C	58.98100	56.16480	81.44990	632.50835	579.78525	295.24144	1
20010	H	58.79600	57.04280	82.10490	2072.59196	-1605.40223	1733.43787	1
20011	H	59.55900	55.40180	82.01390	-3029.52462	728.38312	-452.09881	1
20012	H	59.56000	56.60080	80.60790	489.73541	-3015.18638	751.05713	1
20013	C	56.89100	56.57580	80.03690	-738.17933	-69.24703	-539.44626	1
20014	H	57.59600	57.08480	79.34490	-2014.10563	2110.85900	1175.55937	1
20015	H	56.23000	55.99780	79.35490	-1758.04412	1809.40399	1876.36966	1
20016	C	56.10400	57.58680	80.84990	612.09942	72.72418	665.19675	1
20017	H	55.43400	57.04080	81.54790	2508.33937	1884.31890	185.24347	1

20018	H	55.39900	58.12580	80.18290	-15.38957	59.75542	-3149.29738	1
20019	H	56.80600	58.30380	81.32690	2076.32778	-1737.11946	1597.65195	1
20020	C	56.78400	53.35880	80.02290	-745.79591	510.06983	-136.26126	1
20021	O	56.23600	52.76380	80.96890	586.46816	523.06369	37.22129	1
20022	N	56.27700	53.27880	78.79190	10.70433	587.60088	599.13778	1
20023	H	56.73500	53.86180	78.12490	943.23205	-1979.60866	2249.71654	1
20024	C	55.13000	52.49880	78.47790	-298.45793	790.62413	-348.10402	1
20025	H	54.47900	52.42980	79.33690	841.10892	1699.95694	2502.69370	1
20026	C	54.26500	53.22480	77.40490	751.08208	510.32211	-46.41126	1
20027	H	53.70300	54.02080	77.93790	-1912.50921	-2486.88140	263.83563	1
20028	H	53.51500	52.55080	76.93890	-2514.75430	-1579.36864	1041.97877	1
20029	O	55.06400	53.77880	76.36790	-403.81631	635.29029	-248.82320	1
20030	H	55.77900	53.17280	76.16290	123.48385	3123.82324	345.40259	1
20031	C	55.34500	51.08080	78.13790	727.16410	-447.36364	309.39236	1
20032	O	54.38400	50.33480	77.74290	440.45538	-652.77722	-55.99166	1
20033	N	56.56600	50.60580	78.30390	-110.12572	-766.71739	331.33620	1
20034	H	57.18900	51.23380	78.76590	-206.09660	1793.80309	-2582.87050	1
20035	C	56.93000	49.22180	78.07690	647.42298	-640.49008	-4.87502	1
20036	H	56.17700	48.60980	78.54990	-1685.57563	-2009.33410	1733.18203	1
20037	C	56.90500	48.80080	76.58590	547.78093	503.05454	517.03139	1
20038	H	55.84500	48.89880	76.26890	-1916.10626	2467.70100	375.89510	1
20039	H	57.16400	47.73180	76.43290	1243.65199	2688.00758	1050.04261	1
20040	C	57.61500	49.74880	75.55590	-527.85145	657.26409	345.25500	1
20041	H	58.66700	49.92380	75.86590	50.75156	-3096.96792	-557.03030	1
20042	H	57.07500	50.71580	75.64090	810.84637	1730.29012	-2505.59484	1
20043	C	57.50000	49.15880	74.14190	-223.35265	495.37736	726.09066	1
20044	H	58.09000	49.79580	73.44890	-2574.82200	-1810.75131	51.97719	1
20045	H	58.01800	48.17680	74.12790	2255.03114	444.43995	-2153.50318	1
20046	C	56.08000	49.16180	73.63190	566.76327	-673.03576	220.94543	1
20047	H	55.39300	48.50380	74.20690	1469.41986	-1730.98496	-2182.57190	1
20048	H	55.70700	50.20880	73.64390	2310.54238	135.47811	-2134.07279	1
20049	N	56.00100	48.71280	72.26790	-368.51878	-341.35732	-687.30492	1
20050	H	56.26500	49.45680	71.59090	161.08552	-2616.85465	1728.81374	1
20051	H	55.01000	48.47780	72.05990	1481.87613	2106.56126	1798.00185	1
20052	H	56.61600	47.89280	72.09290	2552.09690	-659.51715	-1719.47830	1
20053	C	58.25800	48.62980	78.70690	528.68676	544.68588	494.17694	1
20054	O	58.67000	47.50480	78.41790	-485.64995	-551.48467	284.81516	1
20055	N	58.87400	49.39780	79.67090	-11.15353	-841.05502	75.23653	1
20056	H	58.55300	50.33080	79.81490	2295.09230	2050.43469	-650.28071	1
20057	C	60.05300	49.01480	80.43090	-739.76577	51.35025	524.23380	1
20058	H	60.85900	48.83280	79.73490	-211.97496	1445.24612	2777.44621	1
20059	C	60.48400	50.11080	81.40890	-592.92340	417.79370	-561.22024	1
20060	H	60.55300	51.07380	80.85790	-1983.46346	-902.11708	2263.60544	1
20061	H	59.62900	50.22680	82.10890	-1608.99885	-1669.53969	-2136.84080	1
20062	C	61.81200	49.86180	82.09690	-17.39217	53.57775	901.39075	1
20063	H	61.77700	48.88480	82.62590	486.97202	2619.74135	1660.67321	1
20064	C	62.94700	50.01980	81.06690	703.63325	-577.47312	-52.21045	1
20065	H	62.97300	51.01480	80.57190	-2307.21941	1828.12275	1104.24845	1
20066	H	62.94200	49.14980	80.37590	-379.88308	-367.68946	-3110.90518	1
20067	H	63.86500	49.83680	81.66490	2804.40415	1331.11270	-510.19502	1
20068	C	61.98100	50.95380	83.20990	-530.35700	-529.07068	-531.23309	1
20069	H	61.11500	50.89480	83.90290	-2600.96689	-13.23639	1763.31772	1
20070	H	62.95000	50.78680	83.72690	-2858.15912	-1165.87505	-625.01334	1
20071	H	62.00600	51.98380	82.79390	-1979.55886	-1095.81766	2180.26988	1
20072	C	59.83400	47.69080	81.19690	28.16078	588.78346	-703.32129	1
20073	O	60.73700	46.80980	81.21890	-396.42664	-156.47903	656.28573	1
20074	N	58.64700	47.46780	81.86090	189.50305	-795.22824	-225.45440	1
20075	H	57.93700	48.16280	81.93990	-2343.97394	-2095.72374	151.12772	1
20076	C	58.32400	46.20480	82.43990	-698.23026	578.72050	-95.57311	1
20077	H	59.16000	45.72380	82.92390	-136.09305	-1222.11680	2887.34584	1
20078	C	57.25300	46.40580	83.55490	438.60519	-369.65632	701.24722	1
20079	H	56.46500	47.09480	83.18390	-2984.15346	-796.47279	-613.66978	1

20080	H	56.84700	45.42880	83.89290	-1528.64299	2388.34080	-1366.96455	1
20081	O	57.79400	47.05480	84.72390	-58.51501	-274.67543	-747.85507	1
20082	H	58.33600	46.39680	85.16390	-3067.73636	-108.12397	680.97552	1
20083	C	57.74300	45.15880	81.47690	-761.43432	366.34712	-351.86501	1
20084	O	57.44700	44.02980	81.86390	658.42406	-57.23348	-441.32801	1
20085	N	57.64000	45.44880	80.18090	-28.83271	-201.47557	-828.86920	1
20086	H	57.87600	46.33480	79.79090	-2407.00087	1967.31608	477.22477	1
20087	C	57.07300	44.51080	79.22090	222.25047	528.66122	-717.09076	1
20088	H	56.64100	43.64980	79.70890	-2195.30224	2068.21296	885.19037	1
20089	C	55.93600	45.12680	78.34290	-520.52782	-146.23133	726.73201	1
20090	H	56.29600	45.99180	77.74590	2182.80936	100.04034	2253.02174	1
20091	H	55.54800	44.49680	77.51490	1246.64597	-603.21103	-2833.27020	1
20092	N	53.71900	46.31980	78.70290	-452.32544	534.44687	-479.57797	1
20093	H	53.67500	46.71180	77.78490	2143.22087	691.28098	-2202.42025	1
20094	C	54.76900	45.59380	79.19390	746.12048	318.95916	403.86066	1
20095	C	52.84700	46.50780	79.73890	-655.23277	360.15652	514.97758	1
20096	H	51.89400	47.02380	79.61890	820.15980	-3006.18718	-451.25623	1
20097	N	53.29900	45.96080	80.86590	-522.22342	-366.13709	547.70996	1
20098	C	54.52600	45.35480	80.48390	149.93693	171.97960	873.87990	1
20099	H	55.14700	44.83680	81.20490	-1934.56761	1912.99514	1569.65665	1
20100	C	58.04800	44.00880	78.19490	735.63683	259.59731	459.54437	1
20101	O	57.88200	42.94680	77.55890	259.17027	-502.59429	540.59931	1
20102	N	59.14200	44.76280	78.02990	-230.88063	-767.62611	-277.16269	1
20103	H	59.21600	45.65280	78.47390	2721.07718	-1531.93880	-383.15218	1
20104	C	60.37000	44.45780	77.32690	473.70491	-634.32786	440.10410	1
20105	H	60.06600	43.86780	76.47490	1924.74792	-1447.26938	-2032.90251	1
20106	C	61.19700	45.73880	76.87590	-755.21103	-28.76892	503.24446	1
20107	H	62.10800	45.47580	76.29590	-205.32545	-2886.01693	1224.11527	1
20108	H	61.43300	46.19080	77.86290	-2219.75341	860.90680	-2068.62879	1
20109	O	60.39300	46.65880	76.10090	297.03439	658.41511	308.52724	1
20110	H	59.93500	47.30180	76.64590	-933.61401	1922.18738	2301.14223	1
20111	C	61.25600	43.57680	78.15690	-180.20461	-160.99100	868.69469	1
20112	O	61.74400	44.02380	79.23190	667.69655	408.95211	81.23428	1
20113	O	61.55900	42.43480	77.70390	606.02463	-496.79187	-99.16065	1
20114	N	68.09800	39.69880	83.86190	572.14840	348.49268	499.13078	1
20115	H	68.31400	38.85080	84.42290	910.88142	2167.50233	2074.67999	1
20116	H	68.24600	39.59180	82.83790	1776.28789	-2242.63956	1296.88740	1
20117	H	67.12500	40.02180	84.03590	1021.91205	1010.50969	-2812.12598	1
20118	C	68.95200	40.75780	84.30590	778.07659	145.19269	439.13499	1
20119	H	68.94300	40.82480	85.38390	1946.89076	224.15770	2447.69469	1
20120	C	70.47100	40.56280	83.91090	-111.17474	612.18102	650.97023	1
20121	H	70.98000	41.53880	84.06090	2031.63668	2398.07471	-140.54322	1
20122	H	70.47900	40.45980	82.80490	230.87820	-2500.71031	-1910.58185	1
20123	C	71.15500	39.33080	84.51890	-125.96207	-756.64873	479.63392	1
20124	H	72.17500	39.10180	84.14190	2817.89958	-1317.06781	463.57001	1
20125	H	70.62200	38.43880	84.12690	2587.53815	176.90232	-1797.22989	1
20126	C	71.32300	39.38980	86.03290	464.33305	679.77286	-405.47193	1
20127	H	70.30800	39.45380	86.48090	141.44274	-558.29009	-3108.29175	1
20128	H	71.82700	40.34380	86.29990	-1193.87842	1305.33389	2585.34378	1
20129	C	71.99000	38.13380	86.56490	194.03726	-858.91623	229.05791	1
20130	H	71.54000	37.18180	86.20890	2224.79382	-2113.60034	688.02257	1
20131	H	73.02200	38.05280	86.16090	-2221.81265	-1829.88731	1254.02116	1
20132	N	72.01700	38.08680	88.06190	-229.59529	310.00148	733.44118	1
20133	H	72.40100	38.94980	88.49690	-1217.21774	2185.16780	-1919.72237	1
20134	H	71.06600	37.95380	88.46190	-1433.98301	-2002.52624	-1974.52569	1
20135	H	72.60700	37.30680	88.41590	2887.40422	1133.45820	-547.80871	1
20136	C	68.42100	42.10180	83.76190	-828.68968	-100.29749	353.52751	1
20137	O	67.82500	42.17680	82.71690	-522.46483	-578.24881	-145.69599	1
20138	N	68.61900	43.27580	84.43490	-646.73735	539.43822	-50.62206	1
20139	H	69.20800	43.27780	85.23890	2269.61228	2046.31764	731.39343	1
20140	C	67.99400	44.54780	83.99690	242.22327	239.65341	-857.65584	1
20141	H	68.34000	44.71780	82.98890	859.28505	-1424.96824	-2682.87345	1

20142	H	66.91700	44.46680	83.96490	-771.71817	-607.43786	-3001.32564	1
20143	C	68.37200	45.68480	84.92590	184.71477	-323.15887	821.12600	1
20144	O	68.20000	46.83880	84.64490	-683.00458	-369.89724	136.18410	1
20145	N	68.83800	45.43480	86.17690	-151.39229	591.14501	-593.20456	1
20146	H	69.14100	44.52880	86.46290	2037.86272	2008.17543	1293.47752	1
20147	C	69.04600	46.53980	87.06590	-543.11290	-347.51654	-657.51677	1
20148	H	68.12300	47.09580	87.14390	66.79450	-2805.07552	1417.01724	1
20149	C	69.42500	45.95680	88.48290	-271.04632	-712.62990	-516.04010	1
20150	H	69.61000	46.79780	89.18490	-408.86347	2761.07606	-1457.13173	1
20151	H	70.26400	45.23680	88.37490	2380.76341	925.05122	1824.20722	1
20152	N	68.12900	45.25980	90.58990	462.36708	307.07757	-647.40092	1
20153	H	68.44200	46.05880	91.10290	-328.47456	2959.17630	992.16865	1
20154	C	68.28000	45.18480	89.23290	520.81394	325.89567	-685.24677	1
20155	C	67.11100	44.45380	90.92790	646.22292	-342.19029	537.41111	1
20156	H	66.88800	44.18780	91.96090	1811.91205	2561.03972	-212.46332	1
20157	N	66.50500	43.97780	89.88790	-539.24208	462.16351	-462.61130	1
20158	C	67.24500	44.40280	88.80090	235.07908	628.65201	602.06080	1
20159	H	67.06100	44.12980	87.76890	2201.34033	768.29515	-2124.52362	1
20160	C	70.13100	47.50080	86.71590	173.75021	437.41516	-791.55036	1
20161	O	69.95600	48.68880	86.84090	222.56843	-629.44933	414.01667	1
20162	N	71.22300	46.97380	86.14590	204.81638	808.13477	108.88488	1
20163	H	71.30800	45.98380	86.05590	1395.89859	-1037.40305	2609.96915	1
20164	C	72.34500	47.79380	85.73390	660.79876	626.73078	-9.96498	1
20165	H	72.45100	48.61880	86.42290	-1545.46175	574.38727	-2691.05549	1
20166	C	73.65200	47.05680	85.70090	-425.71347	46.73580	792.00379	1
20167	H	73.55600	46.00080	85.36790	3039.37973	629.25178	-526.64808	1
20168	H	74.35000	47.50180	84.95990	-1972.90628	1037.14966	-2232.97782	1
20169	C	74.30700	47.04680	87.09390	480.98230	149.99186	746.86726	1
20170	H	74.48500	48.04780	87.54190	2371.12486	2027.46513	-411.96702	1
20171	H	75.34400	46.64680	87.06490	1467.72174	-1261.11581	2468.31487	1
20172	C	73.53900	46.29480	88.22990	59.57164	863.48185	266.66990	1
20173	O	73.14300	46.94180	89.21590	701.60397	-339.67769	-151.87416	1
20174	N	73.26100	44.98580	88.05190	-504.81886	156.89550	-670.43680	1
20175	H	73.59700	44.45680	87.27190	3145.80569	6.48472	-99.37089	1
20176	H	72.71800	44.56680	88.77890	2894.65267	211.77240	-1230.25333	1
20177	C	72.00600	48.49580	84.37690	-652.52051	175.99455	-624.18738	1
20178	O	72.38900	49.64980	84.14890	350.31640	169.84020	-698.03500	1
20179	N	71.16500	47.88080	83.49290	-303.15304	-767.22376	-195.94143	1
20180	H	70.90700	46.92780	83.63290	363.98006	-1765.40643	2566.99020	1
20181	C	70.59400	48.62080	82.36290	-863.52263	-289.81833	-73.54308	1
20182	H	71.41900	49.01280	81.78590	1034.78521	2208.28216	-1998.36773	1
20183	C	69.70100	47.63480	81.51590	-165.67591	-344.49176	-839.80251	1
20184	H	69.09700	47.05380	82.24590	657.60912	-2146.65452	2192.75733	1
20185	H	69.01800	48.11480	80.78390	2983.72361	-664.97893	727.25700	1
20186	C	70.56200	46.67680	80.62690	282.31392	211.65759	828.22551	1
20187	H	71.33500	46.24680	81.29890	-1917.83989	822.52708	-2367.84591	1
20188	H	71.11300	47.16180	79.79190	-946.23148	-445.65707	2955.44761	1
20189	C	69.74500	45.52780	80.02090	523.04167	-391.51330	622.48364	1
20190	H	69.31500	44.92580	80.84990	-1230.52272	1844.36171	2220.02125	1
20191	H	70.38800	44.89380	79.37490	1014.29078	-779.65970	-2886.48899	1
20192	C	68.59400	45.99380	79.11190	-665.02027	-12.29125	-637.30567	1
20193	H	67.85700	46.48980	79.77890	2251.65045	-497.05708	-2150.38313	1
20194	H	68.97400	46.63180	78.28490	914.76839	-2519.43065	1633.33235	1
20195	N	68.02900	44.78280	78.47990	-648.23767	412.23324	341.40103	1
20196	H	67.98800	44.08980	79.25490	455.28824	-1690.80126	2600.92417	1
20197	H	67.10500	44.86980	78.00990	1931.05353	1360.88336	2064.70363	1
20198	H	68.67200	44.54580	77.69790	415.92101	2949.46587	1002.53661	1
20199	C	69.71700	49.79980	82.79390	-618.73070	-325.49733	576.16595	1
20200	O	69.79800	50.86580	82.22390	538.81227	474.22327	-336.61224	1
20201	N	68.85600	49.66080	83.84290	593.72544	431.35354	-425.40192	1
20202	H	68.79800	48.77280	84.29290	-979.05634	2661.76826	-1370.23644	1
20203	C	68.00000	50.77580	84.28590	714.36436	-557.77114	93.40731	1

20204	H	67.57400	51.25780	83.41790	2427.90400	1118.77448	1646.74543	1
20205	C	66.81200	50.11480	85.12790	-332.60095	-306.88801	782.72538	1
20206	H	67.22400	49.50880	85.96190	-139.47885	1648.92335	-2684.57783	1
20207	H	66.27300	50.96480	85.59790	-1695.27368	917.34281	2476.55495	1
20208	C	65.87200	49.30880	84.17590	394.90314	649.91124	-510.18056	1
20209	H	66.45800	48.61780	83.53290	-1810.62980	374.50712	2535.42826	1
20210	H	65.40700	50.13980	83.60490	-2339.09592	-443.18660	-2067.66409	1
20211	C	64.58100	48.69080	84.76490	226.09863	672.50352	560.17978	1
20212	H	63.91200	48.26980	83.98490	-2067.14675	-2147.84361	-1021.12150	1
20213	H	64.00700	49.44380	85.34690	2912.33529	1182.06847	97.33367	1
20214	N	64.98200	47.51680	85.61290	-664.91701	242.15192	-469.41606	1
20215	H	64.97100	46.61780	85.17490	-2237.00020	366.26508	2170.62053	1
20216	C	64.91300	47.44980	86.91190	516.27658	617.48760	-434.97523	1
20217	N	65.22000	46.31280	87.50190	290.93333	-638.29790	-485.27461	1
20218	H	65.23700	45.48880	86.93590	-2930.42837	-15.47315	1132.05777	1
20219	H	64.79200	46.14780	88.39090	-218.77295	1128.27858	2916.41874	1
20220	N	64.55700	48.39180	87.74590	367.16060	729.35435	193.37928	1
20221	H	64.32200	49.30080	87.40390	1717.77950	-1468.61692	2181.59809	1
20222	H	64.48300	48.15980	88.71590	897.63727	603.06479	2943.91369	1
20223	C	68.76300	51.77380	85.17190	-286.17697	629.33475	-602.70637	1
20224	O	68.31700	52.89480	85.38790	454.31736	-471.09918	-452.45749	1
20225	N	69.99200	51.44480	85.66490	2.71915	-340.40751	763.10549	1
20226	H	70.22400	50.48180	85.78290	-2461.59986	944.13598	-1726.90626	1
20227	C	71.03900	52.33780	86.14090	-581.93133	505.91242	475.10551	1
20228	H	70.60600	52.99280	86.88290	-1990.94727	-1244.51668	-2105.66098	1
20229	C	72.06500	51.49980	86.96290	573.76024	-556.61345	430.33180	1
20230	H	72.56500	50.79680	86.26290	-1933.07539	2227.85206	-1102.62695	1
20231	H	71.46100	50.99980	87.75090	560.48785	3081.56903	-280.89386	1
20232	C	73.17300	52.34480	87.63990	59.98324	699.62155	-589.78389	1
20233	H	73.64300	52.97080	86.85090	1255.30795	-185.30317	2868.22625	1
20234	H	74.04000	51.75980	88.01390	320.04030	2012.40000	2384.03258	1
20235	C	72.66500	53.24480	88.79790	-478.04769	560.97048	523.67235	1
20236	H	72.29600	54.16380	88.29490	-1899.74746	-2178.60620	1237.00935	1
20237	H	71.81600	52.78380	89.34490	-611.61823	2477.06376	-1846.76659	1
20238	C	73.72900	53.65480	89.76990	779.73216	-157.16668	437.01378	1
20239	H	74.54200	54.24280	89.29390	-2182.34275	-1073.31267	1986.81002	1
20240	H	74.15700	52.71680	90.18490	-257.98359	181.43153	3119.20826	1
20241	N	73.08500	54.51480	90.80690	-312.13178	-450.87323	634.09692	1
20242	H	72.42900	53.95380	91.38690	1691.60202	-1867.58021	-1898.08776	1
20243	H	72.53100	55.23180	90.29690	245.41774	3096.51651	469.38741	1
20244	H	73.73600	55.06480	91.40390	2155.77025	-2112.73157	887.20414	1
20245	C	71.68500	53.15880	85.00390	622.85733	-426.77001	-521.33755	1
20246	O	71.94000	54.39380	85.13790	209.30480	-65.43527	748.84559	1
20247	N	72.06400	52.55680	83.85790	-513.81699	-561.98131	357.08517	1
20248	H	72.02800	51.56080	83.83890	-1341.10324	-2231.97483	-1778.41156	1
20249	C	72.45900	53.18580	82.59290	270.89472	717.25955	481.93228	1
20250	H	73.31700	53.82280	82.75190	-2567.95505	740.50116	-1672.49836	1
20251	C	72.73700	52.17980	81.49090	-527.05995	-457.92153	577.27441	1
20252	H	73.16400	52.69180	80.60190	-871.78771	-2304.71920	-1967.09080	1
20253	H	73.43100	51.39180	81.85490	1351.55292	498.07726	-2807.48892	1
20254	H	71.81100	51.66480	81.15690	-243.12557	2448.19247	-1971.94397	1
20255	C	71.42300	54.10280	82.09390	-691.77939	-586.23721	100.32104	1
20256	O	71.72400	55.20980	81.62890	-554.90869	-246.77717	497.83383	1
20257	N	70.15100	53.68580	82.18190	-344.01806	458.23455	-629.94891	1
20258	H	69.93300	52.74080	82.41190	-2054.59677	-911.74532	2193.24440	1
20259	C	69.05200	54.61880	81.81290	-663.78664	376.71292	492.33719	1
20260	H	69.27300	54.93580	80.80490	2241.01921	930.53964	-2008.67081	1
20261	C	67.72000	53.76380	81.88590	637.38847	-552.42789	335.48284	1
20262	H	67.86000	52.87180	81.23890	-2065.60674	-2289.26734	623.79050	1
20263	H	67.52600	53.54180	82.95690	-1561.18409	-2707.03761	370.42269	1
20264	C	66.42000	54.44080	81.37090	428.16621	-47.04363	-810.77053	1
20265	H	66.26400	55.30580	82.05090	-683.94594	-584.35067	3007.66367	1

20266	C	66.51600	54.88780	79.91790	-175.62812	-435.09582	774.49107	1
20267	H	67.34800	55.61980	79.84090	-806.33307	-2374.20799	-1909.34041	1
20268	H	66.83700	54.05780	79.25390	1896.34991	2069.85276	-1425.70100	1
20269	H	65.61300	55.35880	79.47290	-1670.07846	-79.20129	2659.20964	1
20270	C	65.08700	53.64980	81.60090	-733.23207	300.29283	-461.75133	1
20271	H	64.19400	54.26480	81.35690	-2513.57008	1571.23124	1049.99450	1
20272	H	65.13500	52.68680	81.04990	-597.64101	-3074.51200	-317.04187	1
20273	H	65.04700	53.31080	82.65790	-2824.26134	-1354.05935	309.17022	1
20274	C	68.94000	55.86580	82.65390	-72.35284	-829.56281	365.53057	1
20275	O	68.94800	56.97480	82.06590	-448.98894	136.69942	628.64884	1
20276	N	68.95500	55.70480	84.03490	278.08921	-556.32186	563.10603	1
20277	H	68.90000	54.78480	84.41390	1044.81786	-533.73438	2910.35253	1
20278	C	69.01700	56.76980	84.97390	-535.92622	-435.82794	589.76596	1
20279	H	68.18000	57.41880	84.76190	-1647.45543	-1801.11554	-1995.28869	1
20280	C	68.98700	56.10080	86.37390	385.01593	767.72484	-307.57984	1
20281	H	67.97000	55.65380	86.34790	1888.20486	1407.57866	2075.57676	1
20282	H	69.84200	55.41280	86.55090	-1619.99118	813.48318	2562.50341	1
20283	C	69.01600	57.12980	87.55390	-624.32867	582.34300	308.88132	1
20284	H	68.64300	58.10980	87.18590	2089.26267	-1167.40158	-2050.00407	1
20285	H	70.04000	57.51080	87.75690	2154.55868	1392.64978	-1826.21459	1
20286	C	68.28500	56.64680	88.80690	-56.98660	-653.10276	-644.95100	1
20287	H	67.27800	56.32580	88.46590	-516.84085	-2480.39706	-1877.23848	1
20288	H	68.78000	55.77180	89.27990	-2708.38037	-133.86664	1587.47164	1
20289	C	68.18300	57.76180	89.88990	-301.55837	-724.17842	463.32912	1
20290	H	67.70500	58.60680	89.34890	-1411.51799	-1850.10519	2113.79583	1
20291	H	69.18300	58.07080	90.26390	2505.21264	-25.05664	1895.41186	1
20292	N	67.28600	57.24180	90.94090	-427.35756	-729.30933	-71.60393	1
20293	H	67.23400	57.85680	91.77790	-2217.05297	399.78465	-2202.06030	1
20294	H	66.34800	56.94180	90.60490	2025.02079	1888.25288	-1495.97933	1
20295	H	67.76700	56.37380	91.25190	2451.71403	-668.69683	1849.01909	1
20296	C	70.26400	57.65280	84.87290	241.76368	-476.27354	-747.45930	1
20297	O	70.14300	58.87780	84.98790	-352.00909	641.15756	-303.68038	1
20298	N	71.49100	57.15780	84.71690	523.89146	-578.23634	313.71041	1
20299	H	71.63100	56.17080	84.69590	191.59395	-1748.19240	-2618.33745	1
20300	C	72.71900	57.94580	84.52690	-331.87025	620.69531	570.99214	1
20301	H	72.79500	58.56780	85.40690	-1954.42550	2421.14515	-472.54501	1
20302	C	74.01800	57.10780	84.51390	-90.52778	855.99416	289.60251	1
20303	H	74.13900	56.57280	83.54790	1095.82774	-2285.40230	-1872.96926	1
20304	O	74.08600	56.29880	85.65490	-368.43632	-695.57568	72.57526	1
20305	H	73.52300	55.52680	85.55590	2454.60387	-869.58241	-1774.32266	1
20306	C	75.19200	58.07780	84.76890	18.69959	-910.31488	-71.63354	1
20307	H	75.21200	58.81580	83.93790	3117.04446	66.42821	-416.04279	1
20308	H	76.17100	57.55180	84.75690	2080.31979	-2327.89268	-394.75131	1
20309	H	75.14700	58.74180	85.65790	1241.68768	321.38165	-2880.91332	1
20310	C	72.59200	58.81480	83.22690	-332.57037	260.84769	-816.76451	1
20311	O	73.01500	59.98280	83.18890	-342.83715	-21.05914	-719.99236	1
20312	N	72.00200	58.27580	82.17390	265.99787	-474.49940	-652.99269	1
20313	H	71.78800	57.30480	82.23390	1712.41435	745.21129	-2538.81690	1
20314	C	71.67800	58.96180	80.92490	195.03254	-849.65981	-272.68048	1
20315	H	72.62500	59.27280	80.50790	161.54240	871.21970	3010.79805	1
20316	C	71.09500	58.12480	79.80190	-410.79276	-506.97801	-646.39630	1
20317	H	70.05700	57.80880	80.03990	-2608.66229	1041.90119	1414.45996	1
20318	O	71.89200	56.91180	79.71290	478.08734	457.88590	419.47237	1
20319	H	71.56000	56.30780	80.38190	-2280.70442	2128.77265	-430.74338	1
20320	C	71.17200	58.81080	78.46790	505.92222	21.70086	748.31272	1
20321	H	72.19700	59.09080	78.14290	1928.56641	922.08949	2298.03620	1
20322	H	70.51100	59.70180	78.53390	-411.33798	3062.13109	593.45666	1
20323	H	70.87600	58.20880	77.58290	633.75977	-1571.55403	-2657.07423	1
20324	C	70.83300	60.20580	81.08790	-912.72187	-35.80337	-55.34504	1
20325	O	71.24500	61.35880	80.80990	295.10042	-476.02553	548.15284	1
20326	N	69.70300	59.95480	81.76090	-228.78229	-416.05940	692.20455	1
20327	H	69.43500	59.01180	81.94290	-1317.97085	1569.50928	2380.82814	1

20328	C	68.79200	60.93480	82.26090	-458.66653	36.73231	-795.03063	1
20329	H	68.27700	61.41580	81.44290	-289.04454	1163.99415	2902.68645	1
20330	C	67.64800	60.18880	82.90290	567.99923	-683.92811	-206.01598	1
20331	H	68.05500	59.43180	83.60690	-1278.27981	2173.20884	1875.05957	1
20332	C	66.77000	61.10180	83.78390	324.32109	658.50292	-543.38922	1
20333	H	65.86900	60.56480	84.14890	2407.00446	640.88392	1913.04682	1
20334	H	66.36600	61.97780	83.23390	-1847.25847	2365.13960	-951.09275	1
20335	H	67.30500	61.44380	84.69590	-2709.72009	1600.20873	-20.07739	1
20336	C	66.87700	59.43380	81.79990	-554.76589	-580.77607	-442.42867	1
20337	H	65.98800	58.91880	82.22390	1819.57357	-2565.46117	44.51815	1
20338	H	67.56900	58.76680	81.24290	2703.55368	-1098.30029	-1177.09817	1
20339	H	66.48400	60.21480	81.11490	1607.94260	-16.54917	-2708.42040	1
20340	C	69.33700	61.96280	83.14390	169.41188	748.50247	-496.10866	1
20341	O	69.12900	63.14880	82.91090	-220.16816	-647.16608	392.85936	1
20342	N	70.16800	61.60980	84.15190	637.50710	-180.99071	514.27285	1
20343	H	70.42600	60.68180	84.41090	572.44504	-1722.00824	2563.66015	1
20344	C	70.81100	62.52780	85.05990	763.55127	-90.30022	480.94846	1
20345	H	70.02500	63.10980	85.51790	-1692.24116	-1787.33670	-1968.80163	1
20346	C	71.57800	61.78180	86.15290	-648.39234	65.61318	632.56494	1
20347	H	72.12500	60.95180	85.65690	-2584.37879	1100.14803	-1426.47151	1
20348	C	72.63700	62.69880	86.91090	508.23624	452.91061	-610.45347	1
20349	H	73.14200	62.11380	87.70790	-1398.76934	-1335.44963	2476.50596	1
20350	H	72.14800	63.58180	87.37590	-37.26404	3115.76084	-424.61865	1
20351	H	73.44600	62.89480	86.17490	-1422.22576	-1984.85421	-1993.63522	1
20352	C	70.63500	61.17080	87.20590	552.00393	531.65998	483.26520	1
20353	H	69.64800	60.89180	86.77890	-1579.47180	137.91482	2711.59627	1
20354	H	70.45800	61.96580	87.96190	2867.07509	893.72701	925.00068	1
20355	C	71.26700	59.95680	87.91890	84.39957	-813.60657	-415.19974	1
20356	H	70.48700	59.54080	88.59190	-1871.27492	-1679.13835	-1901.92928	1
20357	H	71.59500	59.21580	87.15890	-1925.74738	-1981.88814	1500.56651	1
20358	H	72.13800	60.22880	88.55390	-2474.32391	-79.39147	1935.29185	1
20359	C	71.66200	63.52580	84.35490	435.65974	632.55091	-493.90992	1
20360	O	71.52800	64.71780	84.59990	-445.84338	-350.72100	546.62306	1
20361	N	72.44000	63.06280	83.35390	-627.02548	556.39101	-118.19203	1
20362	H	72.41000	62.08380	83.16990	383.84384	-135.92728	3112.55464	1
20363	C	73.23300	63.90780	82.52590	362.39557	-426.64716	712.07262	1
20364	H	73.88400	64.42880	83.21190	548.12828	1391.91520	2760.61253	1
20365	C	74.22100	63.07780	81.65290	-149.12935	809.11784	-401.64750	1
20366	H	73.76600	62.28180	81.02690	-2508.59263	-11.29969	1895.72048	1
20367	H	74.79000	62.50380	82.41590	2270.24357	-1218.23418	1794.73879	1
20368	C	75.19500	63.90380	80.72890	-546.25556	264.79055	676.51373	1
20369	H	74.55500	64.48980	80.03390	-770.91263	2581.68519	1621.07082	1
20370	C	76.09000	64.93880	81.32490	10.79118	-877.59966	-251.80790	1
20371	H	76.90300	64.44380	81.89790	1436.57286	-2322.37376	1551.61064	1
20372	H	75.62900	65.65480	82.03890	-742.40897	2217.42357	2099.85397	1
20373	H	76.67100	65.48180	80.54890	-1952.37794	-2389.68158	614.38726	1
20374	C	76.03300	62.90280	79.89590	-462.52171	-254.04080	737.93655	1
20375	H	76.48300	62.22980	80.65690	2597.06825	1526.36507	-907.61133	1
20376	H	76.84200	63.38880	79.30890	1493.32365	-1395.89410	2380.86759	1
20377	H	75.43400	62.30680	79.17490	2297.91662	-2142.76094	-70.83047	1
20378	C	72.43700	64.90980	81.66490	-225.51182	778.97903	412.83319	1
20379	O	72.81300	66.08780	81.57690	-437.05328	-600.29137	-279.71521	1
20380	N	71.36300	64.44380	80.99590	-327.84715	573.58488	522.09923	1
20381	H	71.19000	63.46780	81.10790	1195.00195	1442.99251	2519.91848	1
20382	C	70.42600	65.14580	80.24290	-627.49429	556.92213	358.84352	1
20383	H	71.03900	65.71780	79.56190	-2617.06162	-1464.67174	-965.84898	1
20384	C	69.50000	64.18580	79.47790	244.58674	-7.86921	872.05543	1
20385	H	69.27400	63.33580	80.15590	14.06284	1064.78090	-2966.00371	1
20386	C	68.14600	64.84580	79.02290	715.97755	-206.36765	-524.54766	1
20387	H	67.51200	65.16380	79.87790	856.94058	-3026.00509	18.07280	1
20388	H	67.58600	64.15180	78.35890	-526.86321	2585.20359	-1720.79642	1
20389	H	68.45800	65.75480	78.46590	-664.59282	-2855.71992	1137.20684	1

20390	C	70.28000	63.43880	78.39190	-475.11112	-679.25380	377.45444	1
20391	H	70.44600	64.25280	77.65390	-152.93739	2024.89369	-2409.85080	1
20392	H	71.27200	63.03780	78.69290	-1943.41974	2068.33878	-1370.82799	1
20393	C	69.41000	62.39680	77.58790	23.78904	618.73215	664.34063	1
20394	H	68.96100	61.73580	78.35990	-2870.98804	555.68997	-1176.29594	1
20395	H	68.57700	62.83380	76.99690	973.22887	-2602.95414	1464.43998	1
20396	H	70.16900	61.86880	76.97190	-1507.36810	-2076.57864	-1828.51547	1
20397	C	69.70600	66.19980	80.98090	611.90070	-32.57079	-676.46951	1
20398	O	69.55800	67.36380	80.51690	440.78933	316.90339	566.40349	1
20399	N	69.14000	65.92480	82.22190	-563.64659	575.32766	254.17591	1
20400	H	69.22700	64.99080	82.55990	-2546.75969	-1685.43835	-772.91701	1
20401	C	68.75000	66.92180	83.19690	-552.41564	-558.56522	463.94420	1
20402	H	67.89500	67.41080	82.75390	-1206.00901	2107.82656	1997.53689	1
20403	C	68.34200	66.10180	84.47590	403.66664	-490.82064	649.22373	1
20404	H	68.06800	66.67780	85.38590	740.91520	-752.85466	-2967.32508	1
20405	H	69.24300	65.50480	84.73090	-2012.57951	-2075.32950	-1252.78755	1
20406	C	67.11800	65.15880	84.29590	-83.67110	-74.89202	-909.53009	1
20407	H	67.27600	64.54180	83.38490	-1073.54999	-2565.17986	-1480.50021	1
20408	C	67.17400	64.17980	85.52090	460.95808	-515.50962	-599.13926	1
20409	H	66.20600	63.64480	85.41390	2397.08861	1927.49171	-651.09076	1
20410	H	67.27400	64.75380	86.46590	-2869.85286	1242.90802	-354.59379	1
20411	H	68.06800	63.52580	85.43190	1294.38050	-788.15091	-2761.80874	1
20412	C	65.84000	65.91780	84.21390	867.88328	266.86433	-38.57492	1
20413	H	65.86700	66.56680	83.31290	2134.99966	-2070.77577	-1025.59095	1
20414	H	64.97100	65.22780	84.18490	2228.47620	-826.73611	-2062.74858	1
20415	H	65.68500	66.60280	85.07490	-1730.18241	-1805.67315	-1916.74896	1
20416	C	69.78900	67.93480	83.58990	-669.78685	590.00057	-198.08022	1
20417	O	69.52000	69.15080	83.59590	-330.49488	-501.32361	512.77342	1
20418	N	71.02500	67.45980	83.92190	-671.44398	451.09628	-252.33206	1
20419	H	71.29900	66.50280	83.86090	1263.83761	2404.96265	1577.80273	1
20420	C	72.04000	68.25880	84.44690	12.43074	420.97127	803.71447	1
20421	H	71.72900	68.65180	85.40390	-1705.16054	687.37629	2550.35971	1
20422	C	73.35000	67.44380	84.73490	-747.41729	-368.33650	371.96345	1
20423	H	74.10400	68.14980	85.14490	2986.10525	-698.14654	-696.97013	1
20424	H	73.20500	66.70780	85.55390	-706.38084	-2782.19233	1286.98793	1
20425	H	73.77200	66.98480	83.81490	2025.39785	-2217.41883	927.30008	1
20426	C	72.37500	69.33780	83.44090	-765.84709	-336.03465	-375.15385	1
20427	O	72.35400	70.52480	83.71590	531.60806	466.83134	340.76811	1
20428	N	72.52600	68.93380	82.15690	564.12353	-253.84989	566.61362	1
20429	H	72.48400	67.96680	81.91890	-314.81308	2477.98286	-1917.84791	1
20430	C	72.88600	69.73780	81.06290	277.65989	529.10933	-691.35934	1
20431	H	73.82700	70.20980	81.30690	-2880.40862	100.79266	-1274.94318	1
20432	C	73.15900	68.74380	79.88290	34.36333	904.61594	-118.40888	1
20433	H	72.24600	68.13780	79.70290	1999.54534	-785.60437	-2298.99484	1
20434	H	74.00200	68.08380	80.18090	-1461.50521	2589.81628	-1039.85540	1
20435	C	73.42400	69.35880	78.57890	802.95351	-420.50731	-39.22834	1
20436	C	74.73300	69.62180	78.20490	-892.04944	-170.97013	116.06176	1
20437	H	75.61300	69.41980	78.79790	509.71363	-2656.48449	1597.86512	1
20438	C	74.94800	70.16980	76.88990	501.57512	-145.89548	738.95212	1
20439	H	75.94500	70.40780	76.54990	-2062.67637	-760.48947	-2259.37280	1
20440	C	73.86900	70.43680	76.05490	-120.65328	-901.44540	-42.28973	1
20441	H	74.11800	70.79380	75.06590	-815.94961	2963.08163	-695.42788	1
20442	C	72.34100	69.62080	77.69590	-642.39369	-1.05379	-656.00186	1
20443	H	71.31700	69.47980	78.01090	-918.60612	1687.30015	2490.34961	1
20444	C	72.56000	70.16080	76.43590	-553.31052	-658.73107	-311.56045	1
20445	H	71.70500	70.39580	75.81990	-2803.80628	425.91313	1370.77547	1
20446	C	71.85900	70.76280	80.73490	357.59302	-606.12368	-580.26266	1
20447	O	72.02600	71.98080	80.52490	246.59321	292.18909	686.51055	1
20448	N	70.56600	70.38080	80.67190	-579.23755	539.79530	-304.60005	1
20449	H	70.32800	69.41380	80.71090	1725.41270	2048.84289	-1649.50001	1
20450	C	69.44000	71.27380	80.50690	-835.54156	347.39919	-144.21704	1
20451	H	69.51600	71.89380	79.62590	-667.86940	-2418.62952	-1901.53640	1

20452	C	68.15900	70.43480	80.33790	502.82823	-180.23693	733.49378	1
20453	H	67.91400	69.83780	81.24290	-1466.56316	1425.53450	2390.19653	1
20454	H	68.37400	69.74180	79.49790	1818.13835	2229.53619	-1270.33072	1
20455	C	66.92100	71.17580	80.05790	-388.14025	-228.08235	-797.11912	1
20456	C	66.57200	71.44880	78.74590	-800.44749	442.75501	-55.39110	1
20457	H	67.31800	71.24980	77.98990	977.15023	1485.62864	2591.91995	1
20458	C	65.36200	72.05980	78.40290	-429.74261	560.31165	-582.13009	1
20459	H	65.06300	72.19480	77.37390	2876.06108	178.39252	1249.47696	1
20460	C	64.52500	72.43380	79.47390	282.18653	-522.64791	689.21628	1
20461	H	63.62600	73.01480	79.32790	-1617.44121	2071.06712	1733.95866	1
20462	C	66.02700	71.52980	81.08290	-421.25756	-448.33810	674.61359	1
20463	H	66.30100	71.35380	82.11290	-3039.23074	-818.82495	-131.76491	1
20464	C	64.89600	72.27080	80.79890	302.28465	560.77481	-650.65446	1
20465	H	64.14400	72.56780	81.51590	2262.96875	-344.06780	-2154.66870	1
20466	C	69.33500	72.26180	81.71990	783.29873	-102.68020	-450.21499	1
20467	O	69.08000	73.41680	81.52690	-377.02007	694.18054	47.02147	1
20468	N	69.63000	71.85980	82.96790	429.16608	-326.31243	645.11695	1
20469	H	69.70200	70.91080	83.26390	-1654.39128	-2673.14766	-184.08662	1
20470	C	69.74000	72.75980	84.02890	-879.24586	-118.37682	-228.23466	1
20471	H	68.80600	73.27580	84.19490	2214.35427	-1065.83465	1959.36725	1
20472	C	69.97200	71.99480	85.34890	-259.03649	519.95733	700.32299	1
20473	H	69.16700	71.24180	85.48590	1963.98958	1789.07772	-1682.11755	1
20474	H	70.95100	71.47480	85.41890	-261.32279	-3134.05308	-142.84297	1
20475	H	69.93600	72.73580	86.17590	-1653.36562	1786.38234	1991.95455	1
20476	C	70.81600	73.85580	83.78590	296.03433	613.59929	601.13933	1
20477	O	70.62400	75.02280	84.15090	-639.07849	-333.17333	-333.17520	1
20478	N	71.92800	73.46580	83.15890	215.77116	687.67294	-438.92147	1
20479	H	71.88900	72.59580	82.67490	-2322.62746	-1320.60787	-1669.93115	1
20480	C	73.00100	74.43080	82.80690	-60.52574	505.51068	-758.84717	1
20481	H	73.28100	74.87180	83.75190	556.31376	-260.79097	3082.67980	1
20482	C	74.19600	73.61780	82.23390	-182.61564	-426.62038	-788.85015	1
20483	H	74.96200	74.36980	81.94790	-94.89338	2301.20883	-2146.54057	1
20484	H	73.88900	73.19180	81.25490	-2501.11075	282.04569	-1896.63157	1
20485	S	74.87400	72.35080	83.38990	-394.92036	303.77970	-260.00484	1
20486	H	73.67600	71.91480	83.75190	2081.38285	-1804.24523	1512.43397	1
20487	C	72.62400	75.52980	81.86190	-620.71856	158.62633	651.43853	1
20488	O	72.81800	76.70480	82.13490	777.95765	-104.45792	11.68727	1
20489	N	71.91800	75.07780	80.72890	-228.00471	-529.15225	-620.32588	1
20490	H	71.92300	74.09580	80.55290	-2083.51628	-2344.09634	-286.47068	1
20491	C	71.54200	75.91280	79.63390	155.42880	285.55874	-852.49322	1
20492	H	72.31800	76.64380	79.46390	682.43095	2638.28760	1569.92876	1
20493	C	71.62200	74.98880	78.37290	-20.37741	-543.34072	-733.02230	1
20494	H	71.04500	75.42080	77.52690	541.20451	793.88229	2993.74599	1
20495	H	71.17500	73.99780	78.60090	1742.37550	-1666.60932	-2017.66499	1
20496	C	73.02200	74.78780	77.81290	61.70109	602.11210	680.60857	1
20497	C	73.70700	73.56580	77.87990	102.69375	663.89250	-620.15308	1
20498	H	73.23900	72.61380	78.08190	2247.23856	600.46480	2110.13018	1
20499	N	74.94100	73.72080	77.23790	658.75799	-433.39922	-288.91116	1
20500	H	75.57100	73.04880	76.91690	-2964.47081	-152.45527	-1061.65727	1
20501	C	75.03800	74.99780	76.86390	312.39758	-446.40941	724.64360	1
20502	C	73.88500	75.72880	77.20590	95.39523	-664.22236	-616.48672	1
20503	C	73.84600	77.15180	77.05090	595.93544	-457.06153	506.73611	1
20504	H	72.96800	77.73480	77.28890	-108.41052	3140.34280	190.57743	1
20505	C	74.99200	77.74080	76.45190	-391.25899	-654.92157	-502.97887	1
20506	H	74.97600	78.77380	76.13690	2071.13153	2364.85940	-10.34101	1
20507	C	76.13500	75.64780	76.26290	267.79791	367.50781	-792.10054	1
20508	H	77.00800	75.08280	75.96990	-1850.58696	-2078.20722	-1474.87729	1
20509	C	76.07400	77.02980	76.04390	259.28936	717.23029	497.99242	1
20510	H	76.95300	77.55880	75.70590	-2234.26855	1243.81347	-1844.85262	1
20511	C	70.21200	76.64580	79.76090	-796.44164	346.90135	291.78737	1
20512	O	70.11700	77.79280	79.22390	-403.37842	-249.72626	634.38027	1
20513	N	69.22300	76.15280	80.47990	-743.90175	392.56767	112.15853	1

20514	H	69.32500	75.27080	80.93290	-2387.91572	1962.98996	603.40948	1
20515	C	67.91700	76.79680	80.50690	-234.14640	-612.77389	635.35631	1
20516	H	67.50100	76.72480	79.51290	-2657.90546	586.61038	1587.05541	1
20517	C	67.04200	75.89380	81.32190	248.29829	-868.98166	-115.39297	1
20518	H	67.50300	75.63980	82.29990	1789.97501	-2444.72445	-840.44232	1
20519	H	67.00500	74.91080	80.80590	2387.77954	1489.98580	1396.74492	1
20520	C	65.64000	76.49380	81.61290	-716.85641	-496.90060	280.51405	1
20521	H	65.63400	77.50380	82.07590	-2859.88869	-394.04495	1262.76110	1
20522	C	64.73900	76.55180	80.32490	-190.84838	-392.66461	802.70889	1
20523	H	64.91700	75.65380	79.69490	2026.34317	-632.23737	2317.97766	1
20524	H	63.67100	76.57880	80.62790	-3055.99920	-761.67452	-105.19469	1
20525	H	64.89500	77.50380	79.77390	1262.99409	2145.17464	1921.00230	1
20526	C	64.90600	75.60280	82.61490	213.47330	480.21257	-742.69183	1
20527	H	65.60700	75.23780	83.39590	-1781.11252	1896.39801	1771.56094	1
20528	H	64.05500	76.15680	83.06690	1737.97054	-1255.56394	-2299.26822	1
20529	H	64.60100	74.61180	82.21590	1324.65009	-1924.22409	2105.71085	1
20530	C	67.88300	78.25880	80.97990	-727.01793	-420.78343	-365.14205	1
20531	O	67.19700	79.02380	80.29190	486.37647	472.84692	398.38258	1
20532	N	68.52100	78.78280	82.02490	-55.67475	833.14887	-121.32656	1
20533	C	69.31500	77.97980	82.97190	-779.60307	287.22913	384.57240	1
20534	H	68.96900	76.92580	83.03290	-435.01923	2322.24841	-2077.63935	1
20535	H	70.36000	78.03480	82.59890	-128.46864	-1711.82206	2636.96651	1
20536	C	68.47200	80.19080	82.39590	118.55891	-847.70446	-313.45492	1
20537	H	67.44000	80.42380	82.61490	-723.12595	-2318.46173	-2001.57386	1
20538	C	69.25900	80.17180	83.75390	-404.90442	588.93397	-567.46988	1
20539	H	68.88300	80.87580	84.52690	2871.51761	1211.51990	394.31535	1
20540	H	70.32300	80.40280	83.53390	1013.38486	2830.74964	-917.27071	1
20541	C	69.11600	78.74880	84.28590	821.75306	199.20080	330.00506	1
20542	H	69.94800	78.54280	84.99390	2716.04460	1573.88846	-127.87139	1
20543	H	68.10900	78.61380	84.73490	1971.27042	-1682.05559	1781.62244	1
20544	C	69.05500	81.12380	81.23090	621.74854	121.46666	651.78921	1
20545	O	68.57200	82.24780	81.04590	352.46462	669.19174	218.92168	1
20546	N	70.09900	80.67380	80.54090	-763.64812	-237.66844	286.47718	1
20547	H	70.39500	79.77580	80.85690	1825.96903	-1978.29223	-1621.43128	1
20548	C	70.60700	81.42980	79.40390	-221.20548	877.27987	129.78830	1
20549	H	70.77000	82.44380	79.73990	-1952.75811	-2361.74275	728.38846	1
20550	C	71.94100	80.76680	78.92290	433.01949	-738.04554	-303.76659	1
20551	H	71.86800	79.65880	78.87490	1427.15967	866.49008	-2663.70379	1
20552	H	72.71000	80.96280	79.70090	2491.99726	-1127.55227	1544.77654	1
20553	C	72.44600	81.21980	77.54890	544.92681	365.19204	-628.15294	1
20554	C	73.03200	82.49780	77.40790	119.30009	888.67053	-168.93695	1
20555	H	73.19700	83.12680	78.26990	2991.19652	-928.54855	-215.41398	1
20556	C	73.38000	82.91680	76.12890	-275.75226	689.20129	536.83544	1
20557	H	73.80300	83.90780	76.04790	279.57033	3047.19941	738.93218	1
20558	C	73.21100	82.08580	74.99290	-491.76033	-746.67195	188.57366	1
20559	O	73.66500	82.54480	73.75290	650.82087	-311.22770	-301.27528	1
20560	H	74.19700	83.33680	73.85990	-749.00924	2285.61093	2035.27253	1
20561	C	72.14500	80.45680	76.39290	-387.13295	-826.71248	-9.33084	1
20562	H	71.53000	79.57280	76.46990	-244.03537	-3110.59560	-393.23317	1
20563	C	72.59800	80.86680	75.14790	353.69255	-780.62741	-296.43406	1
20564	H	72.46700	80.20280	74.30690	2562.29264	-1629.33359	-794.83973	1
20565	C	69.60500	81.53480	78.26890	-284.92785	-734.00912	463.65683	1
20566	O	69.34000	82.63880	77.79490	691.35372	-335.39963	154.19752	1
20567	N	68.89900	80.39980	77.87590	711.51531	442.73410	47.88856	1
20568	H	69.15900	79.51980	78.26490	-1648.75348	-2013.70731	-1771.79205	1
20569	C	67.79400	80.35980	76.99690	787.79125	-97.55859	-435.35576	1
20570	H	68.02800	80.90180	76.09190	-816.63774	-1678.82778	-2532.08108	1
20571	C	67.37900	78.88380	76.66290	777.84194	153.26924	-438.64669	1
20572	H	67.35800	78.20080	77.53890	2467.11337	1468.69270	1276.08677	1
20573	H	66.31400	78.74980	76.37590	1799.39135	-973.64395	-2383.53095	1
20574	C	68.31100	78.32080	75.65290	-705.25669	501.89880	-304.93057	1
20575	C	68.11000	78.68280	74.28590	533.59764	542.89476	-496.15951	1

20576	H	67.23800	79.29980	74.12290	1009.12056	2084.39778	2129.37894	1
20577	C	68.99100	78.15880	73.25190	204.71512	-687.42304	557.14316	1
20578	H	68.92600	78.57780	72.25790	-1779.18635	-169.82652	2594.55253	1
20579	C	69.92600	77.15880	73.58790	-495.17626	114.12480	761.64787	1
20580	O	70.77300	76.70680	72.57590	617.60050	259.32096	-410.18511	1
20581	H	70.57700	77.24380	71.80390	-2377.30488	-1730.95893	1128.23690	1
20582	C	69.24800	77.30080	75.92290	393.48833	-445.23166	686.59809	1
20583	H	69.32500	76.81380	76.88390	2432.54882	1986.14299	-108.92899	1
20584	C	70.03300	76.73280	74.90990	268.21968	483.99985	-724.37097	1
20585	H	70.81500	76.02580	75.14390	1691.71228	2139.10077	1563.53039	1
20586	C	66.60900	81.16880	77.39390	-510.15849	535.88567	541.94057	1
20587	O	66.03000	81.91280	76.59390	-562.59245	-29.98994	-557.81211	1
20588	N	66.26200	81.14380	78.69490	-430.12318	461.06752	-564.22658	1
20589	H	66.72900	80.59280	79.38290	225.60819	-420.10098	-3107.63141	1
20590	C	65.22400	82.07880	79.20490	666.80812	-614.12506	-34.68515	1
20591	H	64.38800	81.88480	78.54990	-2069.77189	-1517.12054	-1824.32272	1
20592	C	64.68300	81.72780	80.60790	-837.93004	-44.52736	-367.49663	1
20593	H	65.60700	81.77480	81.22190	-1930.74285	1277.79209	2137.28689	1
20594	C	63.60600	82.80080	81.01090	499.55969	-398.35731	649.99818	1
20595	H	62.70300	82.86080	80.36690	-2013.04249	1127.11753	2147.89753	1
20596	H	63.25600	82.57980	82.04190	-2211.99161	-828.61076	2087.93316	1
20597	H	64.00900	83.83280	81.09290	-2816.39215	-736.52817	-1203.92838	1
20598	C	64.11400	80.29080	80.63890	606.98847	-594.27891	324.62081	1
20599	H	63.25500	80.13980	79.95190	2843.84020	596.01762	-1190.07659	1
20600	H	64.84000	79.61680	80.13490	-1855.40709	-2543.66909	-90.17938	1
20601	C	63.65900	79.83980	81.99690	527.16891	447.82244	-586.28745	1
20602	H	64.50200	79.89380	82.71890	2471.91691	-658.17484	-1823.32103	1
20603	H	63.43900	78.75180	81.95090	2378.40743	-184.80357	2047.32749	1
20604	H	62.80200	80.44580	82.35890	-739.15916	2925.35186	893.08802	1
20605	C	65.58000	83.61280	79.03390	-668.87574	-189.82880	600.29945	1
20606	O	64.77400	84.26080	78.37690	-455.26397	-99.76538	645.83111	1
20607	N	66.82900	84.06580	79.36490	-671.55587	222.80235	-466.74625	1
20608	H	67.45400	83.43180	79.81190	-2956.74293	-175.31124	1080.48037	1
20609	C	67.14848	85.42555	79.01351	-794.77172	-346.48084	-18.04269	1
20610	H	66.40017	86.12865	79.37831	-163.15970	-1338.42981	3408.28865	1
20611	H	68.12727	85.57651	79.50732	-1908.94692	-2891.00670	-1632.64879	1
20612	C	67.22715	85.74941	77.41232	-766.58746	638.11216	-290.13945	1
20613	O	66.76040	86.84867	77.11799	-153.91875	-225.17470	66.30946	1
20614	N	67.89100	84.89680	76.61290	349.47837	-661.98279	384.43249	1
20615	H	68.32900	84.14080	77.09390	881.12469	2663.55032	1424.31624	1
20616	C	67.91510	85.15220	75.17914	173.63576	927.79959	-349.21030	1
20617	H	68.55113	86.10064	75.00991	1334.76171	-1566.42064	-2374.77745	1
20618	C	68.53600	83.92580	74.53290	-684.58583	-543.11628	-273.03382	1
20619	H	68.10500	82.98380	74.93690	-1573.95899	1819.73773	-2032.45044	1
20620	C	68.34900	83.93880	73.05490	-867.92048	290.18588	100.01343	1
20621	H	67.38300	83.53880	72.67890	551.31919	-3031.68844	617.08689	1
20622	H	68.68700	84.91880	72.65490	-2387.55708	1917.70533	758.49530	1
20623	H	69.02400	83.17980	72.60690	2565.01676	-620.57813	-1697.45723	1
20624	C	70.05800	83.94780	74.75490	-867.10462	17.60983	306.27352	1
20625	H	70.56200	83.01280	74.42890	-564.66550	2793.94571	1341.61255	1
20626	H	70.17300	83.76380	75.84390	1851.07309	1315.25961	-2170.48739	1
20627	C	70.73964	85.25037	74.18339	-96.47682	662.74969	24.18739	1
20628	H	70.51241	86.13298	74.81135	2895.62464	-907.45558	161.75402	1
20629	H	71.84974	85.21415	74.25989	-2243.08714	1142.33984	1408.27602	1
20630	H	70.50118	85.40081	73.07489	-1416.37637	-2431.22559	-733.20556	1
20631	C	66.36120	85.12981	74.59090	711.89096	241.86490	-120.03054	1
20632	O	66.21609	85.91526	73.66779	292.10910	120.99451	276.11465	1
20633	N	65.47600	84.30180	75.09290	-422.70430	436.82380	-588.91212	1
20634	H	65.70400	83.60980	75.77290	-84.32858	-2430.43684	1997.81685	1
20635	C	64.05600	84.33580	74.67990	-318.30538	224.05262	-824.07556	1
20636	H	64.10600	84.16680	73.61490	-2588.17039	-1212.04062	-1325.50766	1
20637	C	63.18100	83.19080	75.19690	297.31517	-481.66584	714.56729	1

20638	H	62.22600	83.07180	74.64190	2739.85345	655.49407	1390.24786	1
20639	H	63.77500	82.27180	75.00590	516.93564	-1981.01331	-2382.95225	1
20640	O	62.80900	83.14980	76.55590	282.19169	160.03859	721.07292	1
20641	H	63.47300	83.61580	77.06990	2988.76605	32.74383	-956.87008	1
20642	C	63.39882	85.76613	75.12136	-6.77955	31.62686	-1127.85543	1
20643	O	62.45323	86.21008	74.50772	-955.60722	83.22041	-260.36816	1
20644	N	63.81075	86.17393	76.30550	-441.97190	-174.59081	61.21346	1
20645	H	64.48882	85.62521	76.83678	1033.71056	-1531.43285	75.07215	1
20646	C	63.26928	87.54548	76.71632	911.89541	16.41080	68.87652	1
20647	H	62.18764	87.41175	76.53953	-3730.67886	1790.16285	1227.45598	1
20648	C	63.39703	87.75025	78.19801	431.37768	165.30127	118.86775	1
20649	H	64.39430	87.77979	78.60741	-109.99858	-3272.92983	849.68098	1
20650	C	62.77283	89.09410	78.58793	-1057.32240	46.68343	-102.67734	1
20651	H	63.24739	89.78485	77.94422	2794.51861	1435.61421	-3098.63029	1
20652	H	62.92250	89.40377	79.66545	758.63880	-583.58687	-926.19382	1
20653	H	61.67416	89.14574	78.42147	1894.22693	711.07586	366.48776	1
20654	C	62.63280	86.63714	78.84168	-301.83138	460.68121	484.09322	1
20655	H	63.04221	85.65699	78.53859	-874.14069	3226.63632	965.88136	1
20656	H	61.55063	86.65558	78.41271	2919.83058	751.94084	1840.42650	1
20657	C	62.57542	86.63160	80.43186	-78.32382	535.64191	700.20883	1
20658	H	63.53130	86.40362	80.94340	713.54950	-4970.64389	-1310.56486	1
20659	H	62.24363	87.63826	80.85378	185.76313	-1589.04562	650.43204	1
20660	H	61.86974	85.79770	80.62287	2534.43605	-1031.54464	-3956.96473	1
20661	C	64.05399	88.66726	75.80785	778.01641	228.99839	-248.26628	1
20662	O	63.54467	89.74659	75.66206	549.51681	-52.88836	50.70185	1
20663	N	65.22526	88.22826	75.32217	-441.83013	-535.34161	-309.76692	1
20664	H	65.64559	87.33629	75.69675	-457.32449	3269.29627	-2005.25354	1
20665	C	65.90495	89.10965	74.34685	-140.62402	-319.84206	-101.95537	1
20666	H	65.94048	90.17377	74.67793	1992.49752	2350.74141	-36.30298	1
20667	C	67.34807	88.61200	74.59488	-907.54566	89.50658	-638.94327	1
20668	H	67.36305	87.51604	74.27806	-2770.78561	2833.41341	-21.01600	1
20669	H	67.47487	88.58597	75.74321	143.36577	872.13733	-322.59842	1
20670	C	68.63614	89.36706	74.06655	-179.91101	-88.25166	-30.08352	1
20671	O	68.60824	90.60045	74.18382	-764.51079	819.79233	227.76724	1
20672	O	69.65000	88.75023	73.69993	-336.25098	-77.35147	-684.34846	1
20673	C	65.24919	88.94903	72.87428	-666.15538	-412.21019	-265.48488	1
20674	O	65.16715	89.89882	72.16671	86.32707	185.09641	-646.73582	1
20675	N	64.63791	87.74476	72.76823	-23.29870	292.12927	-367.36265	1
20676	H	64.78025	87.06801	73.53009	-2395.85199	-936.48633	-185.33349	1
20677	C	64.08304	87.33009	71.51575	463.22597	115.61467	22.90692	1
20678	H	64.81731	87.63611	70.72573	1539.48140	3738.56323	1265.64320	1
20679	C	63.62227	85.79749	71.50449	597.20545	-227.31064	160.43669	1
20680	H	62.79968	85.84775	72.31251	-891.15566	19.06727	152.27209	1
20681	H	63.02087	85.76927	70.60870	920.30092	-785.21819	765.68050	1
20682	O	64.66356	84.85648	71.65456	587.64083	-96.56647	-318.91158	1
20683	H	65.05176	85.14983	72.52792	-989.77908	-477.01790	-2358.37045	1
20684	C	62.63983	88.09711	71.23443	506.45265	755.85180	102.03834	1
20685	O	62.24525	88.26283	70.09351	-288.74887	-10.76247	-440.20593	1
20686	N	61.91870	88.21976	72.34332	86.32084	-147.04365	836.57647	1
20687	H	62.47027	88.08333	73.20161	-1211.05199	1586.99523	-1821.57843	1
20688	C	60.63285	88.89662	72.36240	-31.71811	-662.75474	689.75077	1
20689	H	60.03049	88.59730	71.48536	-183.43472	12.33233	452.51386	1
20690	C	59.80350	88.65296	73.66233	-341.34154	-224.43220	602.50258	1
20691	H	58.73809	89.00100	73.61142	-1434.09828	-323.05204	268.96969	1
20692	H	60.24896	89.26089	74.48064	340.13330	2434.96628	2621.08530	1
20693	C	59.57950	87.12409	74.03554	-578.66689	-333.96247	-353.72381	1
20694	C	59.46838	86.24581	72.92917	313.09481	878.86263	-350.43956	1
20695	H	59.51824	86.62792	71.86149	546.64723	3736.06016	-1060.34233	1
20696	C	59.30100	84.85880	73.12290	17.11612	-616.94622	674.88892	1
20697	H	59.12100	84.20580	72.28090	1145.91002	2426.49186	1644.30462	1
20698	C	59.18800	84.30980	74.35190	543.01516	-532.62079	498.38033	1
20699	H	59.20900	83.23180	74.40590	-128.36272	-1413.16777	-2803.06246	1

20700	C	59.50121	86.54487	75.32936	-311.45280	-135.06315	-610.90124	1
20701	H	59.72625	87.15742	76.23203	-2951.83004	3717.90133	3843.85176	1
20702	C	59.42121	85.15857	75.47888	942.02043	200.93095	-101.26944	1
20703	H	59.40800	84.60080	76.43090	492.51908	3074.37158	450.59690	1
20704	C	60.92212	90.44153	71.91903	451.88666	-171.96767	650.38426	1
20705	O	59.95176	91.10825	71.54004	43.36330	63.49028	1790.15609	1
20706	N	62.11174	90.82882	72.25305	-854.55586	-1081.18359	-559.12697	1
20707	H	62.84905	90.15627	72.59584	606.46427	-4571.60585	-503.54717	1
20708	C	62.66250	92.08922	71.76434	-933.33559	-109.93341	524.85724	1
20709	H	61.86500	92.87544	71.79206	-989.96490	929.13854	-1589.31678	1
20710	C	63.87579	92.46317	72.68348	144.05296	314.09551	-109.88815	1
20711	H	64.86298	91.93500	72.32394	1328.83437	1013.84262	2179.82367	1
20712	C	64.12961	93.99038	72.43076	169.55312	-105.32643	692.76932	1
20713	H	63.92397	94.31106	71.37416	-1359.48952	-117.49054	832.88348	1
20714	H	63.38665	94.64690	72.97127	426.70485	-1404.61136	210.41090	1
20715	H	65.12907	94.21592	72.72167	2334.30877	3117.19741	802.41086	1
20716	C	63.57463	92.30867	74.20211	-575.68509	193.17933	1556.56785	1
20717	H	63.57655	91.17042	74.49792	1960.40909	2181.91034	950.11531	1
20718	H	62.60309	92.74911	74.36024	-240.29001	-1428.34522	2855.15404	1
20719	C	64.51793	93.13227	75.19589	-250.92737	-19.04652	204.64724	1
20720	H	64.38877	94.22679	75.22366	-1068.05531	92.62797	-1311.77940	1
20721	H	65.63067	92.91294	74.93143	-159.73932	2143.27033	-3080.59715	1
20722	H	64.37970	92.72917	76.22494	3948.91834	1911.47754	-53.74148	1
20723	C	63.29618	91.99050	70.25080	39.49362	562.93437	689.31337	1
20724	O	63.47979	93.08333	69.69355	-532.76959	121.22827	-189.13762	1
20725	N	63.61200	90.79427	69.77356	-88.48815	-563.37067	-46.03139	1
20726	H	63.58552	90.00744	70.41473	941.10788	1891.71889	-1607.55463	1
20727	C	64.44913	90.69105	68.60272	320.89657	365.29215	678.91877	1
20728	H	64.95837	91.69250	68.50078	3685.02740	715.71281	-2000.82474	1
20729	C	65.40363	89.42600	68.86932	1.28222	-709.95782	-39.68383	1
20730	H	64.76265	88.56216	69.19349	-879.80675	435.08942	-1885.51649	1
20731	H	66.18910	89.64634	69.61255	-2563.54288	1863.65931	-1614.56234	1
20732	C	66.01490	89.03076	67.54627	-156.42059	151.85300	-303.24083	1
20733	H	65.54141	89.64897	66.72043	906.02218	-1266.74668	1636.93785	1
20734	C	67.51273	89.26344	67.40941	-391.19322	16.76328	-834.71573	1
20735	H	67.86347	90.34614	67.34675	-1344.17983	744.22167	1333.57510	1
20736	H	67.84750	88.80631	66.40361	1984.59000	542.22080	-1756.27699	1
20737	H	68.11795	88.91299	68.17315	52.23918	440.79931	2352.40021	1
20738	C	65.70372	87.57820	67.22275	-1419.32843	172.98325	-730.96140	1
20739	H	66.58300	87.05756	66.65696	2481.80108	-2561.91698	1190.28635	1
20740	H	65.54474	86.98243	68.11281	-590.36462	-2084.39707	-435.51662	1
20741	H	64.68331	87.37119	66.79001	655.66664	1983.56946	2293.55723	1
20742	C	63.43773	90.41966	67.39155	900.15960	783.91466	718.23637	1
20743	O	63.66145	91.02601	66.38186	360.38103	1042.17163	-533.17755	1
20744	N	62.33408	89.60282	67.69794	-70.30861	-685.42518	74.63749	1
20745	H	62.16779	88.95386	68.50842	2009.70470	-147.89715	2163.47986	1
20746	C	61.16825	89.98125	66.92918	433.83382	-64.63196	382.08399	1
20747	H	61.66002	89.95456	65.93871	3329.09899	1895.52477	1652.71623	1
20748	C	60.07266	88.82429	66.90143	-303.47367	-353.01591	447.18922	1
20749	H	60.62964	87.87350	66.62868	272.64933	-281.53047	45.14171	1
20750	H	59.41029	88.94798	66.07779	-397.42144	-70.67103	328.73882	1
20751	C	59.33680	88.67185	68.21537	-494.65047	-106.96607	269.37410	1
20752	H	60.02302	88.28730	68.96448	-2051.66561	-780.04698	1441.79893	1
20753	C	58.68071	89.96325	68.74186	-313.47884	545.48122	-728.60532	1
20754	H	59.52247	90.66161	68.93834	609.70162	284.50469	1478.07458	1
20755	H	58.19860	89.74871	69.62551	496.69659	-3321.83509	1960.10436	1
20756	H	57.98063	90.51973	68.09307	1325.14302	-1657.75235	165.56909	1
20757	C	58.30945	87.55069	68.13400	-474.80810	-609.79142	-763.64103	1
20758	H	57.47549	87.91708	67.48931	750.82613	1106.28442	3846.42778	1
20759	H	58.78954	86.65264	67.64366	-590.07826	-709.88431	520.44068	1
20760	H	57.71045	87.34422	69.03190	835.91366	-3865.28425	685.99969	1
20761	C	60.64382	91.52442	67.08069	290.74491	-140.06496	-1234.69936	1

20762	O	59.80164	91.95351	66.30386	148.42403	350.74843	-391.08482	1
20763	N	61.10948	92.09159	68.17279	473.79268	273.36833	683.86330	1
20764	H	61.77583	91.56829	68.74905	481.70661	516.81995	849.97120	1
20765	C	60.84673	93.43325	68.57630	983.47290	340.24692	1069.83651	1
20766	H	61.26062	93.66123	69.68195	2108.48704	-230.03140	656.81551	1
20767	C	61.49706	94.31506	67.43901	-628.68421	-818.30687	-735.81477	1
20768	H	62.22680	93.65470	66.90567	-1616.20238	-1228.48103	-189.12222	1
20769	H	60.75666	94.63586	66.74264	2537.72308	3228.23615	-1188.47918	1
20770	C	62.18607	95.71044	67.73748	135.62776	53.74188	-261.74571	1
20771	H	63.05871	95.70276	68.49395	-1484.20163	272.83703	827.16646	1
20772	H	61.45474	96.44351	68.20310	-1127.23089	-1152.42342	454.52404	1
20773	C	62.51925	96.32968	66.35890	-510.50826	-530.81570	391.01793	1
20774	O	61.73843	95.86788	65.27391	27.83198	-221.81590	-165.44816	1
20775	O	63.33848	97.24005	66.25969	89.16362	-54.26436	99.54677	1
20776	C	59.29377	93.83407	68.75121	-217.22905	-818.88691	48.36759	1
20777	O	58.88270	94.89738	68.27945	-139.18916	-466.53739	-628.88283	1
20778	N	58.65339	92.96625	69.50651	-609.16534	280.33873	20.02385	1
20779	H	59.09364	92.12045	69.92666	1232.59148	954.74855	3651.92391	1
20780	C	57.41364	93.40144	70.09645	587.36353	-1093.37260	415.88240	1
20781	H	56.91370	94.03813	69.28731	-355.03709	-4053.45219	3384.43901	1
20782	C	56.52710	92.08817	70.40261	-661.38675	-160.99611	555.34363	1
20783	H	56.94339	91.33920	69.67268	-296.15161	-1410.86496	-2864.55681	1
20784	C	56.70396	91.52146	71.83580	647.70479	-964.05184	377.06498	1
20785	H	57.76331	91.03694	72.04485	78.10573	3038.58880	2217.68576	1
20786	H	56.46218	92.37037	72.54768	-1319.39460	581.40843	4026.12610	1
20787	H	56.01531	90.62595	72.02206	2702.26478	2092.00277	455.17128	1
20788	C	55.05862	92.61828	70.16028	-604.13340	236.01807	155.66803	1
20789	H	54.33095	91.77790	69.85987	1356.51101	241.72217	-527.78004	1
20790	H	54.88146	93.29457	69.33943	-1076.96793	4705.09334	-1626.34574	1
20791	C	54.70435	93.43753	71.45253	-389.65374	41.80135	468.72976	1
20792	H	54.66432	92.78669	72.32767	1265.60301	1268.93134	1760.23586	1
20793	H	55.42442	94.26076	71.67409	-1347.31139	52.24130	-228.99649	1
20794	H	53.65345	93.82658	71.34305	-4047.34037	1326.47463	555.66085	1
20795	C	57.84452	94.47422	71.20820	-109.09715	64.95304	-242.47597	1
20796	O	57.22732	95.45542	71.48064	-103.51920	75.97231	-34.65582	1
20797	N	58.84680	93.93680	72.02198	-613.45837	281.89560	627.40327	1
20798	H	59.35203	93.25004	71.51769	-1038.97063	1599.65189	2530.07999	1
20799	C	59.67167	94.96699	72.72148	-697.02977	334.74991	-581.90767	1
20800	H	58.84611	95.60997	73.11315	-2074.04456	-3091.02764	1203.70448	1
20801	C	60.45991	94.27352	73.86574	33.43247	-161.41747	372.51727	1
20802	H	61.29160	93.75444	73.31125	-87.62559	506.91422	-1434.40559	1
20803	C	61.10030	95.15594	74.91902	-417.67540	105.09633	-321.96683	1
20804	H	61.61012	96.09705	74.54713	2608.70598	-1965.09458	-413.40015	1
20805	H	60.37455	95.49646	75.70843	926.67721	-1198.88898	794.35440	1
20806	H	61.86988	94.50838	75.44023	696.63340	-2039.93361	95.74319	1
20807	C	59.48413	93.30581	74.43927	461.67938	301.51946	426.72928	1
20808	H	58.93798	92.74502	73.59256	3430.00534	-121.60401	-2543.01325	1
20809	H	58.58881	93.72193	74.98679	4585.88091	-2890.86732	4955.49765	1
20810	C	60.26996	92.09793	75.19864	-156.01903	-466.18748	-330.11912	1
20811	H	60.87569	92.58296	75.94054	2216.61947	2993.68694	1123.13967	1
20812	H	61.00916	91.54847	74.58523	883.24853	1614.37196	3101.71036	1
20813	H	59.66621	91.36319	75.77756	1344.29036	2293.68399	-630.76368	1
20814	C	60.68089	95.64318	71.65051	-92.19728	-191.57104	-144.85895	1
20815	O	61.43631	95.05393	70.89973	50.52930	-36.18163	118.34628	1
20816	N	60.65015	97.00072	71.84682	426.32938	503.30056	209.89030	1
20817	H	60.25207	97.28566	72.75589	1965.13298	-2203.13261	779.83007	1
20818	C	61.67020	97.76632	71.23343	-906.92786	-392.70324	1026.27266	1
20819	H	61.86974	97.20241	70.27859	2078.65747	-57.30094	1652.58255	1
20820	C	61.12566	99.17991	70.94835	347.37576	157.22103	586.86091	1
20821	H	61.88928	99.96347	70.77391	985.87424	252.57120	-1615.35548	1
20822	H	60.58009	99.49375	71.92042	2490.41006	-237.08974	-290.91948	1
20823	C	60.19040	99.15267	69.62116	691.00587	646.41539	487.25911	1

20824	H	59.81991	100.17563	69.33486	2445.46357	-4085.91767	-953.02297	1
20825	H	60.71175	98.73099	68.76276	2972.77761	-3303.60330	622.75493	1
20826	C	58.93941	98.26556	69.84114	297.23554	-392.98170	99.70051	1
20827	H	58.27606	98.75643	70.65500	-2565.53963	-121.27388	-1205.41742	1
20828	H	59.21885	97.27445	70.24877	-1722.32077	103.93117	-2526.40233	1
20829	C	58.11597	98.12184	68.48819	-53.22675	923.62030	454.11613	1
20830	H	57.67470	99.05185	68.14721	-841.37150	-750.24733	521.94047	1
20831	H	57.40070	97.26583	68.53484	-1017.68230	-1659.96045	-4516.04402	1
20832	N	58.88711	97.46236	67.47186	73.88489	66.87273	262.28228	1
20833	H	62.14563	96.36880	64.51391	1633.73680	-1652.37962	-615.80054	1
20834	H	59.25150	96.53120	67.79575	2504.14793	517.72505	954.77360	1
20835	H	58.45068	97.54708	66.51754	-819.33084	782.58123	700.48164	1
20836	C	63.11835	97.67256	72.12161	341.89986	246.47505	-524.47879	1
20837	O	63.10630	97.87704	73.29410	486.18987	315.20212	-464.12166	1
20838	N	64.18054	97.42186	71.29689	-358.56566	-85.82770	67.39036	1
20839	H	63.90483	97.65326	70.34887	412.13927	-704.95614	-1712.72860	1
20840	C	65.54439	97.81134	71.74247	-813.15935	-19.12025	-387.40688	1
20841	H	65.46319	98.86654	71.80129	-2188.01900	-1021.48784	2446.90025	1
20842	C	65.89639	97.36260	73.18349	-508.58815	192.95577	-227.15957	1
20843	H	65.71662	96.22032	73.21090	-1253.83666	-2477.59342	226.15347	1
20844	H	65.13349	97.82140	73.93091	177.29783	-246.89981	1991.86461	1
20845	C	67.36409	97.62575	73.63378	607.75517	808.20074	371.99366	1
20846	H	67.59028	97.11917	74.56877	1497.06418	-875.29366	-1359.32586	1
20847	H	68.10730	97.11870	72.90059	2158.67958	2087.98906	1735.34675	1
20848	C	67.62411	99.16708	73.92062	126.42186	-690.14968	-66.12072	1
20849	O	67.32920	100.08219	73.19267	599.18304	17.59393	-165.70313	1
20850	N	68.19088	99.36746	75.11736	304.82005	-633.10859	1354.97498	1
20851	H	68.58658	98.71834	75.80516	1650.78290	-617.26942	-494.69665	1
20852	H	68.33915	100.30490	75.52353	1384.41299	-705.48794	-822.42098	1
20853	C	66.67595	97.38988	70.68236	-596.94645	269.85331	557.95842	1
20854	O	66.40525	96.40652	69.94218	373.54661	428.71106	-6.67771	1
20855	N	67.87429	97.94437	70.77372	709.27166	-7.26718	1092.43370	1
20856	H	67.87403	98.69255	71.48637	-1309.76995	-643.45348	910.73957	1
20857	C	69.01034	97.67068	69.95052	-406.09713	249.77037	545.96078	1
20858	H	69.23480	98.68238	69.57368	1249.03470	2587.99183	44.18410	1
20859	H	68.74010	96.93158	69.16336	-138.56796	1465.37732	754.22327	1
20860	C	70.05475	96.98765	71.01805	367.20158	-453.64387	786.42818	1
20861	O	70.19922	97.38246	72.15238	265.83576	286.22052	461.28611	1
20862	N	70.62039	95.97781	70.41853	574.95477	251.71588	801.54237	1
20863	H	70.75207	95.85665	69.33380	4339.91282	680.09693	-2345.17734	1
20864	C	71.42636	95.10795	71.19898	-195.06759	377.44122	26.39350	1
20865	H	70.83924	94.96254	72.18774	3053.23275	1326.55067	213.90830	1
20866	C	71.85554	93.73685	70.55312	103.88330	-542.38404	-93.43065	1
20867	H	72.00328	93.15226	71.49624	1592.81573	942.21601	2817.37305	1
20868	H	72.86503	93.84220	69.99919	-1511.92114	-1231.91081	-945.48833	1
20869	S	70.59298	92.95872	69.46464	192.53212	216.38942	-28.68671	1
20870	C	72.86736	95.82891	71.54208	-260.28447	-170.57006	-592.37729	1
20871	O	73.62793	95.17804	72.26161	-144.05307	164.30134	-479.46692	1
20872	N	73.08232	96.87712	70.82115	130.75313	373.30771	279.44408	1
20873	H	72.39715	97.31739	70.17080	-2387.49474	-2331.05349	465.77485	1
20874	C	74.24713	97.64880	71.02555	-28.26349	187.18656	492.11771	1
20875	H	74.98334	96.78736	71.27075	1080.29349	1440.59911	211.08667	1
20876	C	74.48310	98.37389	69.63622	703.11390	-404.93029	-182.02902	1
20877	H	73.75914	99.24814	69.59709	-2549.97668	-198.53209	2391.64674	1
20878	H	74.22110	97.62196	68.79978	4593.03908	-1455.18350	955.62399	1
20879	C	75.96397	98.80365	69.49397	-639.82100	-699.41277	-1186.80543	1
20880	H	76.01707	99.78756	70.04931	-405.98478	-6.69998	2086.07340	1
20881	H	76.72853	98.04006	69.93090	-3257.85719	2332.10860	-1599.17155	1
20882	C	76.27357	99.04267	67.92451	436.05983	-1595.97569	293.57837	1
20883	O	76.84549	100.10219	67.64426	-784.45154	107.68426	242.78969	1
20884	O	76.12191	98.04522	67.19341	-198.09927	744.69632	-51.75807	1
20885	C	74.00559	98.73299	72.27758	-28.49547	209.20073	916.60384	1

20886	O	74.93331	99.47164	72.51726	-435.98023	-548.83251	144.12774	1
20887	N	72.87892	98.54724	72.92143	-76.14261	-227.92109	229.06778	1
20888	H	72.24439	97.87460	72.41317	-664.69205	-271.01429	-1550.49655	1
20889	C	72.65266	99.09389	74.22390	681.96561	32.39299	258.58037	1
20890	H	73.37957	99.92496	74.55732	2075.64324	-1705.96525	197.87369	1
20891	C	71.12513	99.50444	74.16747	-712.18231	431.41737	-319.67568	1
20892	H	70.54219	98.77784	73.48737	-321.29101	340.78605	-4762.14069	1
20893	H	70.68679	99.38624	75.21423	2042.87626	1915.46090	-214.85886	1
20894	C	70.88388	100.94948	73.68944	302.72484	-778.24582	84.48962	1
20895	C	71.16452	101.82303	74.78377	-74.61931	8.75063	791.98426	1
20896	H	71.66945	101.41767	75.71723	2266.00169	-2217.93323	261.48847	1
20897	C	70.79727	103.18265	74.56602	-101.27143	1165.04115	-584.27942	1
20898	H	71.13614	103.88172	75.36027	-473.59631	420.38807	434.01809	1
20899	C	70.25753	103.67272	73.34650	-489.38483	751.12994	-241.52666	1
20900	H	69.81968	104.71509	73.23340	29.31921	-1042.18600	780.73661	1
20901	C	70.36506	101.33729	72.40138	363.87362	-546.31651	519.03662	1
20902	H	70.06115	100.62416	71.51428	1859.08177	396.00856	-1776.53367	1
20903	C	70.11884	102.74714	72.27854	-98.77227	-225.90014	-155.64021	1
20904	H	69.55666	102.97938	71.41239	-279.17866	-2631.18453	1401.36780	1
20905	C	72.62197	97.92846	75.32462	-557.33298	696.94656	44.87413	1
20906	O	72.24544	98.27071	76.43308	-68.60401	-224.02481	-817.59499	1
20907	N	72.86948	96.66472	74.91170	705.05117	83.85965	-482.39463	1
20908	H	73.25966	96.44103	73.95577	1594.29193	2957.17645	1300.70329	1
20909	C	72.13257	95.66665	75.53365	86.66764	-348.55915	-479.24748	1
20910	H	71.66056	96.07494	76.51769	5456.61101	-2889.69926	1670.03864	1
20911	C	70.97760	95.12531	74.52152	-267.91574	47.33821	-75.62639	1
20912	H	70.69707	95.90268	73.73125	-1935.15715	231.69097	1062.12128	1
20913	H	71.43032	94.29920	73.92031	372.03700	1584.57047	2586.90891	1
20914	C	69.74121	94.76294	75.34056	-556.81808	-555.80046	787.11753	1
20915	H	69.50253	95.67329	75.94573	-902.00261	1822.35505	-2506.06889	1
20916	H	69.75625	93.91989	76.08406	-1040.12070	-1788.87255	358.96500	1
20917	C	68.50285	94.51580	74.31502	-400.36537	1039.45306	1186.62801	1
20918	O	67.38599	94.57553	74.74382	-295.11018	1143.89723	-345.88938	1
20919	O	68.83854	94.17876	73.12906	444.48382	-256.93228	205.23407	1
20920	C	73.04137	94.30074	75.72559	330.32919	-224.49632	-535.45281	1
20921	O	72.53807	93.17322	76.02312	311.22981	953.73629	-732.81486	1
20922	N	74.33163	94.58241	75.64857	108.60199	-202.65025	-1079.36416	1
20923	H	74.43342	95.58558	75.31850	-630.30345	539.52750	1740.28386	1
20924	C	74.96789	94.30062	76.92217	662.17353	1008.22837	-418.40679	1
20925	H	74.58883	93.26366	77.11455	-2347.95216	-468.69727	277.67814	1
20926	C	76.53281	94.56801	76.91057	-291.73144	353.28036	-613.29899	1
20927	H	76.90146	95.45639	77.51200	-952.42737	-2557.16574	-1548.49349	1
20928	H	76.81330	94.69041	75.85007	-2555.88326	-2136.69031	-800.99234	1
20929	C	77.49353	93.39696	77.46362	547.10788	-654.59877	-600.73836	1
20930	O	77.77710	93.30813	78.65393	306.79911	82.35083	-542.45473	1
20931	N	77.88803	92.66686	76.45025	-126.62823	664.95240	783.27227	1
20932	H	77.80904	92.75975	75.44010	-72.90627	424.53153	-1880.39779	1
20933	H	78.67896	92.00101	76.61085	-1348.93323	-1661.31683	249.58963	1
20934	C	74.38297	95.40328	77.96848	-15.87034	965.88360	-469.86396	1
20935	O	74.97702	96.44580	78.33365	-496.19679	-112.53719	278.62222	1
20936	N	73.33418	94.81961	78.38337	1156.62031	-107.42459	-84.50496	1
20937	H	73.06962	93.86899	78.00439	-341.59947	732.05063	-1215.67662	1
20938	C	72.74657	95.33266	79.60211	-1110.73402	664.30733	-458.59644	1
20939	H	73.66445	95.50746	80.19648	-1076.64471	-633.46131	465.10900	1
20940	C	72.04072	96.71021	79.49473	122.10098	-350.11233	-805.60235	1
20941	H	71.63300	96.92083	78.46846	-27.53485	1508.05839	1628.50867	1
20942	O	73.07797	98.15418	79.17332	-33.62956	88.05845	-563.27726	1
20943	H	72.73629	98.22453	78.16617	1335.33274	2913.55828	-1453.03050	1
20944	C	70.99734	96.58970	80.61355	83.50705	347.14984	291.95878	1
20945	H	70.42671	95.60910	80.54868	-2278.96505	-221.97256	-775.44808	1
20946	H	70.24582	97.38376	80.35804	-387.76511	472.80796	4321.46073	1
20947	H	71.45010	96.65656	81.61830	-1693.48307	-1710.69015	884.30332	1

20948	C	71.85878	94.06592	80.17567	-577.34202	-272.59026	1.07324	1
20949	O	71.81296	93.76415	81.37931	-849.63438	-653.40741	-810.57022	1
20950	N	71.17912	93.51856	79.20207	-155.14765	743.12661	-44.99191	1
20951	H	71.36099	93.94130	78.26468	2040.53517	12.67997	43.14337	1
20952	C	70.61621	92.23029	79.45340	-243.91669	164.34283	66.17692	1
20953	H	70.12366	92.37277	80.33839	-1095.60755	-73.66456	4220.55435	1
20954	C	69.57135	92.07858	78.22632	-1087.78798	-73.29801	87.31568	1
20955	H	68.97388	93.06338	78.28411	-3203.78959	-104.40805	-3207.35755	1
20956	C	69.90446	91.78733	76.72249	-47.84361	-41.22951	-356.76750	1
20957	H	70.16418	90.71748	76.64043	-1978.87174	-609.27018	-727.93079	1
20958	H	69.07646	91.97524	75.96228	2828.68013	-682.41980	2583.78426	1
20959	H	70.80794	92.44820	76.45687	2930.63218	-2731.73597	1053.12369	1
20960	C	68.63165	90.91600	78.55164	107.71971	-553.69959	-89.13821	1
20961	H	67.96714	90.76973	77.61265	-27.87404	-3445.54674	-1418.03219	1
20962	H	69.22804	89.99763	78.87079	1763.91690	704.37935	2758.62421	1
20963	H	67.97369	91.25545	79.37490	-75.62065	-2214.46251	267.15019	1
20964	C	71.71886	91.07079	79.30639	-133.11075	815.59069	323.86979	1
20965	O	71.84698	90.13138	80.09648	643.89968	221.31710	-1288.75341	1
20966	N	72.50854	91.27178	78.23346	31.67551	-225.01975	1117.89676	1
20967	H	72.47272	92.05100	77.60317	-654.34958	-240.98889	-921.08071	1
20968	C	73.46106	90.25650	77.95692	-531.23335	216.77553	-632.67964	1
20969	H	73.00856	89.30756	78.30297	2990.79047	-4267.27720	1269.90703	1
20970	C	74.01336	90.12952	76.49161	379.57868	369.57887	-245.97469	1
20971	H	74.72965	91.02738	76.34760	924.36804	-1354.64929	401.08506	1
20972	H	73.21244	90.22441	75.63468	141.51580	458.68272	-4154.64668	1
20973	N	74.39903	87.63091	76.10633	-373.58581	435.46764	847.04146	1
20974	C	74.87978	88.85053	76.42930	623.93018	-912.77630	351.78253	1
20975	C	75.43034	86.78637	76.11837	76.39647	800.31794	-618.72997	1
20976	H	75.37308	85.71473	75.84005	-485.57304	142.86598	927.75641	1
20977	N	76.54119	87.44880	76.52436	-680.40149	228.90438	-54.81577	1
20978	H	77.45175	86.98225	76.69675	4939.24534	639.20546	-3428.73062	1
20979	C	76.27872	88.73298	76.69604	26.52294	-24.06631	-1151.87002	1
20980	H	77.02163	89.51533	76.94540	925.20237	-4671.88109	-1783.14025	1
20981	C	74.72928	90.74907	78.92716	543.46042	301.67259	636.44519	1
20982	O	75.81476	90.29052	78.54173	-1184.47426	122.64286	942.62739	1
20983	N	74.50446	91.53418	79.95507	-165.46903	50.21125	346.89346	1
20984	H	73.51932	91.84208	80.14868	-1277.16519	1896.35377	3334.02098	1
20985	C	75.50894	91.51649	80.97199	-45.84794	-275.02525	37.66263	1
20986	H	76.30443	91.38228	80.31568	-221.88779	-372.04614	1785.83186	1
20987	C	75.42461	92.84293	81.76614	361.43645	-211.23778	-102.97562	1
20988	H	76.26785	92.99211	82.46376	1143.69400	1238.13308	2896.93700	1
20989	H	74.52784	92.74592	82.35803	461.62018	3255.99608	173.78684	1
20990	C	75.30954	94.09816	80.77737	274.55983	262.25884	-205.01155	1
20991	H	76.03266	94.07755	79.93510	3406.57046	-280.18432	1061.05839	1
20992	H	74.28186	93.81076	80.39312	-704.80203	139.45457	86.22779	1
20993	C	75.28094	95.44968	81.56430	220.68389	-264.14760	442.88264	1
20994	H	74.68838	96.28605	81.14735	227.89688	3406.31296	-981.91631	1
20995	H	76.28914	95.78006	81.61086	1066.50641	907.44019	1230.39212	1
20996	C	74.79559	95.28744	83.06171	-90.26826	166.58309	-188.09466	1
20997	H	74.67669	94.25939	83.39913	-1566.12204	2469.90746	-1862.19147	1
20998	H	75.32827	95.89935	83.74771	1833.22932	-628.10653	-773.61967	1
20999	N	73.48899	95.87016	83.04839	581.44656	163.51800	-426.32214	1
21000	H	73.94640	97.51231	78.93811	-541.15096	-89.51436	1182.53559	1
21001	H	73.24897	96.12296	84.02731	813.63467	-1339.72049	1898.77290	1
21002	H	72.74416	95.22909	82.77701	1047.80634	-2122.74599	-1584.71320	1
21003	C	75.27847	90.22621	82.05440	196.73300	-483.71377	-228.63497	1
21004	O	76.18672	89.76223	82.72320	-241.83256	38.03908	264.04580	1
21005	N	73.98943	90.03151	82.14809	-254.21192	-12.45017	181.91901	1
21006	H	73.36594	90.63343	81.57196	1724.27286	3104.91187	2056.75229	1
21007	C	73.46663	88.99047	82.99382	-869.19043	61.84031	15.17177	1
21008	H	74.20900	88.85362	83.81028	750.07545	-1328.24847	816.14853	1
21009	C	71.98322	89.37329	83.43788	-789.71079	-379.51147	-704.42209	1

21010	H	71.60803	88.52931	83.99321	-2894.88079	3326.15250	593.16174	1
21011	H	71.54036	89.52709	82.40180	-1209.72934	960.76041	-1170.10180	1
21012	C	71.98872	90.63532	84.23523	276.87649	-321.93364	-70.81336	1
21013	C	72.10799	92.00057	83.84989	204.85753	27.51959	361.80196	1
21014	H	72.10834	92.48973	82.85873	-713.80693	-56.67575	810.48187	1
21015	N	72.31582	92.76453	84.93390	216.92581	366.65748	146.82913	1
21016	H	72.39484	93.75326	84.66678	290.33564	814.74102	-1551.26547	1
21017	C	72.21545	92.07983	86.09753	-509.08682	544.45690	376.33434	1
21018	C	72.05052	90.65271	85.69483	-788.34141	522.92093	166.77033	1
21019	C	72.05331	89.56492	86.60223	-466.14481	-461.11891	-1324.78157	1
21020	H	71.99437	88.54762	86.29637	-928.62651	-726.32368	-811.68039	1
21021	C	72.06494	89.93332	87.97141	832.55921	-182.30384	517.33201	1
21022	H	72.06015	89.14013	88.74779	180.79365	4168.00811	1254.44059	1
21023	C	72.10720	92.38798	87.51345	-727.43855	139.37462	204.29897	1
21024	H	72.20086	93.42067	87.92669	-2926.86439	1996.32646	784.89343	1
21025	C	72.07118	91.29911	88.38888	-495.75627	-78.14670	851.71249	1
21026	H	71.80577	91.56206	89.48241	-3574.67360	1862.45922	1008.54916	1
21027	C	73.35168	87.60732	82.14512	-511.26822	614.42856	-82.98431	1
21028	O	73.40475	86.57227	82.79031	-328.84017	425.75013	-221.48060	1
21029	N	73.08143	87.79329	80.84585	-150.24939	207.27220	-334.33207	1
21030	H	72.83200	88.67415	80.36472	3747.60557	1689.31913	1390.74497	1
21031	C	73.17505	86.57041	80.03522	1128.29445	344.45568	70.05767	1
21032	H	72.66005	85.93973	80.80709	-1300.01485	-2747.88664	499.34180	1
21033	C	72.37699	86.70262	78.62212	-231.70704	423.30558	221.20283	1
21034	H	73.04062	87.37753	78.01960	-2039.79810	1738.12719	-1081.85723	1
21035	C	72.30440	85.26702	77.94194	139.29899	32.35277	-1232.32526	1
21036	H	73.25929	84.82877	77.79149	120.52842	-1427.87290	-1511.43729	1
21037	H	71.85123	85.33014	76.96682	-2947.99130	289.99593	1945.68791	1
21038	H	71.66062	84.46109	78.38967	1351.38043	2649.88516	-2855.63270	1
21039	C	70.92031	87.22516	78.58597	-490.88423	36.69254	220.45777	1
21040	H	70.75853	87.85113	79.45805	-1766.52533	-119.72623	-278.83406	1
21041	H	70.13507	86.48889	78.77704	2383.26872	-1963.34743	1497.92010	1
21042	C	70.71682	88.03495	77.21626	-948.17734	937.01205	-25.60592	1
21043	H	69.63056	88.06163	76.85470	-5201.73510	-48.73285	4036.76454	1
21044	H	71.05922	89.07954	77.34113	1.08524	3631.40110	-833.56271	1
21045	H	71.14522	87.54058	76.33491	639.32391	816.21591	556.61291	1
21046	C	74.71413	86.16601	79.75454	-194.78666	530.33323	-137.26991	1
21047	O	74.99637	85.06806	79.29356	1011.85391	788.47046	-104.73474	1
21048	N	75.51107	87.20761	80.07493	-726.01439	122.61300	-582.44128	1
21049	H	75.04656	87.92726	80.64487	3069.90331	-2512.57583	-612.69633	1
21050	C	76.94680	86.92125	80.18743	-547.20008	505.59034	350.15823	1
21051	H	77.17068	86.28806	79.33398	-2065.37305	-2043.17087	-1372.08090	1
21052	C	77.56975	88.34777	80.21071	369.52018	1489.11131	10.45996	1
21053	H	77.26475	88.89667	79.31849	2337.49694	1028.77974	4393.52903	1
21054	H	77.11089	89.00780	81.01366	-5005.32114	-1958.41610	1190.19331	1
21055	O	79.04326	88.41906	80.58191	51.70522	-153.17170	245.76829	1
21056	H	79.05557	89.37198	80.79648	-2221.61517	-1886.77099	658.03099	1
21057	C	77.10086	85.93554	81.50079	-147.26520	944.61170	-165.60912	1
21058	O	77.95475	85.08718	81.43609	588.32765	-431.93685	8.43790	1
21059	N	76.34192	86.39729	82.49614	-340.46190	220.16735	297.02352	1
21060	H	75.68522	87.14728	82.32044	1871.75094	-1453.82035	-1173.30244	1
21061	C	76.34418	85.73404	83.73886	-49.08733	92.82177	106.55625	1
21062	H	77.35238	85.30372	83.97214	-1040.18574	-1042.40504	-642.48087	1
21063	C	75.75111	86.60966	84.94099	-248.97787	-283.55425	225.61674	1
21064	H	74.68802	86.72033	84.70134	-2277.97206	-469.36109	2970.88624	1
21065	C	75.97114	85.77930	86.23017	541.74875	-488.60013	439.88704	1
21066	H	75.52830	86.31245	87.10952	358.64977	-1092.84756	-2165.55339	1
21067	H	75.51400	84.69780	86.20590	-1210.19279	-2378.29733	1672.75445	1
21068	H	77.02782	85.71424	86.48012	-1534.59198	-2805.12695	217.72916	1
21069	C	76.53327	87.93833	85.10026	23.12725	-1318.99118	729.78664	1
21070	H	77.65427	87.76720	85.25836	695.29236	-382.45932	-2029.39194	1
21071	H	76.38759	88.54890	84.11362	-1287.67876	1259.73194	1551.00309	1

21072	C	75.91801	88.84977	86.21253	694.71201	912.22706	-824.56526	1
21073	H	75.74092	88.37288	87.19396	2132.90899	237.03261	2187.18366	1
21074	H	74.79961	89.13278	86.06859	3005.27318	-2404.57721	-2398.36931	1
21075	H	76.51669	89.81144	86.32956	2996.35468	-127.78489	1781.11738	1
21076	C	75.78700	84.21280	83.67290	780.31815	-42.05103	-460.38069	1
21077	O	76.22800	83.19180	84.17690	-765.27036	-48.04301	208.39534	1
21078	N	74.61500	84.11980	83.04490	563.20368	-188.35068	-594.00104	1
21079	H	74.13500	84.95480	82.78790	-344.74458	2869.01526	-1243.85815	1
21080	C	73.91400	82.81280	82.88690	-719.42455	390.17044	411.74553	1
21081	H	74.00400	82.22380	83.78790	622.53462	2152.83758	-2205.75129	1
21082	C	72.40500	82.98880	82.63790	723.38832	-305.89760	-453.87018	1
21083	H	71.80800	82.06780	82.46190	-1944.91760	-1720.08361	1783.86333	1
21084	O	72.05500	83.93480	81.60190	-717.74869	-76.49643	334.57649	1
21085	H	72.41500	84.72780	82.00590	2023.09370	-1577.95939	-1812.74049	1
21086	C	71.88900	83.50080	83.95390	605.19602	-360.84239	575.43011	1
21087	H	72.21200	84.53380	84.20790	2191.98616	-1939.79265	-1143.63599	1
21088	H	72.03100	82.81280	84.81390	1804.13016	83.53454	-2571.57819	1
21089	H	70.78500	83.62080	83.92590	-1627.98852	-2139.21008	-1639.27001	1
21090	C	74.57400	81.90580	81.81590	615.11118	-665.98768	50.39140	1
21091	O	74.51000	80.70880	81.83790	-646.40062	129.20151	442.37445	1
21092	N	75.20800	82.54480	80.80190	473.22167	678.21242	155.44275	1
21093	H	75.17800	83.52780	80.63590	-843.16064	-1004.02016	2862.01060	1
21094	C	76.14000	81.91880	79.89590	157.54242	868.30725	229.26375	1
21095	H	75.54400	81.19980	79.35290	2575.64173	1357.49996	-1180.98157	1
21096	C	76.52300	82.92480	78.72290	274.80268	730.76521	-469.81833	1
21097	H	75.62500	83.11680	78.09690	2064.45991	-1558.99425	-1780.98404	1
21098	H	76.66500	83.94280	79.14390	2168.63932	-2264.39534	-181.36611	1
21099	C	77.84600	82.66780	77.99590	-617.88482	139.01027	662.10949	1
21100	H	77.88700	81.63180	77.59590	-1871.15522	2012.70360	-1543.45540	1
21101	H	78.72200	82.60580	78.67690	3002.02647	-856.50807	331.90877	1
21102	C	78.18500	83.71880	76.95690	-107.09657	-886.05157	178.43420	1
21103	O	77.71100	83.55580	75.80090	688.66903	4.89886	373.05333	1
21104	O	78.82900	84.76080	77.27790	519.75083	296.00622	509.88549	1
21105	C	77.35300	81.31380	80.52590	117.92664	726.35021	537.73369	1
21106	O	77.70100	80.15980	80.26390	-53.26553	738.27135	-280.80070	1
21107	N	77.95800	82.09480	81.38790	495.48075	644.69541	-217.44805	1
21108	H	77.75900	83.05180	81.58290	-1885.02414	-2215.29954	-1206.82803	1
21109	C	79.11300	81.64780	82.15290	-457.98023	500.28608	-615.16454	1
21110	H	79.84000	81.34180	81.41590	780.66261	-2555.38934	-1658.29313	1
21111	C	79.73600	82.80780	82.92590	549.17241	-702.71038	171.11183	1
21112	H	79.00500	83.27380	83.62090	1999.56534	-30.14525	2423.97242	1
21113	H	80.07200	83.58180	82.20390	1767.14693	-1970.10006	1693.77958	1
21114	H	80.64900	82.46280	83.45690	-2.29933	2332.10223	-2113.46025	1
21115	C	78.82700	80.48580	83.13890	-369.72256	-599.40209	-583.64553	1
21116	O	79.55900	79.51980	83.22390	151.02221	287.45757	716.81727	1
21117	N	77.64800	80.51980	83.78290	444.56591	348.57190	622.58497	1
21118	H	77.05800	81.29980	83.58990	1779.18934	2071.99204	-1556.86411	1
21119	C	77.12500	79.38880	84.44290	-299.54306	-726.86723	464.00053	1
21120	H	77.86300	79.04080	85.15090	-2731.74188	-1206.94478	-1003.67782	1
21121	C	75.91800	79.80180	85.39390	-762.21498	-221.68741	-457.36341	1
21122	H	75.08100	80.21480	84.79090	1544.49869	-1156.93705	2481.76326	1
21123	H	75.49200	78.90680	85.89490	1941.08079	1924.31596	-1552.78144	1
21124	C	76.28200	80.82580	86.48490	-433.68999	80.49815	799.35650	1
21125	H	76.98000	81.55880	86.02790	3038.75223	526.66718	-600.28091	1
21126	C	74.98200	81.56780	86.85190	-743.94729	-314.23761	-431.80640	1
21127	H	75.18900	82.57080	87.28190	-2664.27821	-1224.78041	-1151.31104	1
21128	H	74.37200	80.96780	87.56090	443.52838	-2206.43547	2199.49783	1
21129	H	74.21300	81.76580	86.07590	-2698.85106	-1172.60111	-1125.07857	1
21130	C	77.11200	80.14080	87.64290	466.13626	-363.27208	-694.04991	1
21131	H	78.19900	80.15580	87.41590	-736.13953	-2435.33703	-1855.73748	1
21132	H	76.72400	79.10680	87.76490	761.84484	-723.60456	-2966.56632	1
21133	H	77.02300	80.76480	88.55790	-1927.48794	-2481.23504	223.08475	1

21134	C	76.81200	78.16480	83.60190	-26.82592	583.22529	698.49627	1
21135	O	76.88800	77.02780	84.09590	681.22562	-368.80145	-136.66817	1
21136	N	76.40900	78.34580	82.33290	114.66656	-327.71632	-770.39121	1
21137	H	76.25200	79.28280	82.02990	-483.74399	1308.05306	-2822.50135	1
21138	C	76.00000	77.24280	81.44990	221.43886	-710.22362	522.39625	1
21139	H	75.30300	76.60780	81.97590	-1977.38274	1232.28114	2116.61964	1
21140	C	75.34000	77.71080	80.16190	-751.87236	357.12298	-385.50321	1
21141	H	74.36600	78.17280	80.43090	-565.96182	2524.84230	-1793.63221	1
21142	H	76.02600	78.35680	79.57290	2899.03508	-1129.43192	425.94841	1
21143	H	75.07000	76.89780	79.45490	-1757.36868	-2496.71814	765.97636	1
21144	C	77.21500	76.45580	81.18090	249.35453	646.81953	588.44193	1
21145	O	77.05800	75.22780	81.01690	80.95629	473.47460	623.69477	1
21146	N	78.42600	76.99280	81.18490	353.50510	-72.86015	757.92946	1
21147	H	78.51000	77.98480	81.24190	2126.23700	-950.17224	2107.29385	1
21148	C	79.72500	76.37280	80.94990	785.96613	-212.30841	396.94714	1
21149	H	79.67100	75.84580	80.00890	-2584.28796	-1693.07951	-615.66348	1
21150	C	80.84500	77.40480	80.87490	-632.04512	614.08060	-254.32493	1
21151	H	81.81300	76.89780	80.67290	1825.76699	-2196.20209	-1313.64380	1
21152	H	80.83100	77.90280	81.86790	-795.73915	1508.53313	2642.69033	1
21153	C	80.72800	78.48680	79.85590	474.14589	136.81949	-766.44319	1
21154	C	79.79900	78.45180	78.78390	-189.58507	-154.53623	-881.91141	1
21155	H	79.19800	77.57480	78.59390	1920.23573	2017.96696	1454.83543	1
21156	C	79.71500	79.51180	77.92990	-495.83879	-673.05800	366.00043	1
21157	H	78.93100	79.51880	77.18690	-2296.60452	317.46210	2132.05000	1
21158	C	80.60300	80.61280	78.00890	-887.28632	133.26319	193.55837	1
21159	H	80.63700	81.41480	77.28690	-1407.85576	-531.31333	-2767.49837	1
21160	C	81.56500	79.61080	80.03390	-35.74170	721.58742	556.30169	1
21161	H	82.29100	79.66680	80.83190	-3120.79393	374.95255	228.33405	1
21162	C	81.49000	80.62980	79.09190	-437.80542	-323.57572	-736.36429	1
21163	H	82.21500	81.42980	79.14390	983.73118	1267.48202	-2707.20231	1
21164	C	80.06500	75.30780	81.89290	27.30115	-618.60110	-672.21477	1
21165	O	80.91900	74.45080	81.59690	669.55248	394.83134	114.57914	1
21166	N	79.44000	75.24380	83.07190	600.03055	-486.27441	-336.42566	1
21167	H	78.65900	75.82680	83.28190	101.08731	2691.73377	1622.30433	1
21168	C	79.63100	74.13880	83.98890	-70.88053	63.60258	902.95116	1
21169	H	80.68900	74.07380	84.19190	2813.27829	-1089.67613	875.60325	1
21170	C	78.87000	74.41180	85.37190	-414.99990	-611.29493	-541.67634	1
21171	H	78.83600	73.47280	85.96590	-1802.79406	-1149.07688	-2315.39983	1
21172	H	77.82200	74.75780	85.24390	735.28626	2930.02592	870.10279	1
21173	C	79.70500	75.33080	86.30090	12.88302	410.03656	810.08980	1
21174	C	79.44800	76.73280	86.29990	325.07925	-574.76938	-630.91415	1
21175	H	78.60500	77.12880	85.75290	2069.89167	1838.29736	1485.77699	1
21176	C	80.18400	77.60480	87.17890	-242.64569	832.26937	-285.37039	1
21177	H	79.91800	78.64980	87.23690	-72.92502	880.94857	-3021.71432	1
21178	C	81.22300	77.03480	87.99790	-590.06330	16.44092	-701.17183	1
21179	H	81.76900	77.73080	88.61790	19.09342	-2099.49312	2340.94424	1
21180	C	80.73400	74.83380	87.05290	-302.81803	444.90462	-740.99522	1
21181	H	80.89600	73.77180	87.15890	-2130.08363	-1155.89099	-2014.64186	1
21182	C	81.50200	75.61880	87.92690	-216.42402	884.75216	26.57408	1
21183	H	82.33500	75.21480	88.48390	-444.31235	1999.57651	-2391.91189	1
21184	C	79.16300	72.79280	83.47990	-516.03174	551.59781	-519.39448	1
21185	O	79.55200	71.72080	84.04290	543.43098	-435.00758	-372.79849	1
21186	N	78.30700	72.68380	82.44790	-842.74127	81.23730	48.92391	1
21187	H	77.94400	73.50180	82.00890	1034.72283	-614.70237	2901.18759	1
21188	C	78.01100	71.39980	81.79690	-313.67359	392.23880	-767.87771	1
21189	H	77.51000	70.87580	82.59890	1351.13833	1384.29953	-2484.13175	1
21190	C	77.14300	71.47680	80.57290	-600.58337	-476.18448	493.83867	1
21191	H	76.78100	70.46380	80.29490	-989.85260	-235.68810	-2983.26254	1
21192	H	76.21100	71.97380	80.91690	-391.91194	-1088.12666	2922.06180	1
21193	N	77.72300	73.44280	79.04490	336.80945	-769.90044	-25.40563	1
21194	H	77.43600	74.19280	79.63990	-1943.86398	-1987.71228	-1480.99796	1
21195	C	77.73900	72.10080	79.28290	339.14265	658.71439	525.86555	1

21196	C	78.21500	73.63280	77.79190	-506.62262	-648.66746	-399.85372	1
21197	H	78.09200	74.62580	77.35890	2922.70215	-606.54080	971.99507	1
21198	N	78.44100	72.46680	77.21390	484.93487	-381.97566	-574.05936	1
21199	C	78.16100	71.51680	78.14890	-693.65672	-586.15218	101.86778	1
21200	H	78.36500	70.47680	77.92590	1211.23453	1925.83611	-2177.43227	1
21201	C	79.20000	70.61280	81.39290	730.93323	476.73181	249.08226	1
21202	O	79.29400	69.44680	81.75690	-87.31612	42.16951	-790.08111	1
21203	N	80.23700	71.24080	80.70990	568.52704	431.88150	-451.64135	1
21204	H	80.12400	72.15080	80.31990	-1149.65240	-2405.00055	-1677.19991	1
21205	C	81.53600	70.68980	80.37790	258.21674	-780.87818	-393.50393	1
21206	H	81.30400	69.88380	79.69790	314.79765	-2655.03250	-1660.70039	1
21207	C	82.43700	71.71380	79.66390	590.88523	255.48703	-648.09388	1
21208	H	82.58700	72.59480	80.32390	632.99086	938.19797	2929.51452	1
21209	H	83.49300	71.39880	79.52090	1354.74289	-2170.45508	-1830.98012	1
21210	S	81.70000	72.38080	78.16590	94.19767	-446.02503	311.04487	1
21211	H	80.97600	71.33580	77.79290	1219.71884	-1563.72376	2432.53615	1
21212	C	82.28600	70.13480	81.59390	-540.84005	550.98076	484.57662	1
21213	O	82.97200	69.12480	81.49390	-436.28164	392.33045	525.78051	1
21214	N	82.03700	70.65580	82.81090	6.28899	-151.64923	824.09626	1
21215	H	81.50900	71.49380	82.92690	-1336.11792	1919.09811	2102.10231	1
21216	C	82.76200	70.16280	84.01490	-512.17584	510.78451	-565.19630	1
21217	H	83.68700	69.72280	83.67190	2439.51831	1691.80363	-1041.58248	1
21218	C	82.99500	71.37380	84.95390	744.21846	-516.55823	69.92031	1
21219	H	83.61300	70.98680	85.79290	-2664.13642	1489.10131	767.28321	1
21220	H	82.07200	71.89880	85.27890	-563.61484	-2073.30590	-2304.88871	1
21221	S	83.97900	72.63280	84.11290	-397.01144	170.82368	351.11502	1
21222	H	85.18200	72.12980	84.34390	-938.37215	707.11658	-2926.23502	1
21223	C	81.93800	69.10780	84.71990	-666.21271	500.18023	369.45573	1
21224	O	82.51800	68.29280	85.42290	-492.56503	-377.88381	-498.13078	1
21225	N	80.65300	69.10580	84.45990	617.44633	-132.70146	550.37538	1
21226	H	80.19800	69.73580	83.83490	-2558.68239	-1828.00004	-168.48568	1
21227	C	79.68700	68.14480	85.04490	-414.70060	252.94468	-779.56284	1
21228	H	80.05800	67.92580	86.03490	-1439.03520	-2776.68828	-365.24589	1
21229	C	78.28300	68.75380	85.06290	-348.58929	763.02345	353.13191	1
21230	H	77.45500	68.03180	85.23190	2179.34118	2180.30691	610.28256	1
21231	H	78.09100	69.16680	84.04990	1965.51469	-958.23108	-2264.97901	1
21232	C	78.00400	69.82480	86.20890	18.93232	197.72398	884.25036	1
21233	H	78.90500	70.47180	86.14290	-1127.50894	652.24411	-2870.13829	1
21234	C	76.81100	70.73680	85.85990	-445.46179	602.41885	516.27520	1
21235	H	76.67900	71.41480	86.72990	-1427.37923	2301.11806	-1606.68973	1
21236	H	77.14500	71.31780	84.97290	-1678.51077	734.77856	-2564.06769	1
21237	H	75.93600	70.06580	85.72890	2454.70188	1187.43975	1559.14909	1
21238	C	77.83700	69.07980	87.51390	256.78752	559.00886	665.26225	1
21239	H	76.86500	68.54180	87.53190	2628.44439	883.92489	1475.49212	1
21240	H	77.89600	69.81380	88.34590	1039.96745	-1663.74612	-2465.11651	1
21241	H	78.56200	68.26680	87.73190	97.91267	2292.23283	2144.86671	1
21242	C	79.65200	66.80780	84.29190	-499.89939	-497.87065	573.19609	1
21243	O	79.37600	65.74280	84.89590	480.47712	-540.34317	-321.51431	1
21244	N	79.98800	66.80280	82.99990	627.33225	-66.11519	550.29628	1
21245	H	80.13000	67.65680	82.50490	1399.56376	-2146.65873	-1828.56647	1
21246	C	80.27200	65.57980	82.21990	345.04682	-447.31261	-721.31110	1
21247	H	79.38000	64.97580	82.30090	1650.38530	1519.17424	-2211.71191	1
21248	C	80.25600	65.98080	80.69390	-334.08369	572.27963	622.10040	1
21249	H	80.91000	66.86380	80.53090	2645.86741	-535.00409	1601.81543	1
21250	H	79.24200	66.28180	80.35290	24.17996	-799.50259	-3049.45710	1
21251	C	80.67100	64.84780	79.76590	91.34875	864.86093	270.29622	1
21252	O	80.29900	63.70080	79.96890	491.28809	510.54753	337.64568	1
21253	N	81.33000	65.20580	78.66090	434.66559	-587.78336	-422.71164	1
21254	H	81.30100	66.17680	78.42390	-92.79501	2773.24980	-1495.12667	1
21255	H	81.92300	64.53680	78.21290	-1624.95742	-662.28272	2604.85185	1
21256	C	81.38000	64.62380	82.85090	824.62520	-11.99987	374.33151	1
21257	O	81.10700	63.45380	83.05790	-131.30189	779.54121	-26.00616	1

21258	N	82.53700	65.11480	83.31390	-339.31920	-721.36209	271.21287	1
21259	C	83.22100	66.26080	82.69590	541.99876	-110.44546	714.18945	1
21260	H	82.94100	67.16080	83.28390	1545.85470	-2007.91833	1853.47843	1
21261	H	82.92800	66.49280	81.64990	905.93180	-1202.84435	-2768.61406	1
21262	C	83.43800	64.25680	84.07790	-240.66065	-339.22390	-820.98939	1
21263	H	83.55400	63.29780	83.59490	2124.14329	-1229.66546	1955.69865	1
21264	C	84.69700	65.12580	84.13990	-796.93056	-125.24448	420.87301	1
21265	H	85.61200	64.50480	84.24490	2279.45514	694.58323	2042.14911	1
21266	H	84.61000	65.77680	85.03590	-1601.06150	-1253.62059	2393.51044	1
21267	C	84.69800	65.91280	82.85790	-749.02680	-523.18608	-22.76480	1
21268	H	85.34200	66.81680	82.82290	1912.45638	-1909.98823	-1613.38983	1
21269	H	85.02000	65.31480	81.97890	2193.15415	-1269.24227	1850.88229	1
21270	C	82.95000	63.89680	85.48290	697.69511	-16.75617	-593.25326	1
21271	O	83.29800	62.85680	86.07890	428.57217	-589.35192	-311.73354	1
21272	N	82.18500	64.85480	86.18890	645.82068	-462.76646	272.96605	1
21273	H	82.04200	65.79680	85.89690	-1849.64782	-2155.75735	-1364.44491	1
21274	C	81.67900	64.58180	87.53990	885.92957	203.76482	31.83323	1
21275	H	82.46700	64.31080	88.22590	1309.38994	1452.35775	-2471.81257	1
21276	C	80.99100	65.83580	88.13590	-476.64914	755.68161	-188.64709	1
21277	H	80.39700	66.35780	87.35590	2519.49885	1875.91449	122.99791	1
21278	C	80.07500	65.51980	89.33090	-485.51541	740.08288	207.84173	1
21279	H	79.23600	64.80180	89.20790	-1421.71086	-681.01690	2716.24615	1
21280	H	79.60200	66.50280	89.53890	-349.83941	1608.09408	-2687.41356	1
21281	H	80.59200	65.06380	90.20190	-2653.86935	1244.66657	1134.91797	1
21282	C	82.10400	66.82480	88.54790	341.08039	750.76400	377.33682	1
21283	H	82.94700	66.77280	87.82690	1058.26083	252.17697	2943.41535	1
21284	H	82.54800	66.39380	89.46990	209.75222	-1466.86417	2768.20379	1
21285	C	81.75600	68.27980	88.67090	766.68587	473.15800	-131.44538	1
21286	H	81.18400	68.37880	89.61690	-1084.69897	-2625.11562	1351.13845	1
21287	H	82.69900	68.86180	88.75190	-1629.90670	-1947.70046	1853.02194	1
21288	H	81.16100	68.59880	87.78890	-1720.56889	-507.26516	2579.63256	1
21289	C	80.71800	63.40580	87.53890	683.54933	525.37521	282.69148	1
21290	O	80.75900	62.52280	88.33690	-298.59033	284.26585	-682.36881	1
21291	N	79.82600	63.35580	86.53090	-566.62785	397.63625	-492.91382	1
21292	H	79.63700	64.12880	85.92890	1418.38124	-2166.98211	-1793.44966	1
21293	C	78.94800	62.20480	86.22690	1.72425	434.54089	-809.68156	1
21294	H	78.49300	61.75780	87.09790	1786.71034	-1480.63809	2115.61906	1
21295	C	77.77100	62.67180	85.34990	-249.35766	-653.93048	-594.24492	1
21296	H	78.14500	63.09380	84.39290	-1171.49152	2061.37804	2060.99536	1
21297	H	77.13300	61.79380	85.11490	2694.88822	114.66173	1607.88303	1
21298	C	76.80000	63.71180	86.07290	-91.33357	-903.89690	84.73427	1
21299	H	77.33300	64.63980	86.37290	239.21745	257.58420	-3133.38059	1
21300	C	75.74100	64.25280	85.11390	506.58859	-687.78010	-324.21865	1
21301	H	76.09600	64.59780	84.11990	1287.60724	-2287.00147	-1740.47961	1
21302	H	74.99800	63.47780	84.82990	-1472.58561	176.09258	-2782.81107	1
21303	H	75.09800	65.00780	85.61490	2431.81597	-1732.59108	981.31642	1
21304	C	76.08600	63.16980	87.28090	-700.51006	-474.68831	-352.69832	1
21305	H	75.75700	62.14180	87.01690	-445.91568	-2546.92932	1787.32991	1
21306	H	76.70900	63.27280	88.19590	1110.91061	2058.54317	2093.75705	1
21307	H	75.17000	63.75080	87.51990	-1082.79162	-1746.74136	2377.32573	1
21308	C	79.71000	61.03980	85.48290	405.84824	566.87794	-595.13298	1
21309	O	79.10700	60.24680	84.78490	-161.99185	548.21819	535.70323	1
21310	N	81.05000	60.89580	85.67690	533.44919	-565.23425	-337.12746	1
21311	H	81.56300	61.63580	86.10390	1083.00552	-1558.87255	2499.16215	1
21312	C	81.67900	59.58380	85.48290	566.41868	-236.18358	662.89105	1
21313	H	80.94000	58.86180	85.16790	-1779.55896	935.28051	2410.77127	1
21314	C	82.84300	59.77880	84.44790	537.99138	-555.58610	470.10495	1
21315	H	83.72900	59.14880	84.67490	1891.56470	1319.59888	2127.45893	1
21316	H	83.19000	60.83380	84.42090	1058.83435	2830.06142	864.61293	1
21317	C	82.46800	59.21580	83.06090	636.62532	-67.41624	-657.69896	1
21318	C	82.09700	57.87180	82.98090	-616.46879	665.01433	-123.55983	1
21319	H	82.06500	57.29180	83.89090	-1041.04369	258.09811	-2969.56608	1

21320	C	81.76000	57.32380	81.74990	-202.38448	-398.99101	783.39511	1
21321	H	81.57400	56.26280	81.67190	1130.34981	2820.92157	-826.66260	1
21322	C	81.73300	58.12080	80.62590	792.16737	-444.58203	-34.48110	1
21323	O	81.35100	57.56780	79.39290	471.29654	615.46945	-160.40697	1
21324	H	80.98200	56.68280	79.44890	-2195.96720	-317.63284	-2244.19934	1
21325	C	82.57200	59.98580	81.93490	659.83917	-599.41313	-188.97373	1
21326	H	82.88300	61.01080	82.07090	2142.39099	-1741.45441	-1513.40529	1
21327	C	82.18800	59.43480	80.71690	-588.71559	-484.68450	-512.22335	1
21328	H	82.27300	60.00980	79.80690	-2935.15819	-991.50955	550.76615	1
21329	C	82.20300	59.06980	86.83590	540.15733	111.71175	714.48925	1
21330	O	82.67700	57.91880	86.94890	331.10550	30.83105	704.60580	1
21331	N	82.03300	59.88880	87.89690	-706.34432	-271.89267	-386.88693	1
21332	H	81.63800	60.79980	87.80690	-2287.23878	229.78604	2139.29466	1
21333	C	82.49000	59.51680	89.18790	-429.20347	-660.19071	-473.10306	1
21334	H	83.47100	59.07480	89.09290	-657.11568	-2946.19267	880.94793	1
21335	C	82.64400	60.75380	90.06890	594.23746	560.14118	-412.36388	1
21336	H	83.36700	60.50080	90.87390	1955.46588	-1228.50243	2127.20429	1
21337	H	81.69200	61.08180	90.53790	2704.79006	-865.49660	1344.79205	1
21338	H	83.13700	61.58380	89.51890	-2831.82718	-1373.82942	-30.85665	1
21339	C	81.62000	58.45680	89.91790	690.34928	501.76332	306.72671	1
21340	O	80.36400	58.52880	89.88090	473.03440	532.29965	-347.94812	1
21341	N	82.22900	57.62180	90.79390	-74.87698	-712.65972	438.65210	1
21342	H	83.21700	57.48780	90.80390	-2531.19794	1333.42174	1295.09487	1
21343	C	81.49200	56.95580	91.86190	-484.62087	580.97427	494.19771	1
21344	H	82.21900	56.51580	92.52890	416.64956	-2022.48046	-2387.80927	1
21345	C	80.59000	57.87080	92.75390	-490.73562	-662.08290	384.23252	1
21346	H	79.86600	58.38380	92.08590	1816.37410	1149.34821	2285.88985	1
21347	H	80.09300	57.24080	93.52290	2202.62792	-1704.50842	-1479.46018	1
21348	C	81.46100	58.86380	93.52190	-583.08386	603.40092	-360.55788	1
21349	C	82.52500	58.47380	94.32090	-96.83068	-762.18108	485.40403	1
21350	H	82.86400	57.44780	94.30990	2841.33140	-962.60301	943.09466	1
21351	C	83.30600	59.40880	95.01490	403.18420	461.44573	662.51970	1
21352	H	84.13400	59.10480	95.63690	2264.94488	-1691.66042	-1398.49004	1
21353	C	82.96400	60.78380	94.84590	563.44879	507.20968	493.64990	1
21354	H	83.47000	61.57380	95.38290	2291.46047	1100.77322	1842.29204	1
21355	C	81.16500	60.24680	93.35090	630.69665	592.55679	271.39685	1
21356	H	80.29800	60.48480	92.75290	-1223.81537	2157.31707	-1941.40482	1
21357	C	81.88600	61.18680	94.02290	-515.77355	731.46685	147.62958	1
21358	H	81.69100	62.24580	93.93990	-140.87734	-1689.51412	2643.20526	1
21359	C	80.76400	55.70980	91.43490	-500.17464	188.56098	-749.21014	1
21360	O	79.70800	55.31080	91.95290	-20.07980	606.17021	490.74313	1
21361	N	81.30300	54.90280	90.49790	-613.18897	137.01729	-574.84867	1
21362	H	82.18100	55.22180	90.14890	-1239.52519	2115.28659	1957.30459	1
21363	C	80.71900	53.68480	89.94390	612.36223	595.14129	-328.81222	1
21364	H	79.65100	53.83680	89.97990	2834.10760	-1176.69575	-710.99315	1
21365	C	81.27100	53.31280	88.53290	-560.34836	452.98662	-570.11317	1
21366	H	80.83700	52.33080	88.24890	1578.65255	-2693.59292	385.49362	1
21367	H	82.36400	53.11580	88.57390	1257.75788	-2242.97224	-1827.20116	1
21368	C	80.98500	54.38180	87.51690	-842.38085	348.28366	7.74413	1
21369	H	81.51500	55.32680	87.76390	2395.00217	-730.48098	-1916.62867	1
21370	C	81.53700	54.10480	86.08490	671.22173	-472.59731	384.01449	1
21371	H	81.59600	55.10380	85.60390	-966.79973	2725.76877	1226.50630	1
21372	H	82.55700	53.69280	86.23790	-2211.60947	-2225.26126	-257.81645	1
21373	H	81.03200	53.33780	85.45890	-1645.61523	-2509.74390	933.98114	1
21374	C	79.54200	54.65580	87.23390	-438.91318	551.49441	-589.28025	1
21375	H	79.04100	54.79480	88.21590	-1489.54258	-1962.09022	-1970.19780	1
21376	H	79.34300	55.38180	86.41690	-2621.10783	1268.91685	1180.27756	1
21377	H	79.14800	53.69780	86.83090	-876.22058	-2193.97233	2067.27869	1
21378	C	80.97300	52.63780	90.95190	-294.66308	223.74628	819.74815	1
21379	O	82.06500	52.10580	91.11790	-626.47854	130.80062	447.55994	1
21380	N	79.89800	52.16980	91.66690	700.99672	-393.49591	252.15640	1
21381	H	78.97800	52.45280	91.40590	-681.63258	2386.12313	-1942.29263	1

21382	C	80.08900	51.23780	92.72590	-237.47494	599.79763	627.86329	1
21383	H	79.15000	50.75680	92.95390	2215.78107	-2233.10999	-167.79085	1
21384	H	80.83200	50.52280	92.40490	-1665.28805	2601.75139	-592.67696	1
21385	C	80.71500	51.67880	93.95290	776.65550	-248.54192	-426.41797	1
21386	O	81.35700	50.96780	94.71090	243.12424	-651.31031	368.95954	1
21387	N	80.54900	52.96080	94.25390	211.98757	-726.81273	369.09334	1
21388	H	80.17900	53.60180	93.58590	2803.25639	227.75806	1399.95341	1
21389	C	81.11800	53.58680	95.39990	-685.69174	594.61897	4.05934	1
21390	H	82.06300	53.10980	95.61590	-2112.39479	-2276.13884	502.42633	1
21391	C	81.44900	55.05980	95.20090	16.05675	-477.49194	767.20087	1
21392	H	82.12800	55.25980	94.34390	-3142.33105	64.73887	92.46630	1
21393	H	80.47800	55.52680	94.93090	1236.55968	-2887.79133	226.48613	1
21394	H	81.73900	55.58780	96.13490	-2907.70078	-1189.64873	-179.67213	1
21395	C	80.21700	53.42580	96.59890	725.72974	-559.59322	-14.76808	1
21396	O	79.01700	53.23880	96.46890	633.46152	-312.66261	349.01780	1
21397	N	80.81200	53.47280	97.79790	-253.56058	538.26796	580.84249	1
21398	H	81.79700	53.59180	97.89590	-553.73820	1892.11503	2434.83529	1
21399	C	80.10400	53.53380	99.00590	-83.91579	658.51692	606.60021	1
21400	H	79.05200	53.39680	98.80390	-472.42510	2324.38280	-2071.82914	1
21401	C	80.72100	52.50880	100.05290	233.58968	-434.99622	-783.60778	1
21402	H	81.81400	52.47280	99.85790	1872.56749	-1434.83900	-2101.36641	1
21403	H	80.40300	52.62580	101.11090	2233.18072	-1205.53046	1855.24459	1
21404	C	80.28200	51.06780	99.72490	740.64847	379.18767	360.40302	1
21405	H	80.89900	50.69980	98.87790	-907.38103	-2108.23571	-2169.25623	1
21406	H	80.52600	50.40280	100.58090	1209.73044	-2451.22492	1556.65493	1
21407	C	78.78400	50.94080	99.35690	-217.71049	-415.53200	-796.90687	1
21408	H	78.65100	51.25080	98.29890	595.16338	637.83785	-3034.80129	1
21409	H	78.23800	51.66280	100.00090	-862.47632	1992.59939	2257.72148	1
21410	C	78.18400	49.58980	99.52590	659.39928	471.49349	-429.22298	1
21411	H	78.30600	49.19080	100.55490	2214.81220	2199.79166	-390.32189	1
21412	H	78.65300	48.87980	98.81090	2552.35577	-729.39431	1682.68986	1
21413	N	76.74200	49.65680	99.25790	419.64495	488.64067	530.02827	1
21414	H	76.66100	49.91580	98.25390	-1358.22428	737.50074	2724.66510	1
21415	H	76.41300	50.36980	99.93990	2247.84457	-1622.33881	1487.61010	1
21416	H	76.27200	48.73580	99.36890	-541.39753	465.54450	3049.52035	1
21417	C	80.22600	54.95980	99.62690	-375.40057	-102.13516	-835.74657	1
21418	O	81.26600	55.62880	99.55690	-512.39704	-305.30105	-529.87790	1
21419	N	79.06500	55.53180	100.15290	73.66002	-573.14662	-632.57827	1
21420	H	78.24600	54.96680	100.20890	2167.21604	2068.83019	941.74550	1
21421	C	78.96600	56.92180	100.51590	-586.63207	-559.92563	-431.97535	1
21422	H	79.79100	57.47180	100.08790	-1673.28905	-839.22354	-2539.50586	1
21423	C	77.72400	57.53680	99.83390	625.78443	193.50274	-644.88255	1
21424	H	76.80700	57.08980	100.27490	1414.55464	-2630.82724	-1018.83450	1
21425	H	77.67100	58.59880	100.15690	-2146.38526	707.25787	-2193.92999	1
21426	C	77.84300	57.42380	98.31090	-240.48154	-882.54119	50.38544	1
21427	C	78.61700	58.35580	97.58790	107.15079	-792.97961	437.15073	1
21428	H	79.29400	59.02580	98.09690	-523.54230	2286.42711	-2100.25588	1
21429	C	78.64100	58.25080	96.16690	852.53770	-143.13388	-306.48573	1
21430	H	79.20400	58.96380	95.58290	-2919.23626	1086.50141	413.47539	1
21431	C	77.93600	57.23580	95.50590	-628.64119	-498.04666	426.86338	1
21432	H	78.04600	57.12480	94.43790	1999.98856	246.97922	-2426.77750	1
21433	C	77.15700	56.45480	97.64590	579.92030	-624.38988	328.11635	1
21434	H	76.68800	55.65580	98.20190	-265.05029	-1298.00640	2845.58841	1
21435	C	77.20800	56.31680	96.28190	563.01934	441.87114	-573.10795	1
21436	H	76.74300	55.47580	95.78890	-1999.53975	2382.98360	427.23241	1
21437	C	78.97800	57.25380	102.00090	-765.50594	342.37163	334.02720	1
21438	O	79.06900	58.41480	102.47090	128.43460	441.95748	627.39383	1
21439	N	78.95100	56.16180	102.83090	543.64501	-564.88512	-342.38822	1
21440	H	78.58300	55.30280	102.48390	-2357.29774	1729.77235	-1154.72275	1
21441	C	78.88800	56.33080	104.26790	679.17118	-605.61759	-144.88744	1
21442	H	78.72600	57.37580	104.48790	2701.74597	368.13041	1563.79394	1
21443	C	77.73800	55.52780	104.91990	588.08092	-616.19941	-358.26986	1

21444	H	77.73700	55.67180	106.02190	-2147.71108	2278.52679	178.17059	1
21445	H	78.02200	54.47280	104.71790	858.28534	-2379.80617	-1893.68340	1
21446	C	76.39500	56.07880	104.37490	-383.79535	-464.25291	-698.00178	1
21447	H	76.33400	56.03080	103.26590	2425.37538	-1985.51195	-359.09172	1
21448	H	76.43600	57.17880	104.52490	2446.90820	832.89736	1785.24220	1
21449	C	75.12500	55.41780	105.00790	101.32343	-461.54444	-795.46715	1
21450	H	74.21200	55.89580	104.59090	-825.78325	-2244.34704	-2061.66732	1
21451	H	75.24900	55.59280	106.09790	-2541.87240	-795.10878	-1682.31856	1
21452	C	75.05000	53.89580	104.84890	-163.65939	-558.79052	-718.04817	1
21453	H	75.91600	53.36880	105.30390	2469.56089	-395.49511	-1927.35616	1
21454	H	74.88900	53.64780	103.77790	-1769.52098	2588.36478	93.79002	1
21455	N	73.87300	53.41980	105.56690	-546.67977	341.26623	-545.45288	1
21456	H	74.07600	53.58480	106.57290	2819.51493	-470.17905	-1338.42872	1
21457	H	73.01100	53.99980	105.60990	-236.68518	2570.82327	-1794.53762	1
21458	H	73.73800	52.42180	105.30890	1436.11924	1826.99246	2105.46168	1
21459	C	80.16700	55.94380	104.98190	-562.18634	-642.96543	316.52428	1
21460	O	80.39300	56.21780	106.18890	-470.53643	-359.15762	-535.59274	1
21461	N	81.09000	55.32780	104.18990	-619.69063	43.27505	554.96531	1
21462	H	80.83000	54.95680	103.30190	-1474.99399	1661.73147	2207.71545	1
21463	C	82.53200	55.16980	104.40690	226.13765	819.78284	300.81604	1
21464	H	82.59600	54.28380	105.02190	-3140.20118	-79.86815	57.79492	1
21465	C	83.29300	54.91580	103.09090	66.83758	737.53381	-535.45073	1
21466	H	82.81500	54.08480	102.53090	-1220.46249	-2210.60774	1869.37159	1
21467	O	84.67700	54.54080	103.24590	-721.25168	-116.57650	-305.93974	1
21468	H	84.78500	53.96080	104.00290	-300.20061	-2268.60807	-2178.96832	1
21469	C	83.23200	56.06680	102.10790	-553.19055	-380.70547	605.74554	1
21470	H	83.45200	55.63380	101.10790	-1789.32235	-2557.03716	409.14435	1
21471	H	83.82700	56.93980	102.45090	-1817.78697	-634.51282	2475.59782	1
21472	H	82.23100	56.54280	102.03790	1183.58087	2418.86174	-1631.03719	1
21473	C	83.20700	56.25880	105.24790	-481.45484	570.84800	-522.89598	1
21474	O	83.00500	57.44880	105.00190	551.04298	-574.82111	-60.89647	1
21475	N	83.99000	55.88980	106.24490	534.03243	232.42701	-624.23858	1
21476	H	84.16600	54.94980	106.52790	92.68837	-92.15621	3131.08234	1
21477	C	84.73700	56.88680	106.99290	825.62441	-392.31486	-109.99574	1
21478	H	84.96900	57.66880	106.28490	-2000.53873	1608.73753	-1819.11862	1
21479	C	83.91500	57.42980	108.20490	906.36631	113.15543	-72.95035	1
21480	H	84.21500	58.48080	108.40390	63.17842	-2977.20480	1029.07161	1
21481	H	82.85200	57.49980	107.89190	1202.89448	1388.87616	2539.98305	1
21482	O	83.89700	56.69080	109.40790	-26.14491	767.95928	125.34871	1
21483	H	83.44200	57.18580	110.09290	1297.80650	1801.40383	2212.90352	1
21484	C	86.04500	56.31880	107.48390	914.97952	-61.74150	-10.40376	1
21485	O	86.23700	55.11080	107.49890	229.61591	378.33656	-664.21723	1
21486	N	86.96200	57.19680	107.92490	597.14599	-123.50356	-602.85420	1
21487	H	86.55800	58.10780	107.88190	-192.35619	-3025.64718	856.28963	1
21488	C	88.24100	56.92680	108.44490	-39.70392	31.43055	-922.93234	1
21489	H	88.79900	56.31480	107.75190	-2308.74034	-399.30065	2082.40514	1
21490	C	88.99900	58.27680	108.62790	533.06131	267.21247	-703.06754	1
21491	H	88.48300	58.99280	109.30190	1621.58566	2506.23513	967.89022	1
21492	H	90.03800	57.98680	108.89590	2283.11093	-1524.00781	-1565.51550	1
21493	H	89.10200	58.71980	107.61390	-2188.71036	-1996.25869	1052.30564	1
21494	C	88.23700	56.08880	109.70490	642.22866	267.23352	578.02159	1
21495	O	89.01500	55.11480	109.84290	674.29431	-417.58623	81.31770	1
21496	N	87.28400	56.41280	110.61790	548.16637	453.94747	-464.45808	1
21497	H	86.91200	57.33580	110.56290	2027.54104	-1421.14751	1940.78371	1
21498	C	86.97200	55.47480	111.74990	-583.22133	-420.93382	-574.57245	1
21499	H	87.90700	55.26180	112.24790	2301.34493	482.26405	-2108.41189	1
21500	C	85.97400	56.15380	112.70390	-434.42365	325.26577	711.77238	1
21501	H	85.55200	55.42080	113.42490	-2652.15769	-446.62730	1611.85439	1
21502	H	85.16200	56.58080	112.07790	1392.34311	-1341.84480	2478.04443	1
21503	C	86.51500	57.41880	113.51390	-518.76209	579.66808	443.45980	1
21504	H	85.63700	57.75580	114.10590	-397.27039	-2877.35012	-1243.82266	1
21505	H	86.86800	58.20880	112.81690	3085.93597	285.05713	557.56108	1

21506	C	87.65700	56.97980	114.46190	-373.18304	533.00404	-638.86655	1
21507	O	87.51800	56.06080	115.23690	-561.92578	-242.26106	-509.74084	1
21508	N	88.78900	57.67580	114.32290	112.31106	827.20148	-17.50210	1
21509	H	88.76800	58.52780	113.79990	-1540.90061	-1709.45619	2136.17914	1
21510	H	89.56800	57.40480	114.88790	31.83797	-2360.60773	-2104.68758	1
21511	C	86.38100	54.13380	111.32290	186.04227	17.84476	-907.08440	1
21512	O	86.84900	53.05580	111.69790	-198.53370	-517.33565	554.93721	1
21513	N	85.41700	54.13580	110.31590	-571.07270	-506.66814	-377.32812	1
21514	H	85.05700	54.93680	109.84490	1272.48260	-2500.38249	1431.54664	1
21515	C	84.85500	52.81180	109.85490	422.34363	477.98314	-662.29753	1
21516	H	84.53200	52.34680	110.77490	305.41600	-736.83651	-3060.04183	1
21517	C	83.70500	53.01180	108.93090	-9.75433	-684.18590	-625.88094	1
21518	H	84.01300	53.65080	108.07590	1434.14690	-2809.32224	-123.33248	1
21519	H	83.34100	52.09480	108.41990	2245.34169	-1331.23701	-1783.46068	1
21520	N	82.20500	53.38680	110.95190	-129.12814	-123.37351	-838.31457	1
21521	H	82.76300	52.85980	111.59290	2115.43274	325.34364	-2323.35424	1
21522	C	82.52300	53.64980	109.61990	-540.65560	-371.89490	620.93352	1
21523	C	81.11100	54.09780	111.23090	-446.76210	109.55486	770.17287	1
21524	H	80.61100	53.96480	112.18990	521.94149	-1096.21733	-2919.64429	1
21525	N	80.67200	54.79180	110.20390	-666.45331	-506.17666	108.82604	1
21526	C	81.57800	54.50080	109.14890	-409.69791	161.45830	781.53908	1
21527	H	81.39700	54.85780	108.14190	-2404.64671	-1642.49524	1180.83233	1
21528	C	85.90800	51.89980	109.19590	-51.36434	492.02505	745.55590	1
21529	O	85.88900	50.70180	109.38790	753.04817	-263.70656	-37.54943	1
21530	N	86.82900	52.50780	108.42890	440.28802	-705.24858	180.35530	1
21531	H	86.68300	53.45680	108.15990	2068.26808	-2382.14230	-97.00836	1
21532	C	88.02200	51.87180	107.84890	687.84369	530.90858	-289.39722	1
21533	H	87.57200	51.13580	107.19990	-1838.47594	-2546.19589	219.49772	1
21534	C	88.70700	52.92580	106.97790	-738.12864	-526.64736	83.75863	1
21535	H	89.07900	53.71380	107.66690	1487.63967	-2251.13827	-1647.74815	1
21536	H	88.02500	53.45380	106.27890	1603.01873	-2662.02562	530.27210	1
21537	H	89.64100	52.60980	106.46590	-665.85474	1160.27859	2828.39221	1
21538	C	88.99100	51.29980	108.85590	661.82690	-508.57586	-403.50394	1
21539	O	89.45100	50.19180	108.67390	-261.51197	-84.85822	-755.02024	1
21540	N	89.27600	51.98380	109.97890	-424.66527	-558.07716	459.47263	1
21541	H	88.76800	52.80380	110.22890	-905.13376	-2832.92282	1030.39139	1
21542	C	90.10100	51.42580	111.06990	-679.22628	543.23924	222.29926	1
21543	H	91.01100	51.07180	110.60790	-931.55511	2643.68285	-1424.58670	1
21544	C	90.26000	52.46080	112.19890	-143.87362	-562.27375	-724.56451	1
21545	H	90.54900	51.99480	113.16490	-2806.66635	1346.09134	364.68259	1
21546	H	89.29800	53.00080	112.32690	-1961.06028	1876.47468	1556.88599	1
21547	C	91.46800	53.42280	111.91590	554.07711	-543.53918	480.44117	1
21548	H	91.24700	53.92980	110.95190	951.11569	-937.59130	2838.44685	1
21549	C	91.52600	54.66780	112.80790	-317.99455	-553.30851	641.25410	1
21550	H	91.94300	54.47580	113.81990	-1363.63520	-1646.74124	-2325.95455	1
21551	H	92.19500	55.45480	112.39790	-1476.00409	2647.15703	-818.10281	1
21552	H	90.49100	55.02780	112.99190	-1674.09359	1651.52184	-2091.62519	1
21553	C	92.83900	52.70780	111.87190	-394.74455	613.22564	-548.39512	1
21554	H	92.94400	52.02380	111.00290	-145.83781	-2017.17187	2400.52263	1
21555	H	93.60500	53.51180	111.82990	2253.68213	2149.78808	417.84540	1
21556	H	93.04000	52.07480	112.76290	1895.46477	1835.56317	-1727.23128	1
21557	C	89.46100	50.19980	111.71690	-547.96712	168.13184	685.77758	1
21558	O	90.15700	49.23380	112.03990	-661.52465	407.88855	-70.00391	1
21559	N	88.19500	50.21680	112.07190	511.12975	-579.90554	349.03531	1
21560	H	87.72300	51.07580	111.88590	-1719.24051	1948.27710	-1772.04816	1
21561	C	87.47100	49.11180	112.69890	401.63311	392.16534	701.22189	1
21562	H	88.04300	48.79080	113.55590	-2396.87845	-1930.18719	640.69576	1
21563	C	86.10000	49.48680	113.13590	609.09279	-214.22935	-669.10143	1
21564	H	85.43700	48.61080	113.30090	-2432.90355	-207.11611	-1991.56016	1
21565	O	85.50100	50.38680	112.30590	210.34657	647.94102	371.65154	1
21566	H	85.67800	50.08280	111.41290	-2036.83915	380.86807	-2375.07761	1
21567	C	86.15600	50.20880	114.52090	-419.66067	228.70361	-784.28352	1

21568	H	85.14000	50.56980	114.78890	-2906.61975	52.20097	-1198.92605	1
21569	H	86.84200	51.06980	114.37390	-867.58561	-3008.30891	367.90175	1
21570	H	86.58700	49.54880	115.30390	-2513.79285	-1578.55899	-1056.06460	1
21571	C	87.33200	47.86380	111.81290	744.96388	-539.93151	58.07691	1
21572	O	87.28100	47.98280	110.59890	402.96599	-511.80725	446.23403	1
21573	N	87.22900	46.69980	112.39890	-242.12019	603.26164	-540.72166	1
21574	H	87.31500	46.64780	113.38990	1729.81744	-1504.06017	-2184.71464	1
21575	C	87.00800	45.43480	111.73590	793.47529	-469.94647	20.09701	1
21576	H	87.60700	45.49580	110.83890	774.51587	2892.98738	-958.92929	1
21577	C	87.63800	44.22280	112.49690	-380.31524	-664.56034	484.48118	1
21578	H	87.57500	43.32580	111.84390	-1405.00239	-1588.99201	-2343.57422	1
21579	H	88.73700	44.38180	112.50190	-2503.19484	-1323.57475	1348.66127	1
21580	O	87.05400	43.98480	113.80390	461.47569	464.54060	421.09403	1
21581	H	87.22400	44.78680	114.30390	-835.70238	-2922.49211	-858.01661	1
21582	C	85.56100	45.12680	111.38790	-844.04850	-314.10052	-135.47984	1
21583	O	84.61300	45.60580	112.09190	52.51541	695.48013	-368.33181	1
21584	O	85.32200	44.42480	110.35290	-393.53940	238.55721	616.83476	1
21585	H	80.24552	97.51177	69.82170	-2203.97439	2774.45925	219.49197	2
21586	N	81.08894	97.39216	69.17606	77.74064	373.01161	219.19944	2
21587	H	81.91105	97.10433	69.70674	984.03137	1350.93135	1179.33617	2
21588	C	81.12403	98.57265	68.38251	-72.22577	-1359.42070	-232.72228	2
21589	H	82.20624	98.66155	68.18763	-373.37624	-430.24295	1627.35341	2
21590	C	80.26537	98.54011	67.03542	241.28132	834.25436	29.00395	2
21591	H	80.23761	97.48790	66.83010	22.12122	1571.01788	3765.50329	2
21592	H	79.24094	98.83010	67.21484	2454.96882	-2275.04413	-1913.64111	2
21593	C	80.83582	99.40257	65.90839	461.46119	-589.66184	940.28250	2
21594	H	80.71285	100.42402	66.40951	1589.22644	-2378.10319	-965.16513	2
21595	C	82.28651	99.14451	65.67684	-223.40295	601.40574	-481.96221	2
21596	H	82.59211	99.82882	64.83465	-3315.07151	2280.75681	-632.51569	2
21597	H	83.03302	99.39790	66.52498	-988.08833	1732.79088	1379.73612	2
21598	H	82.32003	97.96199	65.49377	-1282.30310	-1533.67285	-1635.14912	2
21599	C	80.04675	99.28437	64.60501	294.00209	-373.44555	-14.22494	2
21600	H	78.88365	99.62041	64.63289	2132.47902	483.31960	-1022.14719	2
21601	H	80.61499	99.96498	63.86268	2797.57120	-4122.28627	-270.78469	2
21602	H	80.00774	98.21915	64.25002	-1009.18582	-565.57420	-4075.64879	2
21603	C	80.61261	99.86027	69.15614	-779.82540	-204.41118	-363.39302	2
21604	O	79.90516	100.73543	68.60507	383.26827	590.54177	-201.20594	2
21605	N	81.22223	100.03568	70.33779	947.42103	-580.51925	1128.21349	2
21606	H	81.77931	99.34553	70.85069	-1414.78665	-961.67631	2469.61466	2
21607	C	80.25381	100.81338	71.15527	294.99018	-278.10414	121.04827	2
21608	H	79.44613	100.04009	71.18911	-375.61805	1268.06976	1151.45254	2
21609	C	80.94852	101.15916	72.42867	-421.26118	-957.73411	540.00001	2
21610	H	81.98051	101.60642	72.32048	-385.53739	1978.70737	178.28549	2
21611	O	81.73006	99.81653	73.18388	329.00610	-142.34246	645.24361	2
21612	H	80.99774	99.23978	73.11030	1674.53487	-1776.00480	98.60665	2
21613	C	79.92431	101.86261	73.35512	-548.08259	860.36794	-392.34979	2
21614	H	80.37645	102.50261	74.17852	2557.54246	111.74924	-750.61689	2
21615	H	79.32375	102.58595	72.81690	1513.70468	-1500.01489	1573.49999	2
21616	H	79.34039	101.13525	73.94675	781.15107	-145.50783	-128.22883	2
21617	C	79.81682	102.14222	70.17618	-611.67948	315.36945	929.65388	2
21618	O	80.67040	102.94302	69.82220	217.03584	-320.70400	-44.60890	2
21619	N	78.49275	102.34242	70.36210	-90.08159	-110.86820	564.95092	2
21620	C	77.71653	103.22009	69.53006	218.86649	-332.46417	-248.48957	2
21621	H	78.23652	102.98170	68.60931	-2708.50686	-1441.94494	-3560.19883	2
21622	C	76.22148	102.71367	69.53965	338.05997	252.30797	-772.43145	2
21623	H	75.52796	103.54347	69.31962	-141.96968	-3284.93544	-4366.09237	2
21624	H	75.95826	102.00440	68.75258	-1741.50464	-145.90936	-1521.09628	2
21625	C	76.18255	102.01892	70.93615	204.99968	-262.56799	169.03427	2
21626	H	76.14274	102.71857	71.76649	-2942.43973	-2563.57922	-676.72890	2
21627	H	75.32449	101.32082	71.04248	1380.37966	-185.37434	1755.61461	2
21628	C	77.66132	101.34542	71.00700	168.16198	951.51245	1356.10383	2
21629	H	78.05632	101.15580	72.02553	2759.92067	2846.72771	-2087.10469	2

21630	H	77.71423	100.47901	70.39357	-4209.11269	1956.94027	-1448.48477	2
21631	C	77.74793	104.78003	70.06946	-299.26008	-10.39615	52.72829	2
21632	O	76.87718	105.55517	69.60878	103.19083	179.81900	-408.96953	2
21633	N	78.72644	105.01053	70.90751	469.53877	1.72887	-5.60344	2
21634	H	79.23685	104.14341	71.14987	-743.33809	224.31407	570.09825	2
21635	C	79.05936	106.27441	71.46171	-474.40220	-1227.76910	-14.99596	2
21636	H	78.11481	106.85661	71.27315	188.92374	-115.23930	-1331.69781	2
21637	C	79.43754	106.03223	72.99567	94.71279	-760.20729	-520.04122	2
21638	H	80.44722	106.53300	73.20214	-4142.25380	1984.16703	1251.60105	2
21639	O	79.83378	104.71660	73.40144	-260.36887	-519.61452	-314.03419	2
21640	H	80.81382	104.71535	73.30518	1133.75502	913.38419	1855.37470	2
21641	C	78.27805	106.73323	73.77234	-788.79574	439.82313	16.83536	2
21642	H	77.37901	106.52573	73.22776	1331.45122	1003.94549	-122.66841	2
21643	H	78.16106	106.27396	74.80531	-421.42271	268.16918	868.47965	2
21644	H	78.37437	107.91050	73.76359	1274.31316	1101.26812	1333.45718	2
21645	C	80.40950	106.79956	70.68021	-215.34192	-1003.49298	661.52682	2
21646	O	80.58440	107.98268	70.72728	396.73997	-515.97497	293.08026	2
21647	N	81.20574	105.86620	70.08264	-52.47171	-533.92230	-399.04354	2
21648	H	80.89972	104.89692	70.18844	1709.01957	-1976.05603	1189.98343	2
21649	C	82.61576	106.22868	70.24126	620.78639	100.51051	473.17000	2
21650	H	82.47794	107.29542	70.35573	-1893.63240	-4376.27007	296.37581	2
21651	C	83.30672	105.68127	71.54548	-27.21096	-481.06104	-559.67919	2
21652	H	84.07458	104.82165	71.35549	-3385.09745	-2735.88470	-115.84742	2
21653	H	84.18949	106.33584	71.85139	-362.05123	727.95481	1356.33176	2
21654	O	82.45597	105.44924	72.76053	-99.64758	296.28123	1090.81334	2
21655	H	82.80590	104.57887	73.03662	1317.80671	-3309.92651	-191.97023	2
21656	C	83.46052	105.77159	68.93377	-385.67317	31.94080	312.71540	2
21657	O	83.91472	106.57203	68.14593	52.94135	-169.48440	-136.84643	2
21658	N	83.25264	104.41759	68.71525	-138.79474	-370.39548	463.14758	2
21659	H	82.64545	103.90216	69.32674	-1308.76840	2745.58673	2866.21828	2
21660	C	84.23049	103.82432	67.84948	-499.46842	-152.90827	-1211.00496	2
21661	H	84.98242	104.60081	67.67609	-711.32045	2797.43865	-946.92893	2
21662	C	84.74887	102.52000	68.55384	230.07871	699.40272	-260.94523	2
21663	H	85.12989	101.91587	67.60429	-1166.88035	151.91908	2080.12408	2
21664	C	85.92017	102.64539	69.58259	496.76204	-288.08652	-443.01305	2
21665	H	86.27342	101.69580	69.91422	-2139.75638	-1002.91727	-4029.86329	2
21666	H	86.79787	103.21355	69.18312	-1887.92627	-1282.11423	-747.08396	2
21667	H	85.68265	103.21974	70.56818	-2023.23277	943.28476	-4607.37468	2
21668	C	83.72560	101.57980	69.28144	387.58473	724.06362	-506.49973	2
21669	H	84.09544	100.50607	69.25848	-772.03475	-70.05647	15.87574	2
21670	H	83.70180	101.83958	70.32070	2378.59972	-989.60425	-3522.43561	2
21671	H	82.71188	101.61927	68.81519	1864.31373	-5896.23890	2347.96110	2
21672	C	83.52492	103.44562	66.40702	114.85637	347.38735	-68.76641	2
21673	O	82.43615	102.90028	66.40025	61.62559	595.70270	-137.66335	2
21674	N	84.39787	103.82406	65.46425	-378.58418	206.38815	-579.70658	2
21675	H	85.30474	104.16657	65.77624	1684.10996	-3536.42158	1482.33997	2
21676	C	83.68035	104.10166	64.24912	439.76820	775.26420	1454.32723	2
21677	H	82.72175	103.57338	64.38247	-3788.28219	1589.19077	-666.24183	2
21678	C	83.58443	105.70640	64.26844	433.07503	-117.33178	-88.42648	2
21679	H	84.50065	106.06567	64.75058	1526.46179	-3466.10481	-491.32488	2
21680	H	83.55110	106.09296	63.22995	2137.70859	-354.89833	1009.34825	2
21681	C	82.41694	106.32411	65.06287	499.25643	-579.47694	-469.02489	2
21682	H	81.43965	105.99099	64.62992	2062.03013	-1307.39381	-93.88431	2
21683	H	82.47508	106.08517	66.20283	749.37745	2427.26219	105.01043	2
21684	C	82.44439	107.90145	64.91728	25.30571	-767.57936	-52.50704	2
21685	O	81.72689	108.47753	64.08829	-241.40710	378.11683	-110.52896	2
21686	N	83.13667	108.44105	65.92645	43.61355	-430.69152	73.68896	2
21687	H	83.70540	107.91138	66.60074	5.00312	-294.61137	-2399.86351	2
21688	H	83.26332	109.48118	66.25805	3573.15458	-1250.49415	-451.25549	2
21689	C	84.61754	103.62257	63.03003	-369.60921	-241.52835	148.69096	2
21690	O	85.28919	104.50896	62.50168	300.53955	-96.93360	148.95780	2
21691	N	84.77207	102.30773	62.90429	-315.66316	-547.95222	1014.30955	2

21692	C	85.35005	101.78056	61.70417	15.45555	-469.77434	-424.71292	2
21693	H	86.27713	102.41388	61.53255	1047.79943	-32.42574	-869.88280	2
21694	C	85.59344	100.22584	62.00529	496.65852	24.23655	-478.14644	2
21695	H	84.80383	99.64742	61.43613	278.45829	-925.68296	594.85982	2
21696	H	86.55586	99.81824	61.66812	40.30549	-1895.41441	1875.95655	2
21697	C	85.59598	100.14569	63.52775	-443.03406	363.03598	-579.43865	2
21698	H	85.26933	99.10924	63.88119	1769.39024	121.48120	-652.47291	2
21699	H	86.61826	100.29906	63.85108	-2749.99635	1760.48637	1032.86904	2
21700	C	84.63004	101.31751	63.97393	781.83299	-353.24011	-312.97969	2
21701	H	83.54069	101.05816	63.98696	590.97142	2366.08972	2771.57754	2
21702	H	84.87413	101.91779	64.87313	321.17958	-2754.35300	2991.57344	2
21703	C	84.29830	101.99238	60.41469	-154.67549	549.43569	652.92656	2
21704	O	84.69470	102.26540	59.28510	157.93435	-1077.01057	5.73542	2
21705	N	83.06167	101.79363	60.87124	339.58667	956.94148	89.76747	2
21706	H	83.03868	101.65036	61.90270	2054.94209	-2005.35617	858.05633	2
21707	C	82.00435	102.55170	60.28225	-1407.50344	1138.10303	89.50011	2
21708	H	82.33298	102.83201	59.28796	1145.63215	624.04297	1040.26377	2
21709	C	80.82419	101.43393	60.18152	-99.50972	-192.73972	194.86170	2
21710	H	80.21067	101.38236	61.19596	-1260.07068	-2136.73159	-1090.91546	2
21711	C	80.00328	101.94646	59.00771	191.18885	-558.17174	1297.62697	2
21712	H	80.61589	102.11602	58.10269	-2859.64317	1408.64422	-1326.07524	2
21713	H	79.23426	101.17121	58.75390	2850.61831	-1229.39690	-2478.54816	2
21714	H	79.51084	102.80919	59.27667	1411.97799	2599.35818	-2226.32532	2
21715	C	81.40598	100.05194	59.70498	600.04941	-345.59783	78.67295	2
21716	H	82.31793	99.91047	60.25151	-3351.65435	-929.51100	3746.62904	2
21717	H	80.71151	99.14313	59.88783	-1297.42691	-2381.48810	9.35107	2
21718	H	81.65265	99.82273	58.63769	90.34369	-848.84375	760.66026	2
21719	C	81.49995	103.74805	61.21810	188.61380	28.51271	12.22192	2
21720	O	81.24930	103.48569	62.39129	-109.76024	4.52660	-105.30368	2
21721	N	81.12133	104.87919	60.51858	854.57121	-952.82121	-122.90232	2
21722	H	81.55394	104.81627	59.57498	84.07397	587.31680	603.18393	2
21723	C	81.29679	106.00230	61.40867	-238.66819	-102.20294	-347.58697	2
21724	H	81.62112	105.67108	62.40488	1866.02732	1778.61932	1018.64353	2
21725	C	82.36015	106.96725	60.70610	232.99566	-160.21715	-713.18582	2
21726	H	81.81043	107.54756	59.94192	1149.71658	1214.27193	2947.11994	2
21727	H	82.62438	107.62904	61.55691	-1832.62772	3442.37858	-521.20039	2
21728	C	83.59149	106.19924	60.20698	-365.45344	-160.97216	-188.80921	2
21729	H	83.75905	105.32717	60.85276	1419.55451	358.23656	-830.65182	2
21730	H	83.55140	105.78517	59.25288	2729.78769	2723.89053	377.89352	2
21731	C	84.76411	107.21774	60.36722	-44.44118	-4.01048	-7.71547	2
21732	H	84.54559	108.31482	60.12789	-293.21521	-1196.19452	-467.25044	2
21733	H	84.98341	107.19580	61.43371	-1771.00020	4724.82868	2366.49764	2
21734	C	85.83866	106.47363	59.46435	-369.48070	0.58189	-300.58162	2
21735	H	85.60861	106.45088	58.36654	-1207.87450	-277.71461	1009.57323	2
21736	H	86.78878	106.93955	59.76617	-948.29425	-1071.85936	-2635.47538	2
21737	N	85.97818	105.08549	59.76186	591.82860	325.91893	315.40454	2
21738	H	85.66285	104.25380	59.20104	-1549.13525	-1274.72801	-1898.26096	2
21739	H	78.91197	108.08145	58.25361	1733.06168	-2934.29909	-86.12859	2
21740	H	85.88937	104.81116	60.75115	1847.09234	2053.62650	1314.59220	2
21741	C	79.82328	106.69643	61.49318	-136.24621	-52.97902	126.23821	2
21742	O	78.84468	106.15697	60.95857	-139.00596	920.66947	-149.66407	2
21743	N	79.79846	107.66880	62.34422	751.08826	-1.43123	602.55204	2
21744	H	80.72782	108.08654	62.66712	159.46601	3400.70675	548.64500	2
21745	C	78.62418	108.47299	62.43639	-132.54356	84.74719	-916.56254	2
21746	H	77.90394	107.71094	62.72058	-5249.10243	-903.97572	-2953.89373	2
21747	C	78.85751	109.68551	63.44477	-15.50277	-25.69466	-263.30141	2
21748	H	79.57440	109.38369	64.28105	-1152.28826	-665.93175	-2111.98711	2
21749	H	79.37243	110.53346	62.89357	1633.35955	3217.30782	-1809.60330	2
21750	C	77.38734	110.08708	63.94691	214.92183	1457.94987	-1192.50663	2
21751	H	77.03643	109.07054	64.29302	-957.76681	700.93638	-2894.19502	2
21752	H	77.40973	110.85908	64.77059	4178.73996	-899.20443	-3356.54183	2
21753	C	76.50004	110.69959	62.82032	-69.60484	643.23460	611.12794	2

21754	H	76.89320	111.70194	62.54297	-2080.18609	-589.98569	3743.83500	2
21755	H	76.51451	110.12991	61.90666	-469.12120	2246.86131	-835.89204	2
21756	C	75.05003	110.82815	63.39037	-969.14040	701.66014	23.17791	2
21757	H	74.96382	111.43823	64.36306	3180.50600	-1860.98942	-1459.59654	2
21758	H	74.28589	110.99526	62.57398	-872.72662	-936.82641	-1407.10281	2
21759	N	74.76501	109.45453	63.89464	801.49651	984.41736	192.81445	2
21760	H	75.12467	108.56297	63.26580	-3617.98283	470.15261	-1756.98922	2
21761	H	75.00782	109.10425	64.88994	1197.13630	3862.73220	-2719.38497	2
21762	H	73.66750	109.36073	63.95125	2374.70312	-1515.44022	1297.81246	2
21763	C	78.18780	109.07086	60.93801	-684.92341	-326.31173	354.77080	2
21764	O	78.85514	109.85819	60.19060	187.39289	214.77912	-349.50580	2
21765	N	76.99278	108.60252	60.69256	73.65445	-336.88471	-464.30443	2
21766	H	76.75117	107.91621	61.47005	2493.50609	1111.50848	892.80091	2
21767	C	76.21831	108.53155	59.50565	-624.13201	-284.06219	-8.13794	2
21768	H	76.19724	109.68323	59.19975	-1231.77315	-1351.05609	-366.52448	2
21769	C	76.94532	107.75263	58.41204	152.10135	-335.73592	715.28365	2
21770	H	77.43350	106.84557	58.71894	1026.79589	1264.77692	826.72111	2
21771	O	78.26193	108.76723	57.83035	-199.40088	800.24149	-140.90224	2
21772	H	78.24595	109.57307	58.54812	1816.71793	61.22083	-577.46959	2
21773	C	75.95079	107.44087	57.28591	-325.55500	-188.43985	-244.18959	2
21774	H	75.65552	108.42320	56.78701	242.87445	-843.57925	-304.01251	2
21775	H	76.44114	106.92356	56.38774	-771.77558	2147.79502	-3309.14287	2
21776	H	75.03341	106.90488	57.51428	2594.88873	460.96907	-137.27200	2
21777	C	74.79933	107.72187	59.86779	-727.86366	-178.54675	511.74652	2
21778	O	73.72277	108.14318	59.45068	124.92974	177.34795	-321.07454	2
21779	N	75.11700	106.49861	60.30248	856.83435	504.04220	-339.12310	2
21780	H	76.09421	106.48246	60.50401	643.73026	-1779.41450	2297.63893	2
21781	C	74.14828	106.00731	61.27553	-304.73602	500.28896	-300.88846	2
21782	H	73.42862	106.76031	61.25391	2054.12405	-1543.39285	-356.26931	2
21783	C	73.51612	104.62862	60.75414	-427.58728	904.73209	257.42240	2
21784	H	72.65011	104.47062	61.45164	702.70592	55.31423	1685.14919	2
21785	H	73.08664	104.72773	59.72339	413.83442	-582.82955	-2158.40248	2
21786	C	74.58876	103.53084	60.75008	-256.60927	-630.11284	-767.77434	2
21787	C	74.50142	102.38884	61.55910	551.50747	266.00113	-35.20438	2
21788	H	73.77897	102.18934	62.33123	695.52970	193.28671	1083.60363	2
21789	C	75.47382	103.49909	59.58632	148.08449	-209.39054	-886.18161	2
21790	H	75.46796	104.29663	58.87173	1502.56654	235.70157	107.19171	2
21791	C	75.53803	101.42001	61.36989	75.05288	1040.00387	-291.94838	2
21792	H	75.66755	100.64214	62.15215	750.44565	-1446.84455	218.13332	2
21793	C	76.34025	102.43999	59.37834	-630.45829	1293.59043	50.65334	2
21794	H	76.89830	102.58243	58.42334	-1102.54125	441.34802	592.96233	2
21795	C	76.53775	101.37090	60.37503	-240.71636	660.29462	-0.48801	2
21796	O	77.63059	100.43247	60.28727	-309.48978	340.68932	-67.82445	2
21797	H	77.37376	99.90891	61.11403	-914.07113	-2000.51422	-2188.06526	2
21798	C	75.01534	105.93369	62.61038	26.86302	185.89720	-276.22366	2
21799	O	75.53114	106.99751	63.05029	80.88209	-479.32215	-13.37626	2
21800	N	74.89570	104.80248	63.28306	-294.71895	-381.16766	-324.93744	2
21801	H	74.27893	104.03907	62.93767	2772.08121	-217.43009	314.62306	2
21802	C	76.07714	104.22610	63.80375	-227.32104	-158.08700	261.45666	2
21803	H	75.95488	103.11344	63.71316	-1757.00306	2520.66370	3087.16693	2
21804	C	77.22793	104.74466	62.88718	137.18586	746.55686	3.64500	2
21805	H	76.89912	104.61163	61.79606	1805.77073	-1367.78641	-2307.59400	2
21806	H	77.43076	105.82062	63.05927	-867.08452	-625.92851	2668.02251	2
21807	C	78.59971	104.00887	63.08753	-144.69407	-102.83334	517.71744	2
21808	H	79.35871	104.49687	62.39930	1178.99954	-1055.98462	3229.84243	2
21809	H	79.02129	104.13667	64.15583	-1227.38457	-996.52137	2230.60335	2
21810	C	78.49032	102.45836	62.73817	76.05927	-615.05776	853.72358	2
21811	H	77.72881	102.25824	61.94487	-492.24233	-981.29261	188.67453	2
21812	H	79.41179	101.97698	62.49746	-722.75471	1403.73039	2972.40730	2
21813	N	78.21795	101.91399	64.05533	-704.25862	-744.40629	-183.05924	2
21814	H	77.34076	101.44247	64.29915	-3093.28077	116.39910	194.59088	2
21815	C	79.09231	101.91379	65.00572	879.04327	-511.34096	107.09507	2

21816	N	80.36482	102.46753	64.82808	-422.40141	-540.59316	150.32072	2
21817	H	80.73449	102.92293	63.95905	575.79135	-4015.64010	674.88550	2
21818	H	80.97298	102.46015	65.68827	-719.43781	-4087.09863	-1525.09451	2
21819	N	78.64385	101.43758	66.25903	-243.10159	565.84870	-214.81991	2
21820	H	77.68770	101.18648	66.57110	-1547.62949	-1244.58394	-955.83166	2
21821	H	79.20504	101.59640	67.13922	-2942.47557	-1186.84422	208.43083	2
21822	C	76.50738	104.74412	65.33163	-220.88440	-124.25767	-833.18194	2
21823	O	76.97968	103.90052	66.05001	-43.83107	223.38683	-278.36135	2
21824	N	76.42961	106.05081	65.50948	456.55674	-616.92251	396.36681	2
21825	H	76.01603	106.71409	64.80246	-2719.59469	-628.00329	1539.20195	2
21826	C	76.84360	106.47347	66.81661	84.20867	-747.53651	-178.69462	2
21827	H	77.00395	105.60367	67.49914	163.82945	-3118.10933	1116.20955	2
21828	C	78.12638	107.40005	66.53029	-440.98171	157.81232	-334.77727	2
21829	H	77.79722	108.33421	66.01852	1130.95269	-97.59501	-180.60977	2
21830	C	78.79613	107.67448	67.90196	-670.55059	-274.64745	-62.13292	2
21831	H	78.92814	106.67020	68.39044	99.73801	379.97360	2199.60788	2
21832	H	79.78916	108.23452	67.91864	-353.76031	-228.27497	-323.07610	2
21833	H	78.02452	108.05915	68.63103	-2436.78027	233.11961	1549.84979	2
21834	C	79.15357	106.56355	65.71126	270.78616	-619.53892	-104.41874	2
21835	H	80.17951	107.01569	65.60460	1925.02792	-1882.25887	-875.82659	2
21836	H	79.34712	105.57998	66.25319	397.76113	-904.82218	593.12539	2
21837	H	78.81300	106.32093	64.65182	-1758.77944	-3142.90831	-1259.49944	2
21838	C	75.67808	107.54742	67.16856	-55.80567	178.34451	357.38273	2
21839	O	75.27187	108.35443	66.33585	-260.75776	226.98759	1011.05432	2
21840	N	75.23644	107.30073	68.37382	107.93642	-256.29706	-203.99331	2
21841	H	75.68800	106.62118	69.08632	-2393.99853	-213.66498	-263.44137	2
21842	C	74.23367	108.15831	68.88881	-248.98912	-516.35190	663.20157	2
21843	H	74.16484	109.09205	68.21321	-1788.86935	-2335.56556	-1261.98229	2
21844	C	72.75828	107.50770	68.87205	691.23808	389.03624	-967.36718	2
21845	H	72.78348	106.45847	68.55390	2167.62109	-242.22132	1628.87904	2
21846	H	72.41394	107.48224	69.91402	1913.67732	-111.24210	129.41562	2
21847	C	71.70987	108.25705	68.08555	352.26680	241.58301	160.65104	2
21848	H	72.06727	108.12784	67.00257	-2689.64675	-2238.09014	-484.99052	2
21849	C	70.41281	107.50486	68.36355	259.91785	-650.98112	274.46142	2
21850	H	70.05204	107.53647	69.38839	1220.42018	2664.79482	1004.07270	2
21851	H	69.61838	107.98734	67.78719	-3833.80112	-2426.66885	1860.69338	2
21852	H	70.49106	106.37455	68.17832	-2320.80691	-2778.09004	1067.29826	2
21853	C	71.49426	109.72199	68.43723	-1057.91891	819.66300	56.46605	2
21854	H	70.76520	110.27402	67.73989	-826.27660	3177.14876	-642.82403	2
21855	H	71.22479	109.88370	69.54376	-932.07910	-2357.22920	1198.00374	2
21856	H	72.45054	110.31162	68.37273	-659.31199	57.59903	-397.71354	2
21857	C	74.63462	108.36990	70.44772	766.07197	-965.93206	629.07733	2
21858	O	73.81664	108.23649	71.32311	-32.87966	-978.49119	214.34394	2
21859	O	75.90122	108.89216	70.66376	-460.13090	99.47927	-316.14461	2
21860	H	76.28814	108.93123	69.73619	-394.68518	-1183.57053	405.19334	2
21861		5463						
21862		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000*****	200.0000
		0.2500	400.00	0.00	0.00	0.00	-25972.6645	0.2229
								400.0000
21863	N	57.56085	99.05441	60.57381	57.34284	-315.42497	-587.29842	1
21864	H	57.24857	99.20962	59.62543	-1148.89054	1100.24794	-3390.03508	1
21865	H	57.06960	99.73555	61.16763	-364.24760	999.01903	207.62672	1
21866	H	64.95364	103.32901	61.47345	1247.91277	777.26153	1175.38599	1
21867	C	58.95443	98.75716	60.49356	-301.10350	185.13323	125.31148	1
21868	H	59.51047	99.05793	61.40118	1438.94856	1500.88784	-2587.83048	1
21869	C	58.91834	97.14122	60.40055	-457.94128	95.29282	357.16291	1
21870	H	58.42631	96.82987	61.32562	1183.21921	310.25539	621.00530	1
21871	H	60.01766	96.87418	60.46310	375.57477	-160.81765	217.20628	1
21872	C	58.23647	96.48596	59.18470	-145.70061	-200.77023	28.22940	1
21873	H	57.46280	97.15011	58.68643	-2386.16942	-441.76386	-622.31942	1
21874	H	57.56280	95.62789	59.61132	1121.54147	-1006.24513	-2031.36628	1
21875	S	59.63255	95.79118	58.23193	-595.52181	-141.24332	-348.13167	1
21876	C	59.99192	96.99096	56.83698	91.91193	1389.13184	474.65172	1

21877	H	60.97523	96.81215	56.27331	-5.22117	154.43821	-1600.27930	1
21878	H	59.16743	96.85952	56.03506	30.03546	681.92642	-868.94843	1
21879	H	60.00340	98.07603	57.09179	1606.62908	1287.16642	-1818.96572	1
21880	C	59.49614	99.52930	59.20153	-35.73165	85.85586	-96.70860	1
21881	O	58.74632	99.59185	58.24833	-97.11384	416.54923	-1110.71437	1
21882	N	60.83036	99.82372	59.22608	-463.62687	-266.53621	-103.75285	1
21883	H	61.27876	99.57120	60.12711	1018.78226	1807.58491	1641.59658	1
21884	C	61.64450	99.92398	58.09296	-639.79867	461.52133	786.20804	1
21885	H	60.89701	100.20358	57.31144	-660.90633	-2567.05404	1039.67915	1
21886	C	62.71185	101.08919	58.33272	-110.17299	-520.92085	977.37822	1
21887	H	63.47663	101.08450	57.51050	844.42617	-855.50915	961.80553	1
21888	H	62.17563	102.06731	58.21508	-1244.70867	-3311.96385	1140.08575	1
21889	C	63.30790	101.06109	59.79394	-903.61808	-501.21462	-499.05552	1
21890	H	63.96612	100.21613	59.94944	137.97327	1079.31547	1547.75860	1
21891	H	62.50778	100.92262	60.51523	-1638.53672	-698.05346	-722.09172	1
21892	C	63.96401	102.43380	60.17399	851.46804	-148.90035	-674.33269	1
21893	O	63.65321	103.44645	59.60484	634.28468	78.21967	-282.07908	1
21894	O	64.91979	102.38110	61.20903	418.17781	920.90824	107.15285	1
21895	C	62.46705	98.55563	57.69930	-108.33478	-219.10130	22.09648	1
21896	O	63.00341	98.54841	56.61931	-13.08612	-151.96607	3.55377	1
21897	N	62.70063	97.77312	58.75193	-885.79606	184.94109	219.14416	1
21898	H	62.10148	98.04945	59.55309	-2361.75987	3041.42394	-2820.54252	1
21899	C	62.93137	96.37787	58.41027	-449.73065	-46.18143	75.56008	1
21900	H	62.68931	96.46866	57.31316	-2984.16940	-600.09876	341.24292	1
21901	H	62.17271	95.75328	58.84005	575.60268	-2871.39408	1233.60260	1
21902	C	64.42723	95.99923	58.84843	953.69859	749.37312	-309.25148	1
21903	O	64.76862	94.85353	59.20987	-513.89339	422.10940	337.42167	1
21904	N	65.17499	97.08964	58.85108	-394.80830	365.28864	-130.64361	1
21905	H	64.88762	97.90193	58.33529	-5308.04094	-1569.94467	-1797.76754	1
21906	C	66.40044	97.10173	59.58623	134.21661	48.83579	-409.04689	1
21907	H	66.61523	96.03967	59.83098	-1494.37885	-361.48849	427.18384	1
21908	C	67.53066	97.95417	58.86101	573.31141	571.69088	65.67233	1
21909	H	67.28651	99.02961	59.04429	-303.84689	13.98837	983.63150	1
21910	C	68.85284	97.65262	59.62306	817.05679	218.13227	-343.83476	1
21911	H	69.04477	96.50307	59.73307	-211.16878	499.16219	1081.74599	1
21912	H	68.76761	98.14001	60.62609	-1122.02126	876.45165	-1096.99437	1
21913	H	69.71367	97.99543	59.08549	-1228.92146	-1143.69409	-703.39035	1
21914	C	67.58050	97.46543	57.36977	-179.50950	-667.88067	110.09015	1
21915	H	68.31755	97.99257	56.77318	-633.69056	514.64470	1969.99168	1
21916	H	66.58675	97.72310	56.92611	394.05354	-934.11935	-1673.86804	1
21917	C	67.78076	95.94986	57.07526	-565.30494	910.09653	-97.38579	1
21918	H	67.85172	95.58792	55.98046	-2709.18297	3239.70917	2030.34056	1
21919	H	66.87895	95.44986	57.45867	-589.45539	989.12203	248.62383	1
21920	H	68.67309	95.58039	57.65577	589.31803	-1793.70141	-2020.19026	1
21921	C	66.13717	97.82166	61.04289	-267.63363	-346.80667	-218.74885	1
21922	O	67.07940	97.99041	61.82466	-550.20639	-497.60635	-363.18828	1
21923	N	64.91550	98.34527	61.23240	-615.82017	-394.43867	8.03020	1
21924	H	64.35745	98.26410	60.38533	-329.46709	265.73664	2085.84446	1
21925	C	64.43797	98.48912	62.56737	-1.82412	585.29982	228.93636	1
21926	H	65.31502	98.86731	63.11382	908.24888	2050.80309	-131.67477	1
21927	C	63.16065	99.44566	62.51146	-306.31669	-963.49874	-134.57500	1
21928	H	62.77679	99.44107	63.58093	2313.91870	279.00387	-902.58197	1
21929	H	63.60648	100.44726	62.32327	-2626.58907	786.17904	2444.53702	1
21930	O	62.07184	99.13147	61.61588	1062.55339	538.34685	-344.37657	1
21931	H	61.30374	99.67952	62.05394	-4440.63076	789.47860	1246.29027	1
21932	C	63.90330	97.05194	63.17649	-166.41643	-445.99402	635.55228	1
21933	O	63.57558	97.03435	64.36985	-131.55651	129.38237	352.15942	1
21934	N	63.98084	96.07567	62.27172	-368.93842	-1618.05957	682.93819	1
21935	H	64.23952	96.49984	61.39367	34.05215	-645.60969	-306.76206	1
21936	C	63.50994	94.75633	62.36057	-471.87761	9.23484	-78.90240	1
21937	H	63.68773	94.24378	61.41908	-404.53701	2070.65987	-3562.14310	1
21938	C	64.36159	94.18304	63.55770	-292.18505	-260.16697	1.92868	1

21939	H	64.72585	95.01740	64.19795	-883.40942	-156.45043	2429.12451	1
21940	C	63.38857	93.38459	64.40888	-566.53663	-75.17095	-537.74039	1
21941	H	62.81669	92.60291	63.83094	-1714.47336	1598.94089	3813.25670	1
21942	H	63.85563	92.90278	65.29807	241.48616	-2225.54765	3262.46397	1
21943	H	62.61281	94.04513	64.90872	-372.37274	282.84918	-22.61973	1
21944	C	65.59431	93.50828	63.18281	-303.08560	192.12913	-380.15490	1
21945	H	65.53312	92.57976	62.44784	-4131.75415	531.27607	-2282.91599	1
21946	H	66.00336	92.89196	63.99947	952.52916	802.89585	-2130.70354	1
21947	C	66.79313	94.43273	62.58607	-168.42184	122.31440	-220.38546	1
21948	H	67.66663	93.80431	62.23917	-2546.30628	4657.23807	2346.55317	1
21949	H	66.50051	95.09361	61.70304	771.30329	-1989.49534	1214.79355	1
21950	H	67.16133	95.14877	63.48636	-1302.87382	316.62806	426.94218	1
21951	C	61.83301	94.75402	62.50116	-305.17161	529.47924	-227.48131	1
21952	O	61.14134	94.12444	61.70910	481.36534	221.23263	-761.10726	1
21953	N	61.39612	95.33974	63.61220	-106.03222	290.96572	322.45764	1
21954	H	62.10225	95.71100	64.24059	307.47378	-1519.01516	-1438.34468	1
21955	C	59.99340	95.43390	63.79642	157.68208	-260.10585	-446.83240	1
21956	H	59.54776	94.79955	62.94667	-777.85578	1429.36824	-2424.38937	1
21957	C	59.88246	94.97340	65.31960	76.19818	421.76349	615.62096	1
21958	H	59.91900	95.87219	66.01233	-1899.86632	-125.37802	1221.99154	1
21959	H	60.67193	94.23487	65.63614	1356.95162	446.63451	4526.50851	1
21960	C	58.52660	94.22258	65.38322	339.10851	490.38316	352.86085	1
21961	C	58.56486	92.80983	65.17233	-492.08131	-271.02636	11.01408	1
21962	H	59.45817	92.22865	65.12406	-419.33896	711.40606	-6581.60999	1
21963	C	57.36769	92.18229	65.15215	-234.56456	-475.95586	960.91471	1
21964	H	57.28197	91.09259	65.05024	-4.86399	396.50541	2625.05424	1
21965	C	56.04769	92.82696	65.24527	928.65956	-326.59497	-838.04850	1
21966	O	54.77732	92.17520	65.25506	-51.50437	236.51205	826.63182	1
21967	H	54.23239	92.92475	65.48078	1711.14774	2328.45570	1151.18433	1
21968	C	57.38054	95.00816	65.48354	-375.77258	-326.55858	-350.93357	1
21969	H	57.39123	96.15249	65.57659	2803.82386	-3811.30509	231.78978	1
21970	C	56.18857	94.21480	65.40779	210.93913	-191.69332	-1127.52245	1
21971	H	55.14547	94.67760	65.45365	-669.80040	3565.43772	-1920.63241	1
21972	C	59.34606	96.94950	63.79391	-390.35190	-226.60681	-1045.86776	1
21973	O	58.18387	96.92803	63.47399	-545.31818	-671.55643	-375.67799	1
21974	N	60.12841	98.00579	63.95614	353.72146	450.79328	-31.07254	1
21975	H	61.13665	97.84722	64.02520	1026.44762	-1180.46470	283.88827	1
21976	C	59.76351	99.15255	64.71079	563.14239	79.14318	802.99532	1
21977	H	60.70267	99.78397	64.51419	-2823.42924	-1963.21182	634.93659	1
21978	C	58.32598	99.75633	64.38348	718.42735	102.44724	-380.35832	1
21979	H	57.64373	98.89143	64.64717	-302.29881	-774.48774	2007.84842	1
21980	O	57.76525	99.89917	62.92737	112.60145	997.08971	132.45622	1
21981	H	57.51311	98.96230	62.87099	1175.04341	161.74755	96.47364	1
21982	C	58.10726	101.01321	65.26565	-646.07692	-190.39688	638.59039	1
21983	H	57.99401	100.66142	66.29921	543.06540	-4163.57036	-1755.42025	1
21984	H	59.00889	101.67231	65.28279	-2807.24349	3566.70825	-1094.28906	1
21985	H	57.21181	101.59753	64.93090	1587.09367	-1227.39295	1214.01995	1
21986	C	59.59452	98.59919	66.23093	474.18474	195.66557	-40.26284	1
21987	O	58.52849	98.18213	66.70739	224.59440	-667.90784	-24.19438	1
21988	N	60.76580	98.70776	66.85871	-540.87526	-319.56377	358.65230	1
21989	H	61.54605	99.01144	66.30664	278.07004	874.19435	2550.18010	1
21990	C	60.79905	99.56163	68.10373	-798.23318	86.02139	682.24282	1
21991	H	60.01579	99.06006	68.72764	-82.13483	1816.24158	2396.11761	1
21992	C	62.26098	99.46462	68.72887	391.59172	593.94854	-556.95248	1
21993	H	62.01519	99.41567	69.79974	-1156.52422	677.86569	677.39515	1
21994	H	62.64796	98.45834	68.41808	-3331.22389	718.65205	-477.18419	1
21995	O	63.08492	100.64625	68.50113	45.57348	-1132.13575	920.03868	1
21996	H	63.39411	100.74601	69.48364	-81.69500	1909.29679	460.85450	1
21997	C	60.46203	101.08639	67.89460	26.57256	-492.86669	-573.85400	1
21998	O	60.48086	101.67419	66.83189	-40.07747	618.59622	19.51391	1
21999	N	60.05222	101.57700	69.11630	155.77479	-15.58211	-1088.18182	1
22000	H	59.85735	101.06887	70.02835	925.91029	-1335.26188	-413.31123	1

22001	C	59.11290	102.67172	68.87677	206.96268	181.68255	-93.94492	1
22002	H	58.65422	102.09169	67.96583	-325.97779	700.36379	2461.23266	1
22003	C	58.28156	102.86224	70.15745	-251.62041	-523.53432	-85.75765	1
22004	H	57.47915	103.60523	70.01084	-553.80170	-3374.59155	-1182.20554	1
22005	H	58.89692	103.37827	70.97080	-1397.71366	446.51559	154.79918	1
22006	C	57.70061	101.49677	70.73767	-190.33977	-102.98936	-413.57810	1
22007	O	58.41537	100.49280	70.86159	-631.84914	-386.94435	-71.67728	1
22008	O	56.48600	101.60113	71.04427	554.76333	-40.29553	-374.92178	1
22009	C	59.85273	104.06779	68.43981	1688.16749	-201.34425	-763.48326	1
22010	O	59.13540	104.67256	67.67550	314.05371	832.90285	257.35586	1
22011	N	61.03095	104.38745	68.92675	558.51506	-34.79187	-827.79436	1
22012	H	61.58093	103.67993	69.50945	2723.97930	2285.12172	409.89318	1
22013	C	61.70262	105.49893	68.41739	854.86987	490.38658	1322.62178	1
22014	H	60.91552	106.21568	68.01928	1194.86887	-436.14414	1214.44342	1
22015	C	62.60827	106.04893	69.59037	-220.05194	-716.27737	-788.42996	1
22016	H	61.76310	106.40453	70.27371	-5194.07208	1083.46558	1790.16502	1
22017	H	63.25180	106.90920	69.29086	-555.48417	1662.45884	1723.91029	1
22018	C	63.42144	104.91984	70.32145	-1289.70812	-888.51164	-66.15047	1
22019	O	62.98118	103.83067	70.64262	149.69299	805.52978	-96.07600	1
22020	N	64.64833	105.39380	70.45637	-123.12112	-39.34466	-492.31273	1
22021	H	65.59742	104.84209	70.64027	820.36109	1621.77699	-1217.22131	1
22022	H	64.95076	106.26172	70.02626	-1964.73533	1178.91004	-894.50132	1
22023	C	62.73618	104.97660	67.17822	312.87525	184.70711	-32.91610	1
22024	O	63.61586	105.69062	66.81935	-94.14423	58.58490	-193.25433	1
22025	N	62.42365	103.80088	66.59799	599.20594	-324.01247	-749.35834	1
22026	H	61.82880	103.16708	67.18495	3406.18236	677.01032	2580.87615	1
22027	C	63.19179	103.33382	65.52289	367.66150	116.28444	-270.91106	1
22028	H	64.16030	103.83916	65.69254	4317.67698	159.83552	-717.66507	1
22029	C	63.05467	101.76234	65.54257	-223.00650	-307.64006	-929.48445	1
22030	H	62.87792	101.45573	66.64731	-543.18620	849.70043	1559.61878	1
22031	H	62.18455	101.35992	64.95581	585.71121	-271.71199	-1673.55202	1
22032	C	64.33949	101.09355	65.04809	-84.65835	-256.13608	-89.99760	1
22033	C	65.26526	101.80567	64.20639	-548.08846	86.14706	-38.97318	1
22034	H	65.02259	102.87181	63.90673	69.35934	-1666.74303	-524.20432	1
22035	C	66.45848	101.18863	63.79447	407.70055	195.52419	1044.21502	1
22036	H	67.06874	101.59390	62.99730	2146.30768	1601.42077	587.55332	1
22037	C	66.94760	99.96411	64.34339	733.30886	582.02113	-433.42347	1
22038	O	68.22318	99.42373	63.85717	260.04978	-65.32227	559.72747	1
22039	H	67.90652	98.71626	63.28047	831.71290	219.37256	424.98094	1
22040	C	64.84140	99.88290	65.56761	438.18663	107.80646	295.43167	1
22041	H	64.18048	99.31221	66.21223	1499.24776	2129.85057	-1819.24598	1
22042	C	66.10580	99.33619	65.23038	-120.70242	1212.27733	1062.89076	1
22043	H	66.31553	98.36677	65.69238	2382.81594	1095.16104	3295.88462	1
22044	C	62.80522	103.90006	63.97958	132.16682	-892.81170	-149.37720	1
22045	O	63.61381	104.55357	63.31678	-252.38778	-117.78027	52.59551	1
22046	N	61.69943	103.30090	63.59225	54.38437	594.49308	844.62251	1
22047	H	61.23120	102.80388	64.37198	-28.38374	-1071.60284	1576.60330	1
22048	C	61.12892	103.57566	62.30694	555.01001	266.07192	558.74517	1
22049	H	62.02247	103.69597	61.68287	-2803.79998	1025.90850	3692.68127	1
22050	C	60.03878	102.52139	61.95010	-517.55631	29.01644	-136.12894	1
22051	H	59.19044	102.58045	62.61927	-2021.67704	-1932.41657	1141.39247	1
22052	O	60.44123	101.01096	62.50953	-143.52972	28.16152	42.03924	1
22053	H	59.59805	100.75592	62.88686	-149.93372	-125.70101	-1360.17569	1
22054	C	59.59758	102.81196	60.49186	-422.78291	-353.67284	449.06370	1
22055	H	58.69025	102.13513	60.29664	-2144.91502	-83.85672	-775.42995	1
22056	H	60.37311	102.54410	59.69980	223.31573	-457.70638	696.57320	1
22057	H	59.31550	103.85731	60.25188	314.83574	-4728.11698	1323.86287	1
22058	C	60.37257	105.02308	62.48837	170.59824	27.32143	-135.40987	1
22059	O	59.17188	105.08821	62.58860	83.70533	365.64754	-655.76141	1
22060	N	61.27582	106.02643	62.61758	321.89056	-326.81145	92.14165	1
22061	H	62.25806	105.63106	62.83053	-1396.78759	-127.20385	-26.39640	1
22062	C	60.90853	107.18199	63.35290	232.49396	160.76535	593.52678	1

22063	H	59.83383	107.42936	63.11123	-2208.32372	-1836.65457	-1041.05307	1
22064	C	60.92744	106.80040	64.89665	-249.29852	436.98880	-882.40256	1
22065	H	61.52397	105.89166	65.02092	218.51430	1113.52389	937.32150	1
22066	H	61.42082	107.55831	65.56320	-524.67949	22.46374	1891.87311	1
22067	C	59.45348	106.69098	65.42804	-207.40598	947.67055	443.85891	1
22068	H	58.90652	106.07127	64.65032	237.85490	-404.22187	-2960.71067	1
22069	H	59.60495	106.04780	66.40539	-2667.04981	1346.46070	244.52389	1
22070	C	58.57617	108.04265	65.60731	430.33591	15.47678	-26.42170	1
22071	O	57.38363	107.92829	65.89106	47.87287	352.74242	-309.50983	1
22072	O	59.10211	109.14713	65.37222	380.94445	59.75560	62.68516	1
22073	C	61.99442	108.37636	63.31813	283.29060	-634.37018	-524.39502	1
22074	O	63.10939	108.30628	62.79399	-298.96520	441.74052	658.13890	1
22075	N	61.50237	109.39142	64.04140	-579.28815	895.38960	-380.82435	1
22076	H	60.59907	109.44067	64.51564	1540.63622	-328.45120	668.25041	1
22077	C	62.46712	110.32625	64.50043	-305.17696	50.57354	20.75423	1
22078	H	63.22249	110.14189	63.75309	-925.06371	-3335.30257	1200.24962	1
22079	C	61.81792	111.76813	64.46973	521.00066	-459.17665	-448.08822	1
22080	H	60.90434	111.95411	65.11158	610.89759	3456.39626	1482.65813	1
22081	H	61.49004	111.86406	63.44464	264.35201	1535.83986	1047.47579	1
22082	C	62.86342	112.90861	64.67118	433.46112	897.34511	-850.75930	1
22083	H	62.64729	113.78804	64.00231	-137.47034	-1945.04764	2326.42588	1
22084	H	62.83433	113.16071	65.72062	-3416.23226	398.88294	2720.60805	1
22085	C	64.39284	112.60799	64.16466	369.49562	35.78809	308.72120	1
22086	O	65.01690	111.53750	64.37398	295.56518	864.14990	-87.74129	1
22087	O	64.90478	113.66310	63.71300	-211.36117	-273.38789	-622.54110	1
22088	C	62.82612	109.88815	66.00267	334.41136	-520.58120	-389.06275	1
22089	O	62.00746	109.66631	66.88899	378.04820	202.65923	737.28258	1
22090	N	64.19247	109.78619	66.09444	-704.19558	-621.86760	662.86798	1
22091	H	64.78348	110.17950	65.28549	423.02316	-1514.87254	-751.62497	1
22092	C	64.67405	108.46642	66.49177	317.80348	-687.87234	116.44785	1
22093	H	63.68819	107.99658	66.61587	-2995.70865	-1184.99345	-0.00231	1
22094	C	65.35817	108.05253	65.13679	-815.06928	20.22811	-163.44150	1
22095	H	64.89415	108.58705	64.29154	1126.59612	1575.22341	2075.96056	1
22096	H	66.44865	108.42903	65.07983	-1600.82233	4964.40092	-1378.24100	1
22097	C	65.44743	106.50869	64.97482	-887.48532	-102.19639	-176.54671	1
22098	H	64.41147	106.04064	64.77693	1183.58086	-1456.67413	-807.53667	1
22099	H	65.80912	105.98933	65.94035	2383.34453	-1350.44110	1810.54997	1
22100	S	66.61574	106.21565	63.58584	575.05665	-384.48497	-12.89023	1
22101	C	65.63879	106.87485	62.17593	578.82686	260.94281	197.02964	1
22102	H	64.81367	106.20252	61.77331	-64.63850	-1099.72138	668.58852	1
22103	H	66.23587	107.20380	61.29205	3001.48117	3236.21556	-786.91977	1
22104	H	65.09690	107.77771	62.50570	-1052.41447	-1708.69519	-1646.45472	1
22105	C	65.46395	108.53951	67.91903	432.51513	39.71933	-383.54003	1
22106	O	65.32453	107.62681	68.72453	-229.83387	-277.09932	-194.57876	1
22107	N	66.22751	109.59884	67.91036	-302.42750	-552.62239	-1123.15358	1
22108	H	66.11927	110.31471	67.20235	-62.19578	-34.23159	-887.42475	1
22109	C	67.25030	109.66114	68.95329	-287.96168	227.84045	-104.42813	1
22110	H	67.22060	110.71642	69.22254	2082.87037	-3597.14120	-684.37280	1
22111	H	66.94039	108.98027	69.77248	-3006.16811	-152.72866	-871.79561	1
22112	C	68.76951	109.28350	68.58466	670.81136	739.29392	436.74982	1
22113	O	69.61833	109.19149	69.48163	1028.23078	-217.72396	-328.69887	1
22114	N	69.01863	109.17222	67.25652	436.86897	-295.59906	-736.69576	1
22115	H	68.12083	109.47129	66.83937	1354.07177	-1146.79892	767.58296	1
22116	C	69.34439	107.79765	66.86984	203.80948	129.33601	-177.32140	1
22117	H	68.60984	107.25558	67.55452	-918.63973	-3195.69156	174.02240	1
22118	C	69.09908	107.56082	65.28556	73.16724	83.22966	535.01252	1
22119	H	70.08143	107.45233	64.79072	239.26752	761.53459	-204.69504	1
22120	H	68.75540	106.53556	65.39475	-818.90948	1133.59541	-1827.37366	1
22121	O	68.34512	108.59256	64.55470	-771.02490	774.30886	407.72486	1
22122	H	67.82713	108.04315	63.86798	-2251.42670	1206.96132	-1726.36620	1
22123	C	70.87588	107.40341	67.12733	564.11015	-371.07388	-684.87586	1
22124	O	71.88568	107.96593	66.75404	345.52763	-356.06108	-152.39738	1

22125	N	70.84487	106.23598	67.76796	-666.68070	959.04401	898.24499	1
22126	H	69.90702	105.85897	67.98416	-2006.01951	1567.04511	-1780.69750	1
22127	C	72.08409	105.62066	68.18604	-818.40655	157.89124	-242.46497	1
22128	H	72.94749	106.13524	67.67094	-1538.60738	-2521.96388	563.65295	1
22129	H	71.99683	105.93742	69.23293	-1882.74548	76.39789	-124.13518	1
22130	C	72.17975	104.01576	67.89093	-541.48327	117.48327	-238.79478	1
22131	O	71.24811	103.34371	67.50639	-152.70170	305.24034	76.74392	1
22132	N	73.43337	103.60962	68.05768	-315.66478	-237.45427	-959.90342	1
22133	H	74.14961	104.34387	68.27095	-1705.79479	-2738.85773	-1053.02069	1
22134	C	73.60038	102.21283	68.32268	642.34199	-183.66641	-640.15969	1
22135	H	72.73115	101.73899	67.90607	2337.73395	1263.95232	59.58690	1
22136	C	75.00402	101.85552	67.76262	583.03539	304.40756	-293.68450	1
22137	H	75.43893	100.97769	68.37707	-1278.39722	-2946.05491	773.74978	1
22138	H	75.72706	102.67977	67.92636	4032.05859	-1377.60030	-1272.36814	1
22139	C	74.85492	101.46205	66.21325	422.18042	414.38818	991.06207	1
22140	O	75.88335	101.33054	65.42915	-35.40940	541.36493	-339.67257	1
22141	O	73.67553	101.32326	65.90475	-42.02488	-51.87526	109.96061	1
22142	C	73.75037	101.75699	69.94845	269.24423	664.18531	3.98801	1
22143	O	73.61120	100.58314	70.25210	605.87784	-324.19208	286.73806	1
22144	N	73.99577	102.79789	70.78798	510.69900	73.90032	-1700.36929	1
22145	H	73.85459	103.68920	70.23075	-2274.39300	-1772.71685	-1442.25804	1
22146	C	73.17411	102.62671	71.94678	27.06762	561.99875	60.73680	1
22147	H	73.12867	101.49865	72.17196	-3793.55628	-3318.33753	-1997.54004	1
22148	C	73.72954	103.59189	73.07794	328.31880	738.69506	-72.15936	1
22149	H	73.11376	103.42692	73.96495	741.39865	-859.63217	-1572.80136	1
22150	H	73.62709	104.65789	72.71219	759.95958	2734.10669	-138.41387	1
22151	C	75.21760	103.37297	73.41151	-935.36980	-112.86199	-743.25883	1
22152	C	75.66126	102.09122	73.72311	-293.47785	-823.07987	-1047.31791	1
22153	H	74.98934	101.17798	73.80731	-3502.97707	-1237.65862	-1075.15378	1
22154	C	77.06091	101.95689	73.96773	-987.62577	-84.77008	-850.11089	1
22155	H	77.35677	101.02755	74.41238	-1933.89721	-466.72379	5143.83709	1
22156	C	78.02426	102.93594	73.83244	1124.40862	-1052.91291	272.59581	1
22157	O	79.42308	102.87297	74.15555	433.23045	23.47065	-581.75558	1
22158	H	79.55875	101.85001	74.07740	1339.70971	-1926.74231	2225.44076	1
22159	C	76.13049	104.42407	73.02799	-524.05620	39.00998	696.47147	1
22160	H	75.77823	105.38790	72.59092	1184.45130	-1074.43860	613.62343	1
22161	C	77.42854	104.16659	73.37267	-116.72050	448.74569	295.42516	1
22162	H	78.15640	104.95709	73.19877	1000.96535	2185.52045	529.17790	1
22163	C	71.70144	103.34607	71.74663	807.35466	137.04324	108.32137	1
22164	O	71.69746	104.57276	71.79079	-65.69585	724.21107	409.74300	1
22165	N	70.69285	102.54793	71.56612	-10.48027	230.69615	776.33771	1
22166	H	70.72708	101.52171	71.59746	1918.57665	745.73427	-841.33030	1
22167	C	69.39940	103.15912	71.35556	18.49385	-265.71280	-993.83772	1
22168	H	69.40593	104.08954	71.97155	-394.51559	-5801.85132	-786.55979	1
22169	C	69.35764	103.78083	69.91748	675.84467	-32.09421	19.47540	1
22170	H	70.31314	104.37965	69.72034	1884.31451	-561.71472	2008.89712	1
22171	H	69.30420	102.94000	69.18788	-683.76763	2971.10528	-915.90702	1
22172	C	68.23658	104.92076	69.79147	257.62473	-311.26782	54.33827	1
22173	O	68.35129	105.86114	69.02003	-234.06252	490.97741	369.37383	1
22174	O	67.12372	104.53927	70.36634	-585.33780	-903.17293	13.15847	1
22175	C	68.44911	101.91526	71.77356	679.35642	73.79314	874.99629	1
22176	O	68.87493	100.80286	72.08673	-346.52296	468.45283	802.94377	1
22177	N	67.14749	102.22888	71.63446	1029.91615	-423.65449	249.50990	1
22178	H	66.85617	103.18012	71.27808	838.71923	-2927.80737	3160.33567	1
22179	C	66.15216	101.32520	72.20423	-541.87646	-232.89443	103.20016	1
22180	H	66.92252	100.73207	72.83277	734.32116	-702.99216	-3764.04042	1
22181	C	65.15195	102.25523	72.92408	372.69701	-1386.29624	-639.15024	1
22182	H	64.17118	101.75601	73.11785	-2294.36835	-1063.00906	1152.38896	1
22183	H	64.71223	102.93130	72.13463	667.55278	2289.82023	-562.64455	1
22184	O	65.77713	103.04504	74.18267	-510.82446	322.54273	-43.38158	1
22185	H	66.51887	103.42394	73.76711	444.29506	1581.01302	-3659.82934	1
22186	C	65.35074	100.45401	71.06744	295.60149	-602.06362	594.56423	1

22187	O	64.12452	100.38951	71.04493	94.81367	-418.13872	-45.01091	1
22188	N	66.28683	99.87950	70.31497	101.10835	398.71307	-302.95023	1
22189	H	67.21106	100.23823	70.61243	-1432.92088	-18.51670	39.83693	1
22190	C	66.07167	99.57705	68.93144	231.53330	278.76825	126.55839	1
22191	H	65.12023	98.99244	68.97769	192.07799	3308.74883	1100.02910	1
22192	C	66.09538	100.85906	67.96996	-943.79788	-273.82221	133.99487	1
22193	H	66.52106	100.65368	66.96676	1286.78899	-747.86563	1498.35801	1
22194	H	65.09384	101.34328	67.85884	4691.71888	-488.77599	-1642.58811	1
22195	C	67.01694	101.85631	68.64930	-482.82177	35.16122	-221.00433	1
22196	H	66.57848	102.25075	69.57651	3133.49983	37.14727	292.31342	1
22197	H	67.91043	101.29977	68.92826	-472.26726	-334.13294	-1842.11956	1
22198	S	67.38429	103.15262	67.36366	-169.52065	96.26085	31.24742	1
22199	C	65.78629	103.99268	67.45970	-78.79307	-424.89202	581.60079	1
22200	H	65.19160	104.21566	68.36909	-883.35244	-133.06819	1371.66554	1
22201	H	65.88019	104.96549	66.92191	-1468.46706	-3627.69690	904.04642	1
22202	H	65.02651	103.48987	66.77909	4571.34052	69.74625	624.78981	1
22203	C	67.28016	98.54148	68.42746	-167.57228	-79.42715	101.76261	1
22204	O	68.41446	98.96230	68.39364	-486.08646	-39.10048	-728.04952	1
22205	N	66.78702	97.39432	68.07244	-535.85046	777.46295	523.10853	1
22206	H	65.75082	97.25672	68.12032	2680.27079	-4926.63157	1414.36426	1
22207	C	67.51463	96.25078	67.63100	286.29917	-5.23091	-89.78558	1
22208	H	68.29380	96.33402	68.45397	1110.17002	-1009.83651	234.83511	1
22209	C	66.68698	94.92428	67.56532	-330.37064	-62.51453	-312.90950	1
22210	H	65.76462	94.89448	66.96645	946.06156	1651.23806	-2482.43100	1
22211	H	67.27564	94.13947	66.98893	-914.25033	-1068.51035	-614.66338	1
22212	C	66.40487	94.57060	69.06678	74.53343	682.80050	-443.58725	1
22213	H	65.34892	94.18861	69.25340	-1217.65805	520.93234	-589.68958	1
22214	H	66.66428	95.45298	69.74368	-4167.19910	-2036.60924	126.85542	1
22215	C	67.31207	93.37383	69.45680	484.04439	25.42120	-264.61531	1
22216	H	68.32231	93.50701	68.89119	1764.10561	2891.16111	-28.77259	1
22217	H	66.88538	92.43540	69.03027	1270.70667	236.48394	5.17206	1
22218	C	67.43156	93.14210	71.02437	28.16155	247.78551	539.33889	1
22219	H	67.88975	92.13983	71.20864	-819.86658	-3975.65697	1989.40363	1
22220	H	66.52781	93.35690	71.65247	-2232.67676	-310.28050	2004.75233	1
22221	N	68.38169	94.14082	71.51884	-992.84442	124.20623	-447.31450	1
22222	H	68.70602	93.92885	72.55030	1660.58738	-969.41679	1389.59814	1
22223	H	69.40263	93.95646	70.83838	736.76524	-1868.07995	-1776.45389	1
22224	H	68.00419	95.15276	71.47362	2563.15414	-868.23989	866.97800	1
22225	C	68.16481	96.33464	66.10450	-146.43097	493.27244	-463.52894	1
22226	O	67.56995	95.87994	65.13835	539.92052	-198.57125	10.27518	1
22227	N	69.24876	97.17800	66.03425	326.66953	309.34428	29.07119	1
22228	H	69.46737	97.46486	67.02479	16.60763	1875.63393	1190.20878	1
22229	C	70.40291	96.64849	65.31522	799.29664	-61.86146	-394.47617	1
22230	H	70.50312	95.58157	65.57770	-3640.78174	-145.27753	-2092.48318	1
22231	C	70.14505	96.82395	63.77600	168.12200	-1073.55474	-111.51807	1
22232	H	69.15645	96.45680	63.55302	-1642.23527	836.88757	-2026.21559	1
22233	H	70.11119	97.90569	63.49105	-31.94289	398.42254	2765.40740	1
22234	C	71.24318	96.10267	62.97075	453.15307	-648.76162	614.63765	1
22235	H	70.89222	95.27574	62.36507	2013.98855	-1784.99409	703.74698	1
22236	H	72.00407	95.65939	63.62140	1937.49803	-1871.46429	-822.87318	1
22237	C	71.85978	97.15564	61.90395	-534.35377	-408.00131	-241.21357	1
22238	O	72.95972	96.79370	61.40674	-311.61714	409.72966	115.30915	1
22239	O	71.16679	98.02796	61.40429	270.30539	-676.92400	-432.18561	1
22240	C	71.64975	97.57587	65.77987	182.63322	186.91580	-198.01951	1
22241	O	72.77069	97.19936	65.43443	539.38666	-165.87298	-592.24091	1
22242	N	71.33807	98.71362	66.33783	292.48071	-33.81876	625.25264	1
22243	C	70.61903	99.74160	65.58233	-215.30874	219.84504	-773.61298	1
22244	H	69.60730	99.32981	65.21889	-548.77021	1039.60351	-2363.61483	1
22245	H	71.24961	99.93933	64.65947	4676.08456	-958.06282	-2166.04140	1
22246	C	72.11081	99.19124	67.48047	94.22049	529.89222	882.84103	1
22247	H	72.93012	99.61307	66.92042	628.33704	1196.24977	3349.11657	1
22248	C	71.02690	100.27142	67.91187	-92.20086	146.10766	137.13787	1

22249	H	71.39632	101.04348	68.65427	-1716.93128	-1052.88945	1714.02260	1
22250	H	70.20973	99.87873	68.47607	2283.62708	-813.09823	85.97251	1
22251	C	70.54888	100.96355	66.57546	-600.16657	-839.50224	120.45311	1
22252	H	71.24558	101.82692	66.34215	-2997.04170	-248.19097	-23.35501	1
22253	H	69.59791	101.53376	66.61451	1928.81930	1510.05615	-1296.16545	1
22254	C	72.51241	98.01635	68.50623	-209.10243	-148.06069	568.40513	1
22255	O	72.04185	98.09208	69.62245	59.03163	563.06569	166.29290	1
22256	N	73.33525	97.05618	67.99673	-227.48849	524.78220	-44.01293	1
22257	H	73.45768	97.06663	66.93414	-1874.00439	-2923.31436	189.07034	1
22258	C	73.13725	95.66976	68.47420	747.94010	620.91487	726.90196	1
22259	H	72.53488	95.83347	69.36323	2947.01929	-3574.96871	2445.73734	1
22260	C	72.32061	94.83553	67.45012	-468.56504	338.98483	45.44222	1
22261	H	72.33145	95.31449	66.46380	-500.25505	-269.02671	-651.88689	1
22262	H	72.95488	93.96600	67.13831	2565.05168	656.88387	-376.80190	1
22263	S	70.66143	94.44377	68.13218	-282.09489	-54.45617	105.31302	1
22264	C	74.59810	94.98370	68.60226	77.56685	855.11127	-104.45170	1
22265	O	74.59285	93.81282	68.91736	107.37575	-338.64561	51.24106	1
22266	N	75.65179	95.77290	68.34520	-93.13121	-870.00563	623.20201	1
22267	H	75.46018	96.82945	68.15728	-142.49927	-1672.88451	1275.03039	1
22268	C	76.93226	95.23783	68.74593	733.97847	-315.23402	-333.74696	1
22269	H	76.75807	94.21508	68.32334	300.85770	1758.50346	53.17546	1
22270	C	78.15201	96.01943	68.11890	-541.99087	844.32294	330.01519	1
22271	H	79.13995	95.73967	68.57750	-1416.78998	2801.44367	729.78335	1
22272	H	78.09607	97.04316	68.52598	-3674.46407	-3122.06972	-171.79205	1
22273	C	78.34537	95.96099	66.59071	-301.46825	1113.32919	172.52928	1
22274	C	79.43392	95.25568	65.98742	431.78039	-201.38613	317.75306	1
22275	H	80.19440	94.74720	66.71907	-3689.77943	1669.02700	-579.43081	1
22276	C	79.53602	95.45012	64.57774	-1225.51426	-46.29287	-518.41546	1
22277	H	80.38875	94.94894	64.09731	-867.97499	-1668.91172	3064.84441	1
22278	C	78.50047	96.12487	63.86114	-1260.03735	646.64666	-321.82665	1
22279	H	78.58546	96.19342	62.76252	1345.24987	1493.21095	-318.98140	1
22280	C	77.25477	96.54754	65.85475	-3.60502	-135.76860	530.40874	1
22281	H	76.38020	96.95509	66.42850	-148.50144	-1049.48902	98.93838	1
22282	C	77.38065	96.68947	64.44534	-721.87170	-153.82688	210.83130	1
22283	H	76.68364	97.25626	63.79782	839.86685	-1639.87470	428.92253	1
22284	C	76.98528	95.09370	70.36395	0.84441	558.93081	-120.36275	1
22285	O	77.19785	96.15296	70.96578	4.10333	-462.50164	-415.24953	1
22286	N	76.98035	93.87593	70.92353	-703.49448	618.00576	30.55308	1
22287	H	76.75809	93.11741	70.29817	470.34918	2201.92350	-993.74504	1
22288	C	76.67904	93.91437	72.30005	-19.93765	1035.89722	-413.05866	1
22289	H	75.71446	94.48619	72.42833	891.60984	-2319.08730	1076.51204	1
22290	C	76.50681	92.42695	72.80817	-650.52924	490.18829	724.04291	1
22291	H	77.32364	92.13914	73.50288	-1594.31311	2060.69668	2664.62397	1
22292	H	76.57909	91.63708	72.05040	148.09655	2713.63634	168.97060	1
22293	C	75.13963	92.34143	73.54730	-203.80608	549.92198	-447.13185	1
22294	H	75.20043	91.97860	74.58501	-593.21431	-9.02865	-454.94197	1
22295	H	74.89675	93.46853	73.67475	-419.78167	996.43328	255.39724	1
22296	C	74.16028	91.50244	72.60444	-925.81314	-522.99924	422.25431	1
22297	H	74.21645	90.40590	72.74155	1530.47555	4277.72363	1910.31438	1
22298	H	74.13747	91.84391	71.51065	-814.29965	-594.98533	2049.50397	1
22299	N	73.05113	91.87387	73.35230	27.78327	-318.55262	-783.46875	1
22300	H	73.01480	92.83566	73.73246	1874.75886	1272.77129	768.98630	1
22301	C	72.01390	91.12938	73.47915	93.87290	-595.47716	-1.00476	1
22302	N	71.98077	89.86554	72.92431	312.97585	-582.54509	-287.34985	1
22303	H	72.75519	89.48798	72.44665	3057.12186	1298.38810	-913.28332	1
22304	H	71.13377	89.19329	72.89013	-220.09355	-3355.47125	-212.23372	1
22305	N	71.01439	91.89743	74.14788	27.49430	-495.39465	-348.62908	1
22306	H	71.02448	92.85684	74.56465	-2060.69446	-1618.42460	-1490.28413	1
22307	H	70.11082	91.42653	74.36856	3280.85096	1837.62953	3150.04506	1
22308	C	77.59418	94.71945	73.35142	471.99439	-515.30421	-807.65417	1
22309	O	77.10123	94.71283	74.47275	-230.74872	-594.55525	231.07873	1
22310	N	78.83655	95.12847	72.99814	-393.21023	-528.74412	-282.88272	1

22311	H	78.85436	95.14303	71.97351	-2779.42994	-774.64615	3257.32704	1
22312	C	79.66390	95.79330	73.96430	-845.18396	-538.11611	-800.46145	1
22313	H	80.38238	96.46957	73.38714	-1749.61991	3209.73499	-730.46853	1
22314	C	78.72155	96.66811	74.97967	638.51513	-16.50620	-287.42856	1
22315	H	77.93677	96.11971	75.58295	4336.30454	-657.76058	1067.79718	1
22316	H	79.39651	97.19767	75.76507	1276.34625	719.66649	120.42520	1
22317	C	78.06392	97.74015	74.09812	-22.64925	-277.75671	501.57712	1
22318	H	77.15255	98.17695	74.54981	-578.90694	-2689.14706	-984.05266	1
22319	H	77.70701	97.28366	73.17933	1232.55685	184.76087	-541.08678	1
22320	C	79.13766	98.87502	73.76375	-402.02409	140.27303	129.16378	1
22321	O	78.62597	99.64523	72.90678	-15.09131	-204.13398	9.78192	1
22322	O	80.27459	99.03123	74.19942	365.46832	289.58511	477.29733	1
22323	C	80.41789	94.64884	74.80311	-782.87886	603.05048	-491.13690	1
22324	O	80.23616	93.42620	74.62090	-202.68241	145.81423	239.90962	1
22325	N	81.19903	95.18264	75.80637	132.41876	563.24695	761.95737	1
22326	H	80.93440	96.13014	75.96085	3061.32185	1571.02596	-549.97797	1
22327	C	81.28799	94.36364	76.98271	245.27245	-113.51313	334.57349	1
22328	H	81.01022	93.35306	76.79779	3385.66827	2761.68762	-1226.44279	1
22329	C	82.71839	94.64609	77.66894	151.14313	1337.98551	-193.29157	1
22330	H	82.75879	95.60566	78.29234	-3.83268	3329.72928	1349.46261	1
22331	H	83.47574	94.76076	76.91985	1359.26143	463.76776	1414.31970	1
22332	C	83.09594	93.52595	78.62541	-1000.73021	-309.20613	-27.88216	1
22333	H	82.44513	93.62126	79.52423	1206.64680	-2238.75717	-352.86769	1
22334	H	84.16959	93.41921	78.93948	857.65943	619.68765	-575.38417	1
22335	C	82.78318	92.05651	77.98991	-710.02551	1701.49459	53.91173	1
22336	O	83.47119	91.56254	77.04300	486.93265	-112.06207	509.72799	1
22337	O	81.78888	91.50147	78.51323	-673.38214	140.82539	-12.44753	1
22338	C	80.25284	95.08831	77.99853	350.63382	316.19913	-469.42710	1
22339	O	79.90177	96.22627	77.75764	-199.16921	-257.35412	-665.06052	1
22340	N	79.96341	94.32098	79.05225	132.86537	-164.19290	438.73745	1
22341	H	80.38680	93.41225	79.20324	-1649.57367	-690.57233	1323.23512	1
22342	C	79.53641	95.05183	80.17946	307.18794	84.83558	83.71776	1
22343	H	79.00059	95.95108	79.77374	321.49831	2594.88741	2892.63886	1
22344	C	78.72755	93.96290	80.99036	28.52114	-610.20425	1133.02996	1
22345	H	79.42311	93.04090	80.92090	-2597.10695	-3489.32431	23.72008	1
22346	H	77.84715	93.74979	80.38666	265.30380	-2972.42125	3180.04974	1
22347	C	78.26593	94.36099	82.41923	252.28895	323.78700	203.76654	1
22348	O	78.03875	95.50118	82.80531	-221.05808	-96.56461	572.88062	1
22349	N	78.30958	93.21969	83.17737	-665.70313	303.89784	229.69144	1
22350	H	78.61398	92.33960	82.80526	-894.64582	2830.40034	-2384.97551	1
22351	H	78.45228	93.35825	84.22378	-430.99430	-2118.48981	984.16666	1
22352	C	80.91583	95.39803	81.05206	-47.80238	296.83070	436.67230	1
22353	O	81.67000	94.47230	81.43349	-22.36846	-41.93419	586.86883	1
22354	N	80.99869	96.60277	81.46521	-140.09218	204.57279	-194.29044	1
22355	H	80.20872	97.22769	81.33754	1750.73054	-771.00596	-2117.36454	1
22356	C	82.22776	97.13981	81.88861	364.32280	-143.04340	817.72445	1
22357	H	83.07895	96.60390	81.47703	-1614.99963	-1690.72510	5989.55769	1
22358	C	82.26496	98.68047	81.61036	-1270.27788	-1160.01515	284.65353	1
22359	H	83.24005	99.08983	81.85735	-278.81825	-2083.99091	-1110.96058	1
22360	H	82.13510	98.93763	80.52186	-671.94062	1491.78284	-68.89966	1
22361	H	81.51238	99.13740	82.21780	1928.03804	-356.85769	2982.90271	1
22362	C	82.23221	96.96219	83.53472	-400.61903	457.87662	835.86616	1
22363	O	82.41952	97.95108	84.20573	407.09872	1063.19371	-987.66173	1
22364	N	82.17112	95.62396	83.82587	-424.74437	73.67053	199.61632	1
22365	H	82.06495	94.90531	83.00221	556.82153	-892.07735	322.92928	1
22366	C	81.51571	95.27352	85.08439	-30.03271	-906.62545	655.12830	1
22367	H	81.78759	96.04643	85.86384	-2161.00299	63.96754	-1295.10103	1
22368	C	79.98951	95.43966	84.65963	321.79266	-284.68887	1214.57119	1
22369	H	79.87853	94.76430	83.72306	-508.21724	-114.33590	-87.42485	1
22370	H	79.69817	96.45203	84.26208	-935.61930	491.65174	369.16449	1
22371	C	78.94609	95.18440	85.79767	389.55949	79.17918	-718.68842	1
22372	O	79.35258	94.93363	86.95186	-570.68977	-603.14760	387.33071	1

22373	N	77.65814	95.34088	85.42976	-833.21572	497.44495	-228.19588	1
22374	H	77.40881	95.56742	84.47518	-526.34698	4528.03031	2597.76878	1
22375	H	76.86538	95.29554	86.12672	673.16874	824.95754	1570.08820	1
22376	C	81.98558	93.73546	85.31437	-807.20313	-643.55209	970.28297	1
22377	O	83.04726	93.27017	84.93516	-71.56021	651.11852	-166.44697	1
22378	N	81.07890	93.04769	85.98814	801.81181	878.21457	-193.50273	1
22379	H	80.32912	93.67067	86.50664	1372.97589	-1177.71083	-686.02769	1
22380	C	81.38607	91.66198	86.21177	159.72743	88.51635	-765.70257	1
22381	H	82.31364	91.64726	86.82422	2329.24896	-2175.06778	1397.38628	1
22382	C	80.13560	91.00711	87.02506	-263.78843	105.11731	527.45722	1
22383	H	80.03762	91.53648	88.00393	-2071.99346	424.95396	-629.77990	1
22384	H	80.38062	89.91899	87.20763	1216.79654	586.20971	509.15200	1
22385	C	78.84776	91.17080	86.23028	-68.30199	-1065.83915	331.50352	1
22386	C	78.68650	90.50794	84.96005	-320.30236	-407.22916	-396.21381	1
22387	H	79.54939	89.90549	84.47280	-598.05135	-3164.43161	140.89814	1
22388	C	77.42141	90.49932	84.34219	126.00204	-468.30504	-674.12423	1
22389	H	77.22443	89.84333	83.40669	-603.87635	-6286.16358	39.39800	1
22390	C	76.47285	91.27432	84.99969	-1057.94698	101.30436	-172.83106	1
22391	H	75.47210	91.31378	84.62659	77.11726	-722.85971	315.06923	1
22392	C	77.87302	92.05167	86.81669	908.63810	-319.88872	158.30874	1
22393	H	78.14229	92.59117	87.73974	-2557.65290	-1443.93564	388.04233	1
22394	C	76.63203	92.10608	86.15526	-475.17737	404.24413	824.80646	1
22395	H	75.80817	92.82646	86.50446	-1830.47193	-987.15679	-989.17989	1
22396	C	81.79936	90.68119	85.00536	530.57182	-702.90118	-541.94291	1
22397	O	82.42048	89.65151	85.38368	419.78408	-3.17366	-597.14936	1
22398	N	81.55677	91.07937	83.76087	761.87040	126.68849	-102.32861	1
22399	H	81.22648	92.02664	83.84078	-744.19106	1427.48292	-400.58891	1
22400	C	82.09688	90.33689	82.68277	-376.38397	363.20087	-33.98443	1
22401	H	81.76671	89.25302	82.82425	-3267.25094	-1130.63361	-2709.85688	1
22402	C	81.52070	90.90030	81.34256	359.64567	-35.61022	1038.78083	1
22403	H	82.05452	90.34517	80.57221	-240.23093	307.61934	287.99172	1
22404	H	81.69011	92.03277	81.23922	-361.21610	1687.48344	1850.66505	1
22405	C	80.02565	90.54571	81.13150	-12.20987	357.73852	71.07505	1
22406	O	79.26261	90.29352	82.05739	-319.06452	-395.45011	435.07794	1
22407	N	79.67985	90.64995	79.83618	-329.23722	45.75163	-338.27852	1
22408	H	80.53785	90.80758	79.19384	852.76983	-820.80132	295.92445	1
22409	H	78.73382	90.91478	79.42440	2639.86734	-2490.23626	-1466.40782	1
22410	C	83.77264	90.42247	82.65837	-741.53365	-395.42518	179.75408	1
22411	O	84.39651	89.73581	81.90978	-74.95642	-261.62842	511.27501	1
22412	N	84.24303	91.46678	83.35653	-406.91905	327.54190	300.21497	1
22413	H	83.59391	91.96731	83.97506	4590.27665	1010.95566	-82.52750	1
22414	C	85.66528	91.49586	83.44545	93.65002	584.24736	280.71566	1
22415	H	86.26370	90.92929	82.58503	568.91685	352.68434	352.18378	1
22416	C	85.90824	93.06162	83.54150	671.19807	-411.14144	206.31780	1
22417	H	86.99527	93.27906	83.57319	-2393.23669	-1381.37217	573.27916	1
22418	H	85.51110	93.43857	84.54969	120.63387	-1865.66651	471.89646	1
22419	C	85.36653	93.84876	82.27641	-51.98362	24.83280	-429.33119	1
22420	H	84.27085	93.96659	82.37796	1351.13079	-228.54760	746.22771	1
22421	H	85.67329	93.23069	81.38367	55.82468	-1668.81841	-499.54462	1
22422	C	85.87095	95.29053	82.02038	507.08760	-1180.32107	141.12938	1
22423	H	86.99467	95.32951	82.09009	188.06961	1170.36096	1554.18115	1
22424	H	85.39006	96.04132	82.67977	-2184.54855	-2766.22374	-1146.78317	1
22425	C	85.46264	95.65284	80.47265	-470.09368	547.08354	-138.25465	1
22426	H	84.43969	95.21124	80.24889	546.03886	1353.24138	2296.64612	1
22427	H	85.43756	96.75422	80.20742	-1276.89031	-787.70605	-958.02587	1
22428	N	86.43741	95.12376	79.59301	-66.35280	686.66940	-994.19739	1
22429	H	87.41933	95.06166	79.75073	155.60772	1487.42556	1477.30016	1
22430	H	86.22885	94.14952	79.28000	-471.10017	-2520.32351	2413.25851	1
22431	H	82.33638	97.15049	79.75446	1180.23863	397.30015	-541.72232	1
22432	C	86.21710	90.97046	84.89859	-547.09997	31.62837	285.23759	1
22433	O	87.42689	90.92744	85.17758	880.09404	-10.75917	-22.50758	1
22434	N	85.23261	90.54869	85.73742	-307.52004	-47.66373	89.72077	1

22435	H	84.33354	90.59697	85.22443	-3134.75807	3744.90075	384.93847	1
22436	C	85.46402	90.37400	87.19070	273.82240	-30.23338	-539.52154	1
22437	H	86.54333	90.40779	87.19448	-963.23670	23.59350	590.70537	1
22438	C	84.90160	91.64905	87.80121	-387.70205	-142.30809	440.64591	1
22439	H	84.23833	92.03449	87.07059	-1206.27676	2820.90470	-1999.80496	1
22440	C	84.13390	91.48142	89.09493	-661.78409	-102.09969	659.57122	1
22441	H	84.13212	92.46606	89.67547	1915.99031	-1927.46977	-4033.81104	1
22442	H	84.47548	90.60888	89.75094	1062.79827	-183.29642	2216.62970	1
22443	H	82.99372	91.22942	88.88161	-394.52049	1623.68602	-168.69235	1
22444	C	85.84509	92.79359	87.96260	-385.57064	-235.10417	663.83925	1
22445	H	86.56488	93.02472	87.03986	241.39968	-1258.80969	-275.27290	1
22446	H	85.19736	93.76116	88.02391	-2195.24364	980.68477	1532.47116	1
22447	C	86.76719	92.53530	89.27960	-207.69340	-1330.67564	324.07684	1
22448	H	87.10120	93.45001	89.78720	421.98278	1786.38197	1072.15093	1
22449	H	86.31600	91.85913	90.07478	-725.54306	-5058.74660	-1607.70255	1
22450	H	87.68663	91.93452	88.87668	1411.76495	1124.08944	-2527.37077	1
22451	C	84.87118	88.94213	87.71093	-896.51304	-246.73407	382.23841	1
22452	O	85.65784	88.17975	88.32350	193.37737	-894.78716	-122.67415	1
22453	N	83.58619	88.77567	87.59792	1093.43966	553.36882	-107.58249	1
22454	H	83.09825	89.47047	86.94994	-64.17769	879.53991	797.02767	1
22455	C	83.07007	87.47407	87.80493	-622.92479	-807.60729	1011.55303	1
22456	H	83.64315	87.06201	88.75101	-492.12987	-1986.17219	-182.20486	1
22457	C	81.46714	87.49078	87.83321	-288.91300	583.92117	-957.42825	1
22458	H	81.05347	87.70334	86.85512	-2633.86706	-1175.72458	3198.18215	1
22459	H	81.22925	88.36413	88.43554	105.63844	-118.35809	-821.74968	1
22460	C	80.87235	86.21378	88.43231	15.92383	275.06605	-149.12959	1
22461	C	80.08906	85.45832	87.51308	-366.79674	-54.20568	144.96127	1
22462	H	80.15697	85.63583	86.43094	1529.33675	1170.75891	1719.60662	1
22463	C	79.40000	84.34180	88.00890	144.47270	-887.62377	-155.87244	1
22464	H	78.84100	83.76780	87.28590	-328.20360	-2959.33355	1021.19185	1
22465	C	79.47800	83.93480	89.35490	-642.70599	451.43486	-466.81034	1
22466	H	78.96900	83.02580	89.64090	-635.63027	-442.27836	3049.76432	1
22467	C	80.89855	85.83743	89.79786	-319.02389	497.77724	-89.36843	1
22468	H	81.49328	86.49872	90.45860	2493.60593	-50.99685	-1567.40258	1
22469	C	80.30600	84.65280	90.26790	21.13127	-626.18118	-664.90332	1
22470	H	80.48200	84.28180	91.26690	-2377.19387	-1194.15714	-1686.65329	1
22471	C	83.60197	86.45064	86.63845	-25.77900	838.22299	-149.54524	1
22472	O	83.97917	85.31982	86.89383	-220.54744	494.03394	-217.86666	1
22473	N	83.51588	87.05347	85.44948	-957.47487	-435.22926	748.28055	1
22474	H	83.22605	88.04717	85.30736	1465.79316	807.63552	1049.39588	1
22475	C	83.56315	86.17126	84.34821	291.68538	-773.96385	106.22598	1
22476	H	83.09334	85.22339	84.74479	-685.17615	258.46170	1857.47454	1
22477	C	82.81127	86.86743	83.08177	-10.73207	1076.77546	-126.45154	1
22478	H	82.91985	86.28725	82.13169	358.26945	1506.66533	1182.35941	1
22479	H	83.25034	87.87231	82.95281	-317.90326	-1053.25903	-620.00622	1
22480	C	81.39895	87.06507	83.49578	-62.06920	-473.53789	-335.28456	1
22481	H	81.36392	87.78324	84.32997	-647.83008	-1119.75730	-1765.66262	1
22482	C	80.49944	87.53490	82.33985	6.60934	360.03783	-361.21402	1
22483	H	79.63077	88.06057	82.77632	-2819.75041	-2157.01096	861.67884	1
22484	H	80.12548	86.62192	81.72971	-7.59899	46.03381	-807.29065	1
22485	H	81.04179	88.19123	81.57115	-1774.73727	-27.37210	4128.31565	1
22486	C	80.73265	85.83593	84.02411	-169.16290	284.12977	-456.20011	1
22487	H	80.89050	84.96342	83.29340	286.52784	585.67608	209.20981	1
22488	H	79.63673	85.97120	84.28645	-2332.99081	-1367.29310	-1473.82913	1
22489	H	81.21310	85.47940	85.01243	535.73665	1440.12412	2222.71504	1
22490	C	84.97050	85.42580	84.08910	-618.42842	453.49170	354.66888	1
22491	O	84.87300	84.21580	83.92590	484.78819	-232.13709	572.07571	1
22492	N	86.12930	86.17096	84.09543	153.90626	45.96841	-849.03839	1
22493	C	86.12880	87.62375	84.01711	358.39009	-117.03198	-430.31917	1
22494	H	85.46759	88.00802	84.77338	-1591.87877	-343.94192	-1019.99035	1
22495	H	85.84027	87.96422	82.96547	-764.50073	733.71711	1325.72909	1
22496	C	87.36441	85.48325	84.17263	-176.15204	-357.14120	513.98821	1

22497	H	87.36000	84.75980	83.39390	-1956.53740	-1725.16788	-1765.99997	1
22498	C	88.42126	86.67844	84.00957	91.13787	-141.38902	-436.60274	1
22499	H	88.47648	86.84181	82.84984	-455.27567	598.16659	487.41328	1
22500	H	89.44501	86.60855	84.41165	755.09659	2723.08520	2954.96718	1
22501	C	87.65825	87.96618	84.43206	888.24717	93.88292	302.95916	1
22502	H	87.70869	88.16419	85.51434	517.63815	-1823.36608	-119.87270	1
22503	H	87.93646	88.96573	83.91536	1414.05268	2724.84233	2656.68488	1
22504	C	87.49300	84.44880	85.47990	481.17713	-770.68342	-26.39082	1
22505	O	88.17500	83.43780	85.31690	662.28783	338.86154	-256.54544	1
22506	N	86.94800	84.79480	86.61690	-355.77024	360.43447	-679.89734	1
22507	H	86.39149	85.66438	86.55155	42.78695	-57.62288	2525.52023	1
22508	C	86.99100	84.05980	87.81290	748.44016	418.03311	-302.26836	1
22509	H	88.04200	83.90580	88.00490	-1286.35492	1354.34724	-2536.24087	1
22510	C	86.54200	84.90880	89.03390	418.38191	558.35263	-585.25714	1
22511	H	85.52100	85.32684	88.81898	1615.25536	-410.82888	-1567.42418	1
22512	O	87.39151	86.34049	89.24641	755.00968	-207.58450	15.02082	1
22513	H	86.61062	86.91452	89.07289	-233.07622	1629.78125	-375.47630	1
22514	C	86.58800	84.13880	90.31390	-283.70739	860.17132	100.11513	1
22515	H	86.42200	84.88380	91.12190	-1795.94078	1435.55542	2147.21644	1
22516	H	87.58000	83.65880	90.45790	-435.86088	1217.30768	2865.37132	1
22517	H	85.87300	83.28880	90.33790	847.17946	-2925.10475	789.94646	1
22518	C	86.28000	82.71080	87.71290	348.70998	-610.39722	-581.61753	1
22519	O	86.82200	81.66680	88.07090	487.52202	-368.28329	-500.33258	1
22520	N	85.01900	82.70380	87.12790	147.88702	116.27934	-824.53825	1
22521	H	84.59100	83.60380	87.13890	-2674.73959	1532.87730	-646.48648	1
22522	C	84.34600	81.49680	86.73990	-173.64911	895.38896	-18.27396	1
22523	H	84.30700	80.75780	87.52590	2626.33703	724.73484	-1569.57992	1
22524	C	82.88500	81.78680	86.44690	472.40232	489.18323	601.57630	1
22525	H	82.91900	82.67580	85.78090	-1567.70870	-1396.99338	2344.15697	1
22526	C	82.17700	80.62380	85.67890	-686.10317	-556.20421	-242.24390	1
22527	H	81.07800	80.71880	85.54690	598.41109	-2089.90955	-2275.59134	1
22528	H	82.70400	80.35880	84.73790	461.08637	2498.75301	-1856.94623	1
22529	H	82.32100	79.72080	86.31090	1404.57528	-2171.67960	1786.11393	1
22530	C	82.07000	82.12980	87.72690	829.91579	-260.36295	260.76104	1
22531	H	81.10200	82.37580	87.23990	2005.26066	-1846.06125	-1568.82272	1
22532	H	82.53400	83.06080	88.11890	1997.51249	-773.18170	2299.81178	1
22533	C	81.94500	81.05480	88.81990	-714.77797	295.25802	-489.47011	1
22534	H	82.88100	80.59980	89.20790	-591.02561	3050.46585	-490.56526	1
22535	H	81.31400	80.20680	88.47790	2815.64469	-509.29682	1298.78701	1
22536	H	81.40000	81.55980	89.64590	-697.87421	-1644.06384	2590.27197	1
22537	C	85.05200	80.71580	85.59890	-8.53369	117.84609	-907.35201	1
22538	O	85.24900	79.52680	85.71490	28.89394	785.85224	67.89789	1
22539	N	85.49400	81.43280	84.53190	-394.64883	-637.49170	-394.75551	1
22540	H	85.40200	82.42480	84.48490	-917.73706	-3005.42708	-172.11869	1
22541	C	86.03100	80.79380	83.32290	-685.05291	-509.53067	325.44447	1
22542	H	85.31500	80.12480	82.86790	2087.93761	-1749.15828	1563.17221	1
22543	C	86.55300	81.83280	82.24690	-285.42760	680.70566	-543.31346	1
22544	H	87.16500	81.34780	81.45690	-406.93343	1249.33627	2856.78426	1
22545	H	87.19100	82.46680	82.89890	-1420.16195	-2746.04582	586.62255	1
22546	C	85.50700	82.73980	81.58390	-387.37410	-516.39031	-648.51176	1
22547	C	84.15500	82.39380	81.53690	8.37560	738.15855	534.98096	1
22548	H	83.79200	81.55280	82.10890	-1976.71996	-503.22493	-2401.95861	1
22549	C	83.21100	83.32080	80.93390	-813.75607	351.40567	-239.32063	1
22550	H	82.15600	83.09880	80.98090	2035.65888	1768.92256	-1615.98393	1
22551	C	83.64600	84.52480	80.37890	772.34234	-27.95156	472.41300	1
22552	O	82.63286	85.38866	79.71513	-72.91453	-692.21879	794.11456	1
22553	H	81.83700	84.81180	79.82390	-1080.08605	-2322.12039	1828.02480	1
22554	C	85.92600	83.94280	80.96390	6.05711	-903.27024	-110.87849	1
22555	H	86.96400	84.21780	81.07890	2829.27439	-598.86941	-1226.46106	1
22556	C	84.98800	84.82180	80.36790	-678.00518	496.60885	-369.86313	1
22557	H	85.36288	85.72646	79.87650	-3353.73306	-584.27113	-2761.13606	1
22558	C	87.28100	79.90080	83.70090	-602.48169	658.69385	-208.30911	1

22559	O	87.52500	78.85780	83.08590	-549.44032	561.74256	109.17800	1
22560	N	88.11400	80.46780	84.61090	642.96512	513.19753	-179.98725	1
22561	H	87.81200	81.38580	84.85490	554.47561	2851.08366	1205.19199	1
22562	C	89.22100	79.75680	85.24590	-801.90495	437.56083	62.18517	1
22563	H	89.95300	79.50280	84.49390	-1464.51312	-2546.38990	1124.84143	1
22564	C	89.96200	80.65580	86.28690	-458.29519	-343.52332	707.42201	1
22565	H	90.83200	80.05380	86.62590	2283.07377	-336.40392	-2139.03685	1
22566	H	89.32800	80.96580	87.14490	931.33406	2257.02425	-1986.55878	1
22567	O	90.43900	81.84080	85.66990	610.32611	92.12801	483.01903	1
22568	H	89.67500	82.42080	85.62090	2369.02049	-1179.21299	1691.04846	1
22569	C	88.73400	78.47380	85.93690	-909.04626	101.73149	39.15022	1
22570	O	89.25800	77.41880	85.68690	452.12303	480.50776	425.07062	1
22571	N	87.62200	78.53080	86.72490	-701.95005	282.62632	-385.82932	1
22572	H	87.11900	79.38180	86.85290	1745.97851	2397.36485	-1047.62160	1
22573	C	87.01300	77.34680	87.36090	-113.26819	694.01660	575.81346	1
22574	H	87.78600	76.78980	87.87090	2151.54835	2266.77734	334.12137	1
22575	C	85.83700	77.64780	88.31690	-573.33049	-363.66500	-616.67497	1
22576	H	85.15200	78.26580	87.69790	2170.45817	953.65837	2060.27926	1
22577	C	85.23200	76.35180	88.91690	-584.42856	628.39546	-316.18304	1
22578	H	84.85900	75.70780	88.09290	1913.26524	866.71986	-2344.55790	1
22579	H	85.99500	75.79680	89.50290	-1848.14339	-1493.28883	2060.17481	1
22580	H	84.35600	76.61180	89.54990	-674.86039	3069.33543	124.10768	1
22581	C	86.39100	78.49780	89.48490	354.02269	771.95453	-330.31748	1
22582	H	87.06500	79.27980	89.07290	1427.84035	-2198.47053	-1742.42291	1
22583	H	87.08200	77.89680	90.11390	-991.08893	-1148.86745	2752.86447	1
22584	C	85.32100	79.24980	90.26490	548.11549	-645.98527	-339.45320	1
22585	H	85.66100	79.80480	91.16590	-1839.58327	-1095.46754	2304.62952	1
22586	H	84.50800	78.55480	90.56390	2588.94393	367.32088	-1748.92652	1
22587	H	84.81600	79.99880	89.61990	942.94869	-1655.61062	-2506.74063	1
22588	C	86.59100	76.33380	86.29590	37.20179	705.09135	-582.03551	1
22589	O	86.87600	75.13580	86.32990	263.40507	-247.17595	-706.70502	1
22590	N	85.94400	76.86980	85.20790	-715.74336	-4.18375	448.95949	1
22591	H	85.63800	77.81680	85.14890	838.32427	1784.43455	-2455.06733	1
22592	C	85.54400	75.97380	84.09090	-589.85106	56.62431	-701.66531	1
22593	H	84.97100	75.16780	84.52390	-590.84555	-2292.32178	-2078.06839	1
22594	C	84.70500	76.68680	83.02590	812.00035	-153.54614	-379.98876	1
22595	H	85.34800	77.43880	82.51990	-2032.51842	-1169.11159	-2105.97809	1
22596	C	84.27500	75.71480	81.91990	385.98328	-7.71678	819.03347	1
22597	H	85.09700	75.06980	81.54390	-1047.85130	1847.31625	-2329.86050	1
22598	H	83.47900	75.04880	82.31590	-1135.20078	2167.35756	1976.83175	1
22599	H	83.83700	76.40380	81.16690	-1221.64390	-1777.21280	-2296.52661	1
22600	C	83.45000	77.48980	83.55590	415.02904	385.08012	708.60650	1
22601	H	82.97200	77.88180	82.63290	2751.84028	500.29216	1428.17904	1
22602	H	83.89400	78.25780	84.22490	-2555.14716	-1013.25557	-1541.31490	1
22603	C	82.33100	76.72480	84.30590	-573.33093	-645.33268	-305.08700	1
22604	H	81.47300	77.36780	84.59690	621.70489	408.45907	3052.63070	1
22605	H	82.01000	75.87880	83.66190	-2558.93167	-332.97762	1801.47885	1
22606	H	82.78500	76.35380	85.24990	1982.50157	2424.49246	-276.77835	1
22607	C	86.82000	75.33080	83.39190	633.64313	7.37543	645.91442	1
22608	O	86.93000	74.10180	83.14490	-603.25143	514.93996	22.36745	1
22609	N	87.87300	76.12580	83.05390	-668.26296	292.10033	-438.63187	1
22610	H	87.78700	77.10580	83.21590	964.78945	2390.24356	1798.08006	1
22611	C	89.14600	75.69580	82.51290	626.46137	150.81961	-647.37545	1
22612	H	88.77200	75.17380	81.64490	1618.39587	-2060.16562	-1741.49121	1
22613	C	89.90200	76.92480	82.03590	424.59801	564.74533	-580.80130	1
22614	H	89.27500	77.50780	81.32890	-1811.25018	1035.66443	2354.13974	1
22615	H	90.24800	77.70980	82.74190	964.18930	-2105.74945	2119.73999	1
22616	C	91.23100	76.59480	81.38190	330.76457	-775.30707	330.92615	1
22617	C	91.21500	76.27080	80.01490	-28.59772	910.50041	79.53944	1
22618	H	90.34000	76.17680	79.38890	-472.92306	-1957.49942	-2421.96958	1
22619	C	92.38300	75.83580	79.33690	118.94082	106.98705	890.39808	1
22620	H	92.23500	75.47680	78.32890	1776.04172	-2559.66751	-397.81678	1

22621	C	93.59700	75.74780	79.99190	624.25308	-211.62993	-631.08708	1
22622	H	94.46100	75.44580	79.41890	-286.74729	2950.04185	1059.05801	1
22623	C	92.48600	76.63880	82.03490	847.11558	317.80017	-86.34671	1
22624	H	92.45700	76.91580	83.07890	1214.48412	-2333.47331	1713.23095	1
22625	C	93.65300	76.24480	81.37190	115.99903	622.16726	651.06787	1
22626	H	94.58100	76.33180	81.91690	2963.59074	-681.12503	779.80069	1
22627	C	89.91100	74.63880	83.25790	-903.35201	-96.10774	108.68106	1
22628	O	90.31700	73.58680	82.77890	109.23489	594.74348	-516.45866	1
22629	N	90.07200	74.84380	84.60690	-68.67408	765.07853	-360.08800	1
22630	H	89.75100	75.72580	84.94490	-1906.82177	2504.33977	93.67718	1
22631	C	90.99200	74.14780	85.47890	172.71877	834.47793	317.70845	1
22632	H	91.87600	73.95580	84.88990	-1942.47029	1232.11708	2142.81582	1
22633	C	91.44100	74.96580	86.68890	169.75461	895.44451	-32.20202	1
22634	H	90.54900	75.39680	87.18990	1716.23254	-1244.50565	-2328.82035	1
22635	H	91.98500	74.47680	87.52490	-143.93812	3114.14148	-434.24383	1
22636	C	92.29500	76.20180	86.29890	-752.76381	-253.55780	446.41399	1
22637	H	91.81200	76.81980	85.51190	2489.39924	790.71973	-1755.28764	1
22638	C	92.49600	77.08680	87.49090	612.60728	-40.83853	664.57138	1
22639	H	93.34000	76.67480	88.08490	-647.51045	2185.19990	-2176.92106	1
22640	H	92.75900	78.11980	87.17690	-2283.80133	-591.50604	-2091.43735	1
22641	H	91.62000	77.10680	88.17290	-2016.74418	1687.67690	1724.41877	1
22642	C	93.63900	75.80880	85.71290	-666.17844	-596.80161	179.52286	1
22643	H	94.39500	76.62280	85.73390	2421.79571	-1272.66991	-1553.85365	1
22644	H	94.08800	74.94380	86.24590	214.75996	-1963.48001	2439.94516	1
22645	H	93.51200	75.52980	84.64590	2276.70286	1360.53574	-1695.68753	1
22646	C	90.49500	72.83780	85.92890	-814.14824	-84.26131	400.54954	1
22647	O	91.27500	71.96380	86.38890	-132.46349	-268.58705	722.86785	1
22648	N	89.19100	72.60280	85.69690	-255.16401	122.08979	789.17282	1
22649	H	88.59100	73.30280	85.31790	39.89389	-3144.60655	-66.45142	1
22650	C	88.45900	71.35680	85.94490	723.48278	-371.94380	398.59829	1
22651	H	89.12800	70.64180	86.40090	2330.53934	-2080.58670	343.46997	1
22652	C	87.22600	71.64880	86.78490	628.93547	105.95190	641.74511	1
22653	H	86.71000	70.67580	86.92890	-1832.19757	1647.43117	1951.24989	1
22654	O	86.29500	72.52080	86.19690	718.99266	-294.92835	116.77926	1
22655	H	86.60700	73.42780	86.23990	269.56486	493.91441	-3101.48944	1
22656	C	87.61600	72.22880	88.17090	-738.48817	-496.03654	-217.47822	1
22657	H	86.73200	72.42180	88.81590	-1087.52799	2935.07605	310.64735	1
22658	H	88.12700	73.21380	88.10690	-37.72906	-1909.23681	2493.87076	1
22659	H	88.25200	71.51380	88.73390	1025.24679	2136.63130	-2074.96968	1
22660	C	88.17800	70.69480	84.65590	-50.45776	572.17860	-716.90844	1
22661	O	88.41700	69.53780	84.41390	232.33051	-360.22923	-669.87632	1
22662	N	87.69700	71.45480	83.66790	-645.41248	347.13244	-432.94398	1
22663	H	87.49600	72.42580	83.77290	2619.81576	493.36611	1658.26441	1
22664	C	87.33000	70.99180	82.32790	-518.85451	-528.09049	-541.94431	1
22665	H	86.87200	71.79880	81.77690	-1052.25888	-1586.80486	2498.18214	1
22666	H	86.53900	70.25880	82.39390	3133.90996	-192.42974	116.21042	1
22667	C	88.38800	70.38780	81.46990	-134.42879	-887.79751	-158.04236	1
22668	O	88.07800	69.34780	80.89690	-373.16759	-566.26035	396.88793	1
22669	N	89.50700	71.10180	81.21690	-382.56945	-571.82143	481.75427	1
22670	H	89.71200	71.85980	81.82990	-624.86721	-1575.02937	2642.79307	1
22671	C	90.54000	70.62380	80.30890	-326.05866	684.89496	504.16750	1
22672	H	90.04700	70.37080	79.38190	2545.99165	-1528.54897	1014.57343	1
22673	C	91.49700	71.77680	80.00190	-689.53880	-166.98733	569.17932	1
22674	H	90.87200	72.69580	80.01990	-280.02924	2907.79365	-1184.42513	1
22675	C	92.63800	71.97780	81.09890	357.68200	827.09032	136.09454	1
22676	H	93.11400	72.96780	80.93290	-1450.60608	-648.23368	2708.93437	1
22677	H	93.41500	71.18380	81.09390	-1779.50368	-142.04318	-2602.43373	1
22678	H	92.18000	72.00080	82.11090	2932.36592	-375.46993	1055.84134	1
22679	C	92.06200	71.74980	78.55590	277.79333	-287.01938	808.22593	1
22680	H	91.23500	71.68480	77.81690	-1773.01643	2094.85048	1541.24861	1
22681	H	92.43600	72.79180	78.45790	-1700.52523	2130.76431	1572.99887	1
22682	C	93.19900	70.75380	78.20890	621.50515	-557.64419	-360.59341	1

22683	H	94.09500	70.93880	78.83990	-2529.67869	389.04233	-1846.44203	1
22684	H	93.64100	70.73480	77.18990	897.29307	-2274.97275	1962.54830	1
22685	H	92.87200	69.72480	78.47090	-2542.31628	637.72588	1739.11216	1
22686	C	91.19200	69.33780	80.85890	-849.95865	43.45862	328.99050	1
22687	O	91.46200	68.34780	80.13890	-217.10709	678.60722	-358.65655	1
22688	N	91.48600	69.32480	82.18790	-416.88690	596.93588	-443.17047	1
22689	H	91.23100	70.17480	82.64090	2764.92366	-1189.20059	893.24514	1
22690	C	91.91500	68.12480	82.90290	671.36736	-2.87476	-623.06226	1
22691	H	92.79300	67.74880	82.39990	1133.56769	2477.29230	1564.60967	1
22692	C	92.25100	68.54980	84.34890	-626.76818	-215.90569	618.92128	1
22693	H	91.36300	68.83680	84.95190	2028.09572	-2132.98964	-1113.19804	1
22694	C	92.93000	67.35280	85.13090	-40.91579	546.89107	719.26604	1
22695	H	93.39500	67.66780	86.08990	2814.39815	786.43232	-1170.73680	1
22696	H	93.59900	66.86780	84.38790	680.66775	2167.50407	2166.50194	1
22697	H	92.08600	66.72380	85.48590	-1299.95203	-2084.63292	-1976.25914	1
22698	C	93.12200	69.81780	84.36490	-85.87097	-711.85949	-571.20768	1
22699	H	92.59100	70.79080	84.28690	414.67910	-1823.40109	-2537.36238	1
22700	H	93.47800	69.79780	85.41690	-1802.65629	612.34957	-2516.71922	1
22701	H	93.92400	69.74080	83.59990	-2113.48540	-1556.20673	-1746.88212	1
22702	C	90.88500	67.01480	82.85490	-560.17604	643.61302	-340.86267	1
22703	O	91.19100	65.97680	82.31990	575.22684	277.24387	-472.22652	1
22704	N	89.59800	67.27880	83.21290	524.26395	509.00915	411.22306	1
22705	H	89.33800	68.17280	83.56890	-3104.29147	-448.44894	272.40266	1
22706	C	88.50800	66.28280	83.31090	-546.36324	555.93347	468.75313	1
22707	H	87.63400	66.81180	83.66190	-1061.58852	-2934.61204	389.35155	1
22708	H	88.77800	65.52880	84.03490	10.55105	2346.86330	2086.70722	1
22709	C	88.13700	65.55880	82.06790	310.85332	-559.78602	-655.74751	1
22710	O	88.04400	64.34280	82.03790	297.99695	-575.60490	436.46325	1
22711	N	87.94300	66.29480	80.94490	-137.00757	642.44250	-543.31416	1
22712	H	88.08700	67.28080	80.99990	-2816.45071	981.16264	-1023.44780	1
22713	C	87.72000	65.63780	79.67190	409.75527	-523.64252	-628.67610	1
22714	H	87.02600	64.82080	79.79990	1055.26269	209.07024	2945.60613	1
22715	C	86.96700	66.60780	78.71390	-96.50363	174.73197	-899.78714	1
22716	H	87.46400	67.58080	78.50890	3100.41132	83.77961	492.40403	1
22717	H	86.78100	66.01880	77.79090	2244.79463	362.51811	-2179.42405	1
22718	C	85.61000	66.79680	79.39290	253.03182	779.73252	-410.17787	1
22719	O	84.83300	65.81480	79.48890	37.47156	745.08190	256.45328	1
22720	N	85.34400	67.99780	79.87490	288.96529	778.85602	145.97078	1
22721	H	86.08300	68.66580	79.96190	-2090.44743	-1477.05993	1824.28030	1
22722	H	84.39500	68.15680	80.14790	-3078.34110	132.10681	648.47374	1
22723	C	88.89800	64.98780	79.03490	725.56730	379.20971	-407.24982	1
22724	O	88.72200	64.04280	78.34190	-697.68038	357.86740	-140.39072	1
22725	N	90.14400	65.40080	79.46790	206.17005	-788.69204	-214.25132	1
22726	H	90.25700	66.25580	79.96790	-1065.98865	2023.85267	-2174.79194	1
22727	C	91.31700	64.73480	79.05890	93.71269	519.29579	734.58953	1
22728	H	91.30700	64.62180	77.98490	-2931.29772	1154.91559	-86.26070	1
22729	H	92.21500	65.29480	79.27790	1058.09386	-1921.96269	2239.17693	1
22730	C	91.40100	63.43180	79.75790	307.19372	-793.67896	-327.48745	1
22731	O	91.82500	62.42080	79.26990	-580.71505	335.53104	412.68605	1
22732	N	91.02800	63.38680	81.05790	657.76904	157.06926	-513.16336	1
22733	H	90.80500	64.21680	81.56290	-2520.77814	1604.09448	-1008.37858	1
22734	C	90.91800	62.15580	81.79590	272.45577	-732.55007	-476.09448	1
22735	H	91.86200	61.64080	81.70190	-1069.04265	2392.46453	1734.04641	1
22736	C	90.82800	62.40680	83.27890	329.01022	-793.01168	288.14551	1
22737	H	90.54300	61.55180	83.92790	1675.42279	2646.15876	286.61107	1
22738	H	89.92600	63.04680	83.38890	-2288.58946	-1672.21465	1356.64915	1
22739	C	92.01900	63.17780	83.96190	-509.76875	-339.68900	-688.14800	1
22740	H	92.39400	64.07880	83.43090	2369.14348	459.71170	2004.19969	1
22741	C	91.67700	63.61180	85.38990	-429.89384	656.53258	456.35901	1
22742	H	91.21000	62.80180	85.98990	-2954.60133	-361.20843	-1035.64947	1
22743	H	92.58900	63.86880	85.96890	1881.86793	-747.02512	-2417.75690	1
22744	H	90.99500	64.48680	85.45990	-1865.52047	1325.49624	-2172.38385	1

22745	C	93.24800	62.26580	83.90690	393.27022	144.47070	796.69234	1
22746	H	93.04800	61.32980	84.47190	2317.86464	-1499.53353	1491.55401	1
22747	H	94.12500	62.84280	84.26990	-1441.26038	1876.80917	-2088.92882	1
22748	H	93.55700	61.98580	82.87690	1526.72314	1894.80110	1981.84056	1
22749	C	89.83700	61.22880	81.39190	-673.56171	392.29999	-491.00902	1
22750	O	90.05200	60.01880	81.38790	778.59487	-101.80623	35.24678	1
22751	N	88.67800	61.73480	81.04490	327.52024	-212.84915	735.04661	1
22752	H	88.46700	62.70780	81.09490	-1224.48454	-2122.30223	1962.12456	1
22753	C	87.67100	60.85880	80.39390	537.35759	463.01271	560.59986	1
22754	H	87.32000	60.08580	81.06090	-2112.67471	422.44166	-2307.29397	1
22755	C	86.36900	61.62080	80.15290	433.87130	380.64547	694.38434	1
22756	H	86.66700	62.53680	79.59990	-935.20663	-1903.33518	2312.79831	1
22757	C	85.41000	60.79180	79.24990	-43.61770	142.25521	-910.99776	1
22758	H	85.78800	60.71980	78.20790	-341.41829	2236.52582	2178.93898	1
22759	H	84.42100	61.27980	79.11590	-2235.95014	1459.15621	1660.75727	1
22760	H	85.21300	59.82180	79.75490	-1558.88322	-962.09369	-2570.00536	1
22761	C	85.66900	62.05280	81.46790	56.95089	166.44982	884.42928	1
22762	H	84.86800	62.78280	81.22090	2285.82367	-973.61446	-1935.38889	1
22763	H	85.26400	61.20280	82.05790	1415.76207	-210.19905	-2810.85385	1
22764	H	86.41700	62.61580	82.06690	1683.88527	1797.32319	-1967.03297	1
22765	C	88.14800	60.21080	79.10090	-464.01205	410.83459	661.23382	1
22766	O	87.98300	59.02080	78.84890	-681.96966	364.92232	-191.34311	1
22767	N	88.93200	60.97080	78.26790	599.50119	-481.08076	-349.45192	1
22768	H	88.88200	61.95180	78.43890	946.20447	-2007.23967	-2236.91977	1
22769	C	89.63900	60.42180	77.09990	721.30426	370.11921	401.85220	1
22770	H	88.99200	59.82980	76.46890	-2641.09457	-774.16600	-1541.37773	1
22771	C	90.13200	61.55680	76.21090	-249.73876	332.90145	-826.21242	1
22772	H	90.77500	62.20780	76.84090	2383.78880	1979.62664	-553.06215	1
22773	C	91.04800	61.07380	75.04890	-458.90769	-400.75647	-690.82362	1
22774	H	91.94600	60.50580	75.37390	-1643.60510	-2667.34882	252.83678	1
22775	H	91.50200	61.91580	74.48490	2373.47000	2040.78215	301.13448	1
22776	H	90.55600	60.35680	74.35590	-889.18090	-323.61543	-3013.67162	1
22777	C	89.00800	62.48180	75.66090	2.41465	571.42336	702.92004	1
22778	H	88.47400	61.93980	74.85190	2608.02503	-1680.09225	-494.18834	1
22779	H	88.14100	62.60780	76.34490	-2635.58262	-1486.42667	-879.13109	1
22780	C	89.53000	63.78780	75.11390	-558.13061	-410.42923	583.44340	1
22781	H	90.19400	63.52080	74.26490	937.78538	-2995.70759	55.39792	1
22782	H	88.68400	64.35180	74.66590	-2111.45304	2271.08343	-580.65405	1
22783	H	89.97900	64.42080	75.90890	-2577.15885	1659.78578	-746.17560	1
22784	C	90.77300	59.45680	77.46190	329.05637	-605.52153	-603.74000	1
22785	O	90.96700	58.38780	76.89490	-36.89162	742.63305	264.66326	1
22786	N	91.47500	59.73380	78.58890	-209.46183	-458.02523	663.27245	1
22787	H	91.42900	60.64380	78.99590	1673.14064	1715.00203	2026.56494	1
22788	C	92.46700	58.82380	79.17890	-728.08068	-472.04575	-296.01746	1
22789	H	93.13400	58.59180	78.36190	-2157.87647	2202.47670	-663.86227	1
22790	C	93.39400	59.54580	80.25190	-730.45366	-63.40790	532.29891	1
22791	H	93.67500	58.93680	81.13790	-480.11514	1903.19728	2447.81206	1
22792	H	92.68800	60.32980	80.60090	-1888.57015	2442.64555	-638.24877	1
22793	C	94.60100	60.20980	79.64990	-3.17038	139.77363	-915.12005	1
22794	H	94.23900	60.46180	78.62990	-1497.82791	2213.14065	-1682.09542	1
22795	C	95.06300	61.43480	80.47190	178.10144	820.46697	-374.98231	1
22796	H	95.28300	61.04180	81.48790	-1714.68042	-2400.28468	1078.48133	1
22797	H	94.26400	62.20680	80.47790	-1642.19514	-1985.67416	-1817.20160	1
22798	H	96.00300	61.82780	80.02690	786.27561	-1751.03237	2475.87270	1
22799	C	95.76500	59.20580	79.52190	-727.03968	518.79853	191.27898	1
22800	H	96.08900	58.91780	80.54590	-2582.50637	1683.27393	635.04484	1
22801	H	95.53700	58.21280	79.07790	1394.79679	-2449.70895	1372.41442	1
22802	H	96.53300	59.68580	78.87890	588.50767	-2902.94354	1033.01070	1
22803	C	91.86500	57.57880	79.69390	-585.46378	-299.95709	-646.33610	1
22804	O	92.42900	56.49880	79.48290	532.95971	-21.51262	-593.94772	1
22805	N	90.65400	57.56080	80.28190	-384.15772	-693.58104	273.19261	1
22806	H	90.21300	58.42780	80.50190	-2076.92091	2030.04528	-1232.07644	1

22807	C	89.92200	56.39580	80.60690	-271.79873	-30.09409	-884.24767	1
22808	H	90.56100	55.73180	81.16890	2607.64521	-681.42523	-1632.40807	1
22809	C	88.72200	56.64380	81.52490	-258.24014	820.33596	-323.89875	1
22810	H	88.11700	57.51680	81.19890	-2203.02400	-869.90295	2059.72808	1
22811	C	87.81900	55.37180	81.65790	-272.15218	310.67785	-827.90045	1
22812	H	87.24900	55.30580	80.70590	-1681.65973	2607.81144	524.33392	1
22813	H	88.39100	54.44580	81.87890	2323.15910	1311.67298	-1680.44588	1
22814	H	87.10100	55.43280	82.50390	1539.72277	-1894.79062	-1994.62403	1
22815	C	89.30500	57.08480	82.90890	-337.14599	788.76436	-328.88430	1
22816	H	89.91800	58.00280	82.78290	2330.12044	611.44628	-2034.77314	1
22817	H	89.92900	56.23680	83.26390	-1970.49449	1710.20878	1747.79753	1
22818	H	88.39800	57.27180	83.52290	-1982.06179	-1725.43340	-1743.61534	1
22819	C	89.44700	55.63980	79.32990	-362.02130	579.39707	594.58887	1
22820	O	89.89800	54.49180	79.18290	-452.31241	651.48165	18.98527	1
22821	N	88.71500	56.24380	78.37590	-690.63293	365.25085	-343.51006	1
22822	H	88.39800	57.18380	78.48190	-1685.49488	-206.93043	-2663.24163	1
22823	C	88.13600	55.43780	77.35890	478.36241	-511.56873	-591.56564	1
22824	H	87.98700	54.42380	77.69790	2164.42108	1548.30737	-1691.41299	1
22825	C	86.80000	55.99480	76.89190	514.99122	-65.87512	733.87699	1
22826	H	86.79700	57.04880	76.53890	-1147.62899	2799.00795	-893.68217	1
22827	H	86.30400	55.48680	76.03690	1251.33634	2537.35880	-1393.27456	1
22828	C	85.67600	55.90280	77.97190	-487.62758	-147.45835	744.92118	1
22829	H	86.01400	56.61080	78.75890	1868.93221	1230.59661	2198.00104	1
22830	H	85.62800	54.90080	78.44890	-2221.71982	1005.34716	1979.39634	1
22831	S	83.95900	56.24880	77.57990	-408.26724	-141.71723	343.17326	1
22832	C	84.12800	58.00880	77.20090	-200.84187	-506.55809	-741.40743	1
22833	H	83.24300	58.67880	77.24590	-417.77200	-2977.18794	908.17125	1
22834	H	84.54900	58.20380	76.19090	407.55617	2086.46621	-2333.35067	1
22835	H	84.85200	58.45580	77.91490	2083.96667	1036.17712	-2126.57726	1
22836	C	89.02800	55.25480	76.12090	448.45100	-399.40198	-695.23347	1
22837	O	88.67300	54.33880	75.34490	-486.05266	221.26994	-600.58136	1
22838	N	90.17100	55.99680	75.92590	-671.16278	-218.14259	452.58388	1
22839	H	90.45000	56.78180	76.47390	1344.22147	2731.26508	-816.79921	1
22840	C	91.03600	55.84080	74.74190	-893.83321	196.54963	-68.61397	1
22841	H	91.33000	56.77180	74.28090	-1591.12168	302.17210	-2714.27866	1
22842	H	90.59400	55.18780	74.00390	-576.40564	2947.00891	943.08605	1
22843	C	92.32500	55.26980	75.05690	633.10786	-635.66830	108.59183	1
22844	O	92.92800	54.78180	74.07790	-203.32699	-693.29440	294.05873	1
22845	N	92.85900	55.28180	76.31390	-423.77072	-721.99708	74.73643	1
22846	H	92.39700	55.80080	77.02990	-2182.92949	-317.00795	2231.41823	1
22847	C	94.18600	54.76780	76.54990	-519.65626	741.53402	-163.87150	1
22848	H	94.42000	54.19980	75.66190	2042.92389	2186.73409	-990.76277	1
22849	C	95.24000	55.87480	76.84190	-406.83065	773.69858	-293.62934	1
22850	H	96.23400	55.39980	76.97990	1640.53249	998.87294	-2507.31248	1
22851	H	94.96800	56.43880	77.75990	1804.08947	-533.91802	-2533.35478	1
22852	C	95.32500	56.83880	75.67490	654.95474	604.67323	-210.00064	1
22853	C	94.57400	58.04680	75.56990	731.71339	-400.11289	340.42540	1
22854	H	93.81100	58.35680	76.26890	1621.81396	-2627.07086	559.19251	1
22855	C	94.76300	58.89280	74.47790	-425.21057	-262.96070	-777.13733	1
22856	H	94.19800	59.78980	74.27190	-2214.85488	878.17117	2048.42730	1
22857	C	95.64700	58.60780	73.44990	412.56078	587.45763	550.72522	1
22858	O	95.87200	59.44180	72.41690	-560.11085	-357.88667	413.39932	1
22859	H	96.32200	59.00280	71.69190	1955.31868	-1688.47311	1768.93106	1
22860	C	96.26800	56.58880	74.66090	-711.29179	-522.03013	-245.19670	1
22861	H	96.92000	55.72780	74.64290	-1396.08723	234.46085	-2827.95862	1
22862	C	96.40200	57.42980	73.55890	239.36014	-857.17333	-178.26183	1
22863	H	97.07000	57.15380	72.75690	1810.66320	1092.18531	-2344.28853	1
22864	C	94.25100	53.70880	77.63690	514.36361	686.42840	-329.84905	1
22865	O	94.75800	52.60880	77.40090	-419.00787	-618.77781	-265.43881	1
22866	N	93.66100	53.96080	78.80590	254.13132	-668.26441	426.01780	1
22867	H	93.27600	54.86780	78.95390	-1236.76060	-2600.59858	1246.98660	1
22868	C	93.44100	53.00680	79.89090	-601.81432	604.19439	-349.06548	1

22869	H	94.35700	52.47780	80.10790	1825.75358	1578.63553	2002.46595	1
22870	C	92.94400	53.62880	81.25290	443.80576	-393.77199	-705.11153	1
22871	H	92.05600	54.20480	80.91490	1526.44231	1905.07992	1970.59790	1
22872	H	92.64800	52.84180	81.97990	1216.13596	899.36378	2742.98059	1
22873	C	93.94700	54.46080	82.04690	-395.24330	818.29969	91.04556	1
22874	H	94.47900	55.07880	81.29190	-1518.71544	-2747.20600	171.08257	1
22875	H	94.64500	53.84780	82.65590	2441.23361	-1925.35655	446.86464	1
22876	C	93.27700	55.39580	83.02990	-568.93645	45.01388	697.67726	1
22877	O	92.47900	54.97380	83.85390	277.08816	-652.90903	327.84141	1
22878	N	93.52300	56.72180	82.88790	-589.21039	-84.00996	585.73711	1
22879	H	94.41900	57.02380	82.56290	-2099.22431	47.95983	-2359.45524	1
22880	H	92.86000	57.35880	83.28190	1727.88598	366.51408	-2616.65426	1
22881	C	92.57700	51.86780	79.50590	307.03237	599.38574	600.81571	1
22882	O	92.78500	50.65780	79.79990	-588.61236	398.43318	-367.87454	1
22883	N	91.47300	52.18080	78.75590	358.64088	365.81277	655.88441	1
22884	H	91.20800	53.14080	78.70990	2026.38491	266.84928	2374.73414	1
22885	C	90.61600	51.17280	78.07990	622.80050	-485.14990	433.00641	1
22886	H	90.80800	50.23680	78.58390	-2146.65397	-1357.71144	-1872.82504	1
22887	C	89.08300	51.53180	78.20090	474.89020	-646.62861	410.05360	1
22888	H	88.90900	52.51580	77.71390	-2986.90579	-810.46801	559.95488	1
22889	H	88.49600	50.75480	77.66490	385.07431	2813.55053	1345.41743	1
22890	C	88.66600	51.54680	79.65090	-18.59448	730.56480	533.97343	1
22891	H	89.15400	52.39480	80.17690	1410.85715	2459.48343	-1381.03279	1
22892	H	89.07300	50.61780	80.10390	2468.82731	-1052.29292	-1652.96547	1
22893	C	87.13900	51.48180	79.68990	-434.68627	-793.38035	-118.26329	1
22894	H	86.76700	52.34880	79.10290	819.63088	-1656.38513	2529.15828	1
22895	H	86.88900	50.48680	79.26190	-2962.05142	807.77855	684.02838	1
22896	C	86.57500	51.74980	81.08890	624.52108	584.56640	-330.56326	1
22897	H	86.92000	52.73180	81.47690	-1472.39118	2540.31383	-1150.99503	1
22898	H	86.98500	50.92780	81.71390	426.78497	-2562.75313	-1786.33586	1
22899	N	85.12500	51.68880	81.07790	-327.65326	635.94393	-466.28001	1
22900	H	84.77400	50.75480	80.78390	2059.62684	2254.53092	-772.57995	1
22901	H	84.69900	52.02580	81.96490	-2255.66064	-2169.92629	-334.00927	1
22902	H	84.83800	52.34680	80.32490	2700.67518	849.04682	-1383.60262	1
22903	C	90.95300	50.94980	76.60790	-794.82222	419.33478	162.82826	1
22904	O	90.98900	51.89480	75.82090	-480.24644	-339.16292	-542.84198	1
22905	N	91.05100	49.72080	76.17790	-652.42125	402.56880	347.06871	1
22906	H	90.96200	48.97080	76.82890	1455.59256	2352.58446	-1519.18408	1
22907	C	91.29900	49.34780	74.85290	-199.67264	857.49545	240.30770	1
22908	H	91.82800	50.10280	74.28990	806.87489	-479.31523	-3017.74564	1
22909	C	92.38200	48.18380	74.82990	-235.56528	673.22905	-592.82728	1
22910	H	92.07000	47.34480	75.48790	1994.94448	898.40063	2242.64783	1
22911	H	92.30400	47.74580	73.81190	-1465.24917	-2624.07662	902.06909	1
22912	C	93.85500	48.62380	74.83190	-427.43123	622.41207	502.45541	1
22913	H	94.07900	49.05780	73.83490	-1536.79240	-1549.85098	-2281.87548	1
22914	H	94.46100	47.69280	74.87390	-1015.85140	-903.76807	-2854.69531	1
22915	C	94.33100	49.57380	75.99790	-126.33383	754.23628	487.29172	1
22916	H	93.81300	50.55380	75.93290	2513.79348	1869.68758	277.35752	1
22917	H	94.18600	49.06480	76.97490	-1089.28768	2944.09369	-293.96816	1
22918	C	95.82100	49.84980	75.84490	659.12768	340.02034	512.35935	1
22919	H	96.00100	50.55280	75.00390	1606.27959	-835.05304	2551.70036	1
22920	H	96.33200	48.90480	75.56290	-1868.93442	2260.54528	1135.13105	1
22921	N	96.36400	50.35680	77.12790	81.20232	-835.21473	-23.09563	1
22922	H	95.93900	49.92380	77.97290	364.39057	-1843.26879	-2537.64610	1
22923	H	96.24700	51.38080	77.26290	-215.43952	-2413.36853	-2018.75078	1
22924	H	97.39300	50.20580	77.11590	2218.23074	1042.91871	1953.89131	1
22925	C	90.00100	49.00580	74.10290	-649.43109	-428.40477	458.87613	1
22926	O	90.08300	48.49180	72.98190	-112.65898	635.89307	446.27918	1
22927	N	88.81000	49.29580	74.67490	642.13307	-286.88294	443.47643	1
22928	H	88.70200	49.78880	75.53390	-1339.66650	-686.17315	2747.20915	1
22929	C	87.55400	48.97680	74.08890	807.40947	337.23074	236.54092	1
22930	H	87.68600	49.00780	73.01690	1257.58492	-2804.72326	625.85089	1

22931	C	87.15200	47.53380	74.50490	192.69265	-367.55207	-825.43390	1
22932	H	87.00100	47.55280	75.60590	624.95393	-2726.71050	1414.33315	1
22933	H	88.03400	46.90580	74.25790	-297.94061	1842.96608	2519.41907	1
22934	C	85.88800	46.98380	73.78190	-517.72163	-671.48744	-346.92766	1
22935	H	85.04600	47.70380	73.87690	2156.37604	2132.35386	825.17355	1
22936	C	86.19700	46.73680	72.27590	509.88814	-385.04054	628.24096	1
22937	H	86.97300	45.94380	72.21590	754.15993	1558.26217	-2646.15083	1
22938	H	86.79000	47.58380	71.86990	-2373.73063	8.06651	2052.89856	1
22939	H	85.32100	46.35980	71.70490	1416.40800	2205.52311	-1760.23517	1
22940	C	85.44900	45.69380	74.43390	-575.59521	-683.72804	156.05618	1
22941	H	86.17400	44.86080	74.31090	-2599.21855	1299.81467	1198.89010	1
22942	H	84.50200	45.40480	73.93090	-2901.17415	-258.25554	-1211.83336	1
22943	H	85.30700	45.81980	75.52790	-2860.55318	-599.22074	1152.23141	1
22944	C	86.58300	49.95080	74.48290	467.10690	40.38841	765.05519	1
22945	O	86.54200	50.31480	75.64190	-591.60520	473.35718	-253.86202	1
22946	N	85.76300	50.38280	73.53390	70.85480	-808.54208	198.73130	1
22947	H	85.97600	50.05580	72.61690	1801.88911	1550.27901	2046.56587	1
22948	C	84.62100	51.21080	73.67290	-169.02506	-438.56183	-793.81836	1
22949	H	84.52300	51.36680	74.73690	-1670.48822	2606.29968	-604.10162	1
22950	C	84.88700	52.61880	73.07790	867.09297	228.53306	-163.98279	1
22951	H	83.94100	53.16780	72.88390	1366.84042	587.76508	2757.73719	1
22952	H	85.25400	52.43280	72.04590	-1943.23716	-81.37147	-2490.07071	1
22953	C	85.88700	53.42880	73.88690	641.21360	-636.33986	52.33474	1
22954	H	86.80800	52.87480	74.16590	-296.71855	2776.83533	-1472.81840	1
22955	H	85.38700	53.70380	74.83990	-224.50653	2919.51661	-1175.67359	1
22956	C	86.28500	54.67180	73.14490	-50.67725	-647.09072	-649.04509	1
22957	H	85.41500	55.31380	72.88890	967.76638	2325.71282	-1901.62633	1
22958	H	86.96800	55.30180	73.75390	1562.55506	2005.23223	1841.94832	1
22959	N	87.02500	54.16280	71.89790	-613.51596	357.87667	452.82345	1
22960	H	86.52100	54.27380	71.04090	2251.03426	2194.33652	-154.74492	1
22961	C	88.26400	53.66480	71.80990	-574.32393	369.15566	-626.42116	1
22962	N	89.10000	53.50980	72.82190	573.46650	615.66775	-96.05201	1
22963	H	88.79100	53.70980	73.75190	-331.83540	2641.13313	1671.42228	1
22964	H	90.04200	53.23980	72.62390	2820.03680	636.37764	1219.55910	1
22965	N	88.74400	53.35480	70.59690	239.09338	-458.47432	646.66656	1
22966	H	88.15000	53.32880	69.79290	588.76453	-1071.18775	-2909.93942	1
22967	H	89.71700	53.20780	70.42090	1550.59835	2704.32568	432.95304	1
22968	C	83.32200	50.61480	73.20590	-631.25281	-474.40471	-470.44823	1
22969	O	83.24600	50.07780	72.10590	154.16955	81.40065	755.61937	1
22970	N	82.30300	50.67980	74.02090	285.13236	-353.75363	-721.81545	1
22971	H	82.47000	51.01780	74.94390	-1320.51972	2084.15193	1944.69055	1
22972	C	80.90500	50.41080	73.69990	210.07684	865.93215	193.90642	1
22973	H	80.90700	49.61780	72.96590	2618.24816	1230.87924	1218.80562	1
22974	C	80.09800	49.91280	74.88890	887.87873	102.98276	152.46396	1
22975	H	80.65700	49.07480	75.35590	-613.28966	2741.78292	-1437.77795	1
22976	H	79.13500	49.50380	74.51390	-1337.39175	-2451.62466	-1459.22698	1
22977	O	79.93000	50.94380	75.84990	401.92725	680.62285	12.17402	1
22978	H	80.78600	51.10580	76.25190	2042.19612	-1931.06415	1391.89319	1
22979	C	80.20200	51.63780	73.09290	-294.67002	464.99592	718.26769	1
22980	O	80.82500	52.67380	72.89290	2.14290	-665.84704	404.90586	1
22981	N	78.90600	51.49280	72.63190	800.15382	-240.89606	64.27737	1
22982	H	78.46200	50.61780	72.45690	1962.54868	2036.12175	1366.55138	1
22983	C	78.10900	52.61380	72.12490	-43.08762	-518.84935	-757.77133	1
22984	H	78.62900	53.02480	71.27190	566.72532	3042.40369	574.85855	1
22985	C	76.74700	52.13880	71.62190	-6.00748	690.83885	588.36671	1
22986	H	76.16900	52.99880	71.21990	956.16082	-1450.21470	2607.71660	1
22987	H	76.18700	51.79780	72.51890	-1766.91820	-2487.23243	-776.41636	1
22988	C	76.84800	51.01580	70.56590	-680.31760	336.20169	502.41519	1
22989	H	75.93000	51.16180	69.95690	960.34794	1597.10047	2524.16015	1
22990	H	77.66100	51.23680	69.84290	2352.98473	469.80657	2018.28403	1
22991	S	76.94200	49.31380	71.19890	337.19909	412.75368	154.65424	1
22992	C	75.79700	48.59480	69.95690	822.81620	249.88131	282.45155	1

22993	H	75.35400	47.67380	70.39290	2060.74359	-2366.09647	-132.47549	1
22994	H	76.40800	48.33680	69.06590	-364.61826	-2319.87485	2075.47209	1
22995	H	75.08300	49.32480	69.51890	1732.48659	1351.75257	-2263.39407	1
22996	C	77.92300	53.80080	73.01490	-220.98370	641.16344	603.70978	1
22997	O	78.11000	54.94380	72.61990	507.20748	-571.98677	-184.01056	1
22998	N	77.71000	53.58280	74.34390	112.45206	-796.61967	231.54239	1
22999	H	77.59800	52.67680	74.74290	-1360.67478	-1229.55302	2544.89250	1
23000	C	77.68700	54.67680	75.33990	-682.04171	-106.36014	-610.49811	1
23001	H	76.94800	55.38980	75.00390	-1210.53135	2908.43475	23.36828	1
23002	C	77.20500	54.32980	76.79390	469.29062	13.13921	-790.83834	1
23003	H	77.72800	53.41580	77.14590	2370.63613	-1296.24041	-1617.01128	1
23004	O	75.76300	54.21780	76.78490	246.74145	-472.35287	-590.27785	1
23005	H	75.63300	53.42280	76.26290	3026.59544	-800.63023	-281.48693	1
23006	C	77.39900	55.42680	77.81890	-568.97019	427.32721	564.12234	1
23007	H	76.81700	55.15480	78.72490	2377.70020	2040.06093	265.30622	1
23008	H	78.42900	55.46880	78.23490	220.82873	3109.80303	-446.85938	1
23009	H	77.11100	56.36280	77.29590	-11.43411	-3026.81523	840.02012	1
23010	C	78.99300	55.41280	75.48290	697.95757	-573.76628	-89.93018	1
23011	O	79.01200	56.64380	75.52890	-63.11175	-772.43755	-146.97250	1
23012	N	80.04200	54.60680	75.54790	-402.26277	514.11675	-552.84201	1
23013	H	79.91100	53.62580	75.42390	-2352.64599	2069.82402	318.70266	1
23014	C	81.45000	55.05880	75.60490	203.28338	640.59352	-630.52741	1
23015	H	81.54600	55.60980	76.52890	628.71135	-639.37924	-3026.00901	1
23016	C	82.49400	53.85080	75.62690	595.14304	400.57143	-574.32955	1
23017	H	83.54200	54.17680	75.80090	-2235.84851	-1657.68567	-1480.77062	1
23018	H	82.40300	53.30880	74.66190	673.19822	2405.60484	-1929.09052	1
23019	C	82.13700	52.85880	76.75290	-373.08063	40.92871	-845.48761	1
23020	O	82.51800	51.66580	76.56390	-354.38605	24.61665	693.37048	1
23021	O	81.53100	53.20380	77.76190	284.12498	77.25823	719.25973	1
23022	C	81.81100	55.96680	74.36290	201.59443	704.83893	-557.48842	1
23023	O	82.31600	57.09180	74.51690	407.19084	420.97399	518.20284	1
23024	N	81.46000	55.58180	73.12090	226.26998	-737.12114	-342.84076	1
23025	H	80.97900	54.71980	72.97790	2573.21982	1051.39428	1457.15659	1
23026	C	81.68400	56.29980	71.95890	384.57750	-164.97618	-818.36243	1
23027	H	82.73300	56.54780	72.03390	-1974.24170	1754.81688	-1731.48162	1
23028	C	81.30300	55.39580	70.72990	-586.61785	328.70786	-635.13016	1
23029	H	81.29600	56.08680	69.85890	-2347.84998	-2027.08644	516.75439	1
23030	H	80.24900	55.09180	70.90490	-2706.22542	1288.96343	964.54968	1
23031	C	82.34400	54.32980	70.40590	40.27656	-674.19040	593.67127	1
23032	H	82.91800	54.03380	71.31090	-1069.05665	1990.54140	2183.64709	1
23033	H	83.11200	54.74680	69.71990	-617.05995	-2633.90841	1586.03922	1
23034	C	81.85800	53.05580	69.67590	655.61508	-561.97280	256.89264	1
23035	H	81.45300	53.35580	68.68590	-2522.32768	-602.87286	1774.03817	1
23036	H	81.02700	52.73880	70.34090	-291.10079	-1814.87670	-2562.77661	1
23037	C	82.96900	51.98280	69.53090	-519.84914	-510.12782	534.16558	1
23038	H	83.51800	51.86480	70.48990	1852.32208	1399.27427	2109.45388	1
23039	H	83.71600	52.20480	68.73890	1296.71898	-1527.63214	2405.11738	1
23040	N	82.51400	50.65680	69.16890	530.42691	534.02625	370.02555	1
23041	H	82.10400	50.74380	68.21690	-174.42471	2207.89161	-2254.88183	1
23042	H	83.32800	50.00980	69.15490	-697.52425	2022.61341	2299.10532	1
23043	H	81.81100	50.26080	69.82490	-1895.70458	-2330.05748	916.87689	1
23044	C	80.96500	57.63780	71.82890	826.33937	-331.71141	153.65811	1
23045	O	81.52700	58.63680	71.43890	523.16986	50.70035	-595.67242	1
23046	N	79.66900	57.69580	72.21290	62.45139	409.56300	-748.05525	1
23047	H	79.23700	56.80280	72.31390	1047.96918	-1318.90113	2642.40019	1
23048	C	78.91900	58.95380	72.34290	668.93466	8.64760	604.37743	1
23049	H	79.04000	59.54580	71.44790	-1801.46544	2274.28975	1223.80510	1
23050	C	77.45800	58.71880	72.77690	812.28507	-345.45887	-213.28381	1
23051	H	76.82600	59.62580	72.87990	-1464.45585	-658.36634	2698.36901	1
23052	H	77.44500	58.21880	73.76890	-2755.11863	1063.15487	1090.38235	1
23053	C	76.64300	57.82380	71.87090	565.68760	-81.69041	696.34826	1
23054	C	76.58300	58.10480	70.48090	191.17442	-840.35040	-289.80430	1

23055	H	77.12200	58.96280	70.10690	-2027.91211	1447.77085	-1939.83156	1
23056	C	75.81100	57.35880	69.59390	-626.25240	-139.62751	642.60311	1
23057	H	75.76500	57.60680	68.54390	-1780.74170	-1779.93218	-1896.43867	1
23058	C	75.22600	56.17080	70.00690	502.67737	-711.06597	237.11467	1
23059	O	74.53900	55.28780	69.16190	631.47124	29.23568	456.27273	1
23060	H	74.41500	54.44180	69.59890	-1234.33470	-2724.01531	-980.30574	1
23061	C	75.90500	56.70580	72.30390	-442.83426	-215.54464	759.17842	1
23062	H	75.83900	56.41280	73.34090	-1393.61831	2307.76743	1620.77316	1
23063	C	75.30900	55.81680	71.36490	-143.38104	491.05271	-768.48538	1
23064	H	74.94300	54.87280	71.74090	1870.61073	1909.21757	-1669.14605	1
23065	C	79.49600	59.91880	73.36590	310.03549	-622.19152	573.62197	1
23066	O	79.75100	61.08780	73.13790	161.29134	38.24882	-780.40413	1
23067	N	79.82100	59.45580	74.55290	-645.59120	-337.18352	-440.57348	1
23068	H	79.68400	58.49580	74.78390	2765.67771	-1450.35858	-344.06181	1
23069	C	80.44200	60.30880	75.56290	-734.28892	362.26782	-421.75171	1
23070	H	79.90500	61.24580	75.55490	-2792.31292	-897.72575	-1155.65992	1
23071	C	80.24100	59.73180	76.98690	329.07937	554.50571	-654.93185	1
23072	H	80.77400	60.48080	77.61190	2462.34126	127.12950	1939.85042	1
23073	H	80.74600	58.75980	77.17490	-1131.41524	2485.96200	-1578.84657	1
23074	C	78.72500	59.53680	77.40490	-659.15040	472.49354	-434.86651	1
23075	H	78.16700	60.42180	77.03090	2658.64920	1563.65188	-618.41456	1
23076	H	78.24300	58.62080	77.00190	-2103.48584	-1944.98981	1292.83512	1
23077	C	78.50600	59.36680	78.91590	28.64145	200.53876	879.83748	1
23078	H	78.94700	58.43680	79.33590	-77.54784	2294.75625	2142.82964	1
23079	H	77.42800	59.16480	79.09190	-1973.69052	-1071.09530	2196.37425	1
23080	N	79.05000	60.55680	79.71390	-232.92205	497.60710	634.13661	1
23081	H	79.41200	61.35180	79.22890	829.62815	-2922.84523	-815.56267	1
23082	C	79.10800	60.62180	81.05290	121.67880	-646.72468	-638.70515	1
23083	N	78.65600	59.79180	81.93890	-680.33710	-278.22122	409.58322	1
23084	H	78.00100	59.08680	81.66790	-1758.51946	-2223.70049	1356.87274	1
23085	H	78.68000	60.11080	82.88590	-1985.72939	-1569.31999	-1880.29613	1
23086	N	79.61200	61.72080	81.54490	-337.58761	-584.30655	-517.00108	1
23087	H	79.92100	62.44280	80.92490	-1565.41979	1492.86060	2278.79114	1
23088	H	79.73600	61.78780	82.53490	-1798.38855	1793.76216	-1868.53441	1
23089	C	81.91100	60.65180	75.26890	612.34580	443.77764	-517.12508	1
23090	O	82.34700	61.74380	75.64890	404.44469	677.51636	-55.80654	1
23091	N	82.63500	59.80580	74.56990	-194.80445	74.07543	-829.93939	1
23092	H	82.35300	58.85480	74.46790	-2534.09818	1466.87656	1155.08720	1
23093	C	83.96700	60.27580	74.06590	575.73276	-678.33284	157.97618	1
23094	H	84.51900	60.58080	74.94290	-2020.08267	-266.09556	2389.94338	1
23095	C	84.76500	59.15580	73.29790	802.63368	-158.23136	-402.30804	1
23096	H	84.27400	58.99080	72.31490	-1309.67093	1430.43942	-2494.03726	1
23097	H	84.62400	58.26080	73.94190	-1614.59018	2706.35416	64.72486	1
23098	C	86.25700	59.33680	73.14890	-741.70812	202.46992	487.94101	1
23099	H	86.42000	60.38280	72.81090	2277.59375	-2075.12710	-611.22370	1
23100	C	86.99400	59.10380	74.43890	-137.29936	763.25162	-500.00913	1
23101	H	88.03400	59.42780	74.21690	2311.67705	2064.42048	527.50779	1
23102	H	86.66200	59.73080	75.29390	1760.34186	-1717.90148	1942.49574	1
23103	H	86.94000	58.03480	74.73590	1613.83236	1951.69980	1855.41381	1
23104	C	86.78800	58.36680	72.08090	-38.09675	295.79315	851.64547	1
23105	H	86.63600	57.36080	72.52590	-1367.98749	2400.07169	-1530.64046	1
23106	H	87.88400	58.53880	72.02790	-267.64055	2655.86362	1662.64344	1
23107	H	86.34700	58.51580	71.07190	-2547.99560	1748.39836	617.68570	1
23108	C	83.83400	61.42680	73.15390	-354.64480	-407.89906	-744.37542	1
23109	O	84.63000	62.37580	73.26490	648.14062	411.87515	-185.96437	1
23110	N	82.85300	61.48880	72.22890	-702.02783	-438.82468	-184.48865	1
23111	H	82.23800	60.70680	72.16490	2551.70259	1722.72296	-649.34929	1
23112	C	82.51100	62.67080	71.40490	-180.44389	898.20725	-67.92951	1
23113	H	83.43700	63.02080	70.97290	2736.15189	942.16660	1216.01058	1
23114	C	81.45100	62.39580	70.30990	648.58985	637.19681	52.60743	1
23115	H	80.52300	61.97280	70.74890	-1130.53842	1220.42489	2666.10188	1
23116	H	81.11100	63.34480	69.84290	-1243.55693	-1028.19869	2692.91121	1

23117	N	83.07400	62.04880	68.49190	-72.09256	-817.92844	160.36765	1
23118	C	81.94000	61.60380	69.18490	547.48863	-716.85763	39.39778	1
23119	C	83.07900	61.30880	67.38090	-162.73829	807.53689	-417.27807	1
23120	H	83.93400	61.31080	66.70590	2700.42262	1608.11270	65.40617	1
23121	N	82.06700	60.43080	67.32990	21.15065	698.20229	-493.46019	1
23122	H	81.96900	59.68080	66.67590	2116.59453	2326.94943	-96.22663	1
23123	C	81.28500	60.67180	68.46190	745.64159	350.07244	-394.10703	1
23124	H	80.30900	60.21780	68.57990	2033.02284	196.50651	2378.51407	1
23125	C	81.99700	63.82580	72.29390	-165.90970	-887.54285	-106.51993	1
23126	O	82.45800	64.95180	72.13090	-748.05413	56.91983	-273.20362	1
23127	N	81.10700	63.58780	73.24290	-512.30371	-351.85098	564.88451	1
23128	H	80.64000	62.70880	73.29990	2256.16195	587.08714	-2116.98066	1
23129	C	80.62600	64.63480	74.15290	535.62813	423.97319	593.90494	1
23130	H	80.25900	65.41980	73.50690	1099.07169	2679.89010	-1239.77150	1
23131	C	79.51400	64.01580	75.02690	482.42299	682.57672	356.16106	1
23132	H	78.93200	63.32680	74.37890	1776.31344	-1447.63628	2141.04153	1
23133	H	80.05900	63.34980	75.72990	2042.83635	2141.45031	-1073.18334	1
23134	C	78.65200	64.92580	75.86790	146.11829	896.21227	-111.29981	1
23135	H	79.32500	65.43280	76.59190	1572.66026	-162.20736	-2724.55262	1
23136	C	77.84300	65.91680	75.11090	397.68066	398.06485	-723.21153	1
23137	H	78.40300	66.58380	74.41990	-2086.64999	-2126.87440	-1020.86725	1
23138	H	77.04300	65.37980	74.55790	1421.83921	-2277.51256	1623.99252	1
23139	H	77.34800	66.57180	75.85890	469.35220	679.65577	-3042.08427	1
23140	C	77.73700	63.96780	76.62590	173.72059	-633.55352	-636.05472	1
23141	H	78.25600	63.31880	77.36390	-2273.11237	-1444.05636	1622.53117	1
23142	H	77.23500	63.24180	75.95090	-2034.98824	-468.30590	-2364.38132	1
23143	H	77.01400	64.60180	77.18190	1032.40119	2970.78737	-112.01456	1
23144	C	81.76100	65.29180	74.99290	338.51371	303.40417	781.50850	1
23145	O	81.80900	66.50180	75.10190	441.91437	532.16493	372.24414	1
23146	N	82.73700	64.49880	75.49490	-438.71074	390.93270	-620.66337	1
23147	H	82.74800	63.51180	75.35190	2662.66134	-1430.57157	-860.87617	1
23148	C	84.02000	64.94880	76.06590	570.07449	-676.82637	185.98102	1
23149	H	83.77900	65.63080	76.86790	-1568.41220	1468.68089	2294.83952	1
23150	C	84.77200	63.73480	76.76590	591.31833	-679.25247	-111.61653	1
23151	H	85.81700	64.05580	76.96690	-1294.43509	2329.36057	1670.94555	1
23152	H	84.71000	62.84780	76.09990	2122.06918	2037.89727	-1122.36510	1
23153	O	84.15300	63.55380	78.01490	481.99624	-40.08419	-630.29644	1
23154	H	84.37800	64.25280	78.63390	-1791.30470	2066.63923	1554.08905	1
23155	C	84.93100	65.67980	75.13190	-668.65983	-284.45105	546.13060	1
23156	O	85.56500	66.64980	75.53790	-593.22646	-509.33452	-128.31155	1
23157	N	85.05100	65.29680	73.86190	-264.97826	746.65147	298.61939	1
23158	H	84.70800	64.42780	73.51290	-2112.12096	-134.96352	2323.26722	1
23159	C	85.69500	66.04380	72.82190	567.18923	371.70183	-616.07252	1
23160	H	86.70800	66.33380	73.05990	2758.97835	-1496.28405	-16.80281	1
23161	C	85.74100	65.15480	71.54090	-139.12277	-863.66209	-250.56710	1
23162	H	84.87900	64.46080	71.44990	142.62428	2094.40964	-2357.14046	1
23163	C	85.79600	65.94080	70.19390	448.09140	-357.51663	692.87889	1
23164	H	84.86900	66.50480	69.95490	2545.26475	-1360.53258	1223.72822	1
23165	H	85.96200	65.21880	69.36590	-1483.02878	-28.50688	-2787.29310	1
23166	H	86.63500	66.66980	70.17690	-1298.62715	2551.36513	1314.32383	1
23167	C	87.01400	64.26180	71.59490	-398.47848	628.50707	528.07633	1
23168	H	86.82200	63.39980	72.26990	-897.36194	-2480.49486	1699.58092	1
23169	H	87.92700	64.84480	71.84190	309.69020	-2967.42149	969.38262	1
23170	H	87.23900	63.84180	70.59090	-3029.74422	-812.69627	282.55922	1
23171	C	84.98600	67.39680	72.55390	-388.20567	-802.29636	-191.53180	1
23172	O	85.69000	68.41580	72.40690	204.00267	-510.67779	551.72119	1
23173	N	83.64700	67.48780	72.47490	209.88712	-309.53405	-760.88718	1
23174	H	83.09500	66.66380	72.57690	1587.35745	333.16398	2684.92746	1
23175	C	82.92000	68.76280	72.32790	-522.12723	261.97688	-713.72885	1
23176	H	83.22900	69.31680	71.45390	2017.85139	1696.18342	-1721.77106	1
23177	C	81.43200	68.40580	72.15790	642.18654	-297.34433	558.50114	1
23178	H	80.91900	69.33580	71.83390	-1732.04280	1320.60283	-2284.41409	1

23179	H	80.92200	68.18880	73.12090	-1763.10117	-1739.80244	1934.58287	1
23180	H	81.28100	67.60480	71.40290	-744.24462	1524.10081	2647.34867	1
23181	C	83.14400	69.72080	73.44490	-401.56651	816.77359	116.76247	1
23182	O	83.43900	70.90080	73.25090	533.44374	563.95410	-145.61397	1
23183	N	83.00700	69.24380	74.69190	-39.97664	577.49679	-625.50195	1
23184	H	82.62000	68.33680	74.84090	2961.24189	977.11794	378.73485	1
23185	C	83.27700	70.00580	75.90190	868.18360	27.95767	253.05356	1
23186	H	82.61000	70.85480	75.90990	-2618.14610	-281.83495	1723.37295	1
23187	C	83.12800	69.09680	77.13590	-194.20103	-628.26331	623.09979	1
23188	H	83.48300	69.52780	78.09690	-434.75185	1739.98287	2580.57913	1
23189	H	83.61800	68.12180	76.92790	547.37166	-3045.50053	-553.82756	1
23190	C	81.58900	68.79880	77.42290	501.38341	748.89580	-142.27043	1
23191	O	80.75700	69.59680	76.91990	629.39047	471.66334	27.60771	1
23192	O	81.33500	67.81580	78.15690	-685.65551	-126.81589	-385.37380	1
23193	C	84.71100	70.58080	75.95190	712.37272	56.03895	552.77983	1
23194	O	84.86800	71.75680	76.30490	-398.58340	-423.74005	528.83059	1
23195	N	85.74100	69.79480	75.67590	-420.60342	269.36334	-693.03326	1
23196	H	85.60700	68.83480	75.43990	2131.55193	-2196.38932	691.72991	1
23197	C	87.13300	70.09780	75.63590	-194.25664	-885.16984	-78.06735	1
23198	H	87.32400	70.52680	76.60790	1086.47113	-2112.86238	2048.01621	1
23199	C	87.91400	68.77880	75.41390	484.11481	-588.49556	481.71557	1
23200	H	87.59900	68.21680	74.50790	694.43447	2655.17981	1535.04643	1
23201	H	87.63200	68.11480	76.25890	-2487.21738	1386.93921	1342.35916	1
23202	C	89.44000	68.82480	75.48290	687.32333	574.92272	-170.45234	1
23203	H	89.72900	69.58180	74.72290	292.40196	-1741.75538	2591.10961	1
23204	C	89.94100	69.29480	76.88690	176.79026	685.55266	569.03778	1
23205	H	89.75800	68.53080	77.67190	2538.41880	1853.64798	-97.31015	1
23206	H	91.05200	69.32680	76.88190	1541.41723	714.58211	2636.97240	1
23207	H	89.44900	70.26980	77.09490	2908.37514	811.39892	861.79164	1
23208	C	89.95100	67.43480	75.03090	-440.37549	-435.26089	660.29917	1
23209	H	89.65900	67.25180	73.97490	-2235.33346	-1200.65278	1854.09040	1
23210	H	91.05800	67.51580	75.08490	-2352.04345	2042.37497	-499.88046	1
23211	H	89.58900	66.62280	75.69590	2312.84618	2119.59863	216.90221	1
23212	C	87.46200	71.14180	74.60090	237.27872	-510.70131	704.40633	1
23213	O	88.19800	72.07180	74.83790	236.08794	-369.12582	644.87549	1
23214	N	86.84400	71.04980	73.39090	-212.52087	-785.72387	204.69509	1
23215	H	86.17000	70.32580	73.26190	-2335.64399	-1640.93104	1320.51084	1
23216	C	87.01800	71.85880	72.20590	-804.01431	-379.60713	-225.11485	1
23217	H	88.03400	71.65880	71.90090	-1375.31846	-1174.71095	-2582.66918	1
23218	C	86.05600	71.26180	71.07990	-551.52472	-635.70301	344.33956	1
23219	H	85.03600	71.30180	71.51890	1892.07259	-2212.96784	1164.10830	1
23220	H	86.42000	70.23180	70.88090	-1163.07643	-2073.46781	2051.08699	1
23221	C	86.06000	71.96180	69.68690	-564.94187	622.88925	-381.50936	1
23222	H	85.52600	72.93580	69.71790	1889.54724	-325.31404	2481.59483	1
23223	C	87.48200	72.28980	69.17990	214.81475	-623.62407	-627.25981	1
23224	H	88.21400	71.45680	69.22790	750.41205	3051.66438	220.99950	1
23225	H	87.92000	73.10780	69.79090	-681.47380	2380.22746	-1958.58845	1
23226	H	87.44600	72.71180	68.15290	1930.44647	1434.77548	2018.60962	1
23227	C	85.20100	71.16880	68.59090	65.77431	-584.21557	683.83865	1
23228	H	85.60800	70.14180	68.47390	351.36567	-2854.66222	1250.49403	1
23229	H	84.15200	71.20580	68.95590	-2365.75256	2035.65280	-474.34324	1
23230	H	85.20300	71.73380	67.63390	1735.96716	-20.55441	-2625.03691	1
23231	C	86.64900	73.30080	72.42790	165.30275	-752.36931	470.79021	1
23232	O	87.45100	74.21280	72.17190	115.49290	-364.28724	-693.18047	1
23233	N	85.50800	73.52580	73.11090	155.62338	-283.42482	-782.65226	1
23234	H	84.97100	72.71180	73.31890	2615.16069	-1508.59074	-863.22509	1
23235	C	85.11500	74.80280	73.59690	620.33716	-472.37695	453.51387	1
23236	H	85.32400	75.60080	72.90090	1523.65794	1538.97562	-2285.95655	1
23237	C	83.55300	74.85180	73.84290	669.18378	209.29702	571.77076	1
23238	H	83.38800	74.05380	74.59790	-1791.68459	-1113.73741	2331.73852	1
23239	H	83.04800	74.70080	72.86490	-1456.48194	-2333.06436	1522.17870	1
23240	C	83.06600	76.20680	74.31390	-323.30774	794.82781	321.32763	1

23241	C	83.49400	77.39480	73.61290	-690.60474	359.11199	484.34991	1
23242	H	84.09300	77.25680	72.72490	-734.44688	2297.76149	-2032.06310	1
23243	C	83.02700	78.64780	74.04590	586.02348	-649.52679	-231.87825	1
23244	H	83.34500	79.53480	73.51790	2483.77400	412.76260	1874.51630	1
23245	C	82.11700	78.73280	75.12690	-73.83237	798.97442	-444.16364	1
23246	H	81.80600	79.73380	75.39090	-2030.52580	287.53404	2389.53778	1
23247	C	82.25700	76.31380	75.36790	509.74574	695.25257	-298.40294	1
23248	H	81.88900	75.42480	75.85690	-289.64877	3132.02664	-176.40238	1
23249	C	81.80600	77.52180	75.83390	154.49631	-644.86573	-624.20506	1
23250	H	81.02300	77.59480	76.57490	1610.36273	1953.48617	1862.27773	1
23251	C	85.85600	75.28680	74.89890	551.94871	-315.04845	640.82202	1
23252	O	86.21200	76.46780	74.94090	-623.64636	-325.34870	361.28744	1
23253	N	86.17100	74.39980	75.83690	359.74186	185.71876	732.92331	1
23254	H	86.02200	73.41680	75.76590	-969.78659	626.62849	2923.25589	1
23255	C	86.82000	74.75980	77.14490	87.08210	-704.36475	561.27531	1
23256	H	86.15300	75.48880	77.57990	-2696.71457	374.29449	1581.84553	1
23257	C	86.94000	73.58780	78.11590	405.49713	704.80430	-419.12917	1
23258	H	87.14500	72.68280	77.50590	2422.94955	1809.77411	852.52307	1
23259	C	88.11000	73.73880	79.17790	427.75013	-781.61778	-175.53223	1
23260	H	89.11200	73.50380	78.75790	-2807.49405	12.10367	-1437.13632	1
23261	H	87.89000	73.00680	79.98390	1684.44889	-2018.36985	1713.69353	1
23262	H	88.01200	74.79180	79.51590	-2370.35484	1459.51705	-1483.39932	1
23263	C	85.60400	73.41880	78.88190	484.05100	393.94197	656.55445	1
23264	H	85.67200	72.50580	79.51190	2300.45982	1922.04758	-954.59843	1
23265	H	85.36200	74.27280	79.54890	1145.11528	-2921.78123	-160.98052	1
23266	H	84.74200	73.40480	78.18090	843.48751	-2265.93803	2001.66877	1
23267	C	88.17300	75.40380	76.92690	263.90865	-695.14568	-525.71419	1
23268	O	88.54300	76.32780	77.61390	216.98731	-470.56935	-596.62610	1
23269	N	88.89700	74.85580	75.91890	-243.60281	-510.54149	-631.90316	1
23270	H	88.53000	74.08180	75.40890	-407.24081	2260.88654	2148.80142	1
23271	C	90.29200	75.32580	75.66290	-234.73417	-240.18219	841.54056	1
23272	H	90.89600	75.29980	76.55790	2240.11415	1864.98748	-1186.14884	1
23273	C	90.95300	74.41080	74.56690	334.87763	769.82144	353.55324	1
23274	H	90.23300	74.14880	73.76190	2547.48593	1657.75648	795.47200	1
23275	C	92.24400	75.00980	73.95790	-644.56647	645.23234	116.28143	1
23276	H	92.97600	75.11480	74.78690	-1458.67259	1644.21811	2251.60185	1
23277	H	92.67300	74.27880	73.23890	1795.76073	-2162.47044	1387.94855	1
23278	H	91.99400	75.90680	73.35290	2247.73265	-2186.36975	-104.57226	1
23279	C	91.30800	73.01580	75.20290	574.41658	-208.18284	-677.87929	1
23280	H	90.39500	72.66380	75.72790	-1259.46669	2447.10828	1528.82474	1
23281	H	92.16300	73.06880	75.90890	-2572.27047	-1165.44627	-1401.80332	1
23282	C	91.58000	71.93880	74.11790	-551.05875	728.78144	97.74645	1
23283	H	92.58900	72.13780	73.69690	-1855.94692	1932.00343	1654.80183	1
23284	H	90.83500	71.82580	73.30090	3074.99244	563.03598	295.39384	1
23285	H	91.68900	70.94580	74.60390	1166.42133	2855.07588	-642.34699	1
23286	C	90.27000	76.76580	75.16090	37.40249	534.74287	-746.74704	1
23287	O	91.26100	77.50980	75.35290	-675.93397	-413.21845	-36.48690	1
23288	N	89.15800	77.21180	74.50990	-192.59274	-540.33783	-622.78191	1
23289	H	88.43600	76.60280	74.19090	1194.13194	1548.22509	2458.92348	1
23290	C	89.12800	78.59280	74.10490	377.50393	508.01125	651.07281	1
23291	H	90.03400	78.84180	73.57190	1469.30424	-1257.81007	-2479.54999	1
23292	C	87.93400	78.86780	73.12990	-29.07440	-731.92606	531.65041	1
23293	H	88.03500	79.86580	72.65290	874.83027	-2362.58676	-1878.30949	1
23294	O	86.60800	78.75480	73.78290	494.52937	-520.88501	304.75807	1
23295	H	86.49900	77.90180	74.21090	3133.14724	32.62321	187.58542	1
23296	C	87.97000	77.75680	72.01390	-721.09669	-537.08802	-171.68586	1
23297	H	87.68400	76.74380	72.36890	1930.66671	2474.54389	-219.98785	1
23298	H	87.16200	78.06680	71.31790	1557.84851	-1308.35620	-2396.37134	1
23299	H	88.96600	77.83780	71.52890	194.80847	-1558.04845	2717.03243	1
23300	C	88.96700	79.58880	75.24390	-553.02543	-593.71890	-423.33659	1
23301	O	89.33600	80.75080	75.13190	-480.33427	-511.35593	-369.58633	1
23302	N	88.46200	79.15180	76.40990	-50.08885	-812.88617	-213.00321	1

23303	H	88.27300	78.17780	76.50590	-1758.54857	-1463.49354	-2167.10605	1
23304	C	88.07500	80.00680	77.54090	-28.71935	192.47567	887.54003	1
23305	H	87.30100	80.66680	77.17790	2295.51013	334.11988	-2122.61327	1
23306	C	87.30500	79.28680	78.65090	-600.75589	186.28553	-670.72541	1
23307	H	87.05400	79.85480	79.57290	-2004.71889	1719.40676	-1723.13828	1
23308	H	87.98500	78.45680	78.93890	42.46103	-2585.37115	1782.97069	1
23309	C	85.94700	78.73980	78.20890	-397.08447	316.88538	757.44892	1
23310	H	86.02600	78.13580	77.27990	-2809.43718	1416.73723	-210.73565	1
23311	C	85.44800	77.83980	79.37790	-901.55403	-8.23883	-173.48386	1
23312	H	86.11200	76.94880	79.37190	221.84360	-2791.68866	-1432.60241	1
23313	H	85.48900	78.35180	80.36290	-2616.16425	1752.27728	-142.86320	1
23314	H	84.39600	77.56880	79.14390	-3051.72716	-124.86140	772.55016	1
23315	C	84.96300	79.87180	77.92290	-902.58962	87.58801	141.05840	1
23316	H	85.05400	80.27480	76.89190	2452.58299	1965.27922	39.43196	1
23317	H	85.04300	80.76780	78.57490	-2004.02539	-1894.58962	-1521.98116	1
23318	H	83.95600	79.43980	78.10290	825.88212	-1453.43888	-2665.16199	1
23319	C	89.17800	80.94580	78.08890	-717.73370	495.08186	285.18454	1
23320	O	88.80600	82.04980	78.42590	643.80407	451.28983	9.90323	1
23321	N	90.47200	80.68380	78.13390	-575.46373	-15.62058	618.56191	1
23322	C	90.96500	79.30680	78.36890	-415.30352	-444.98896	-685.51246	1
23323	H	91.18800	78.92780	77.34790	-1625.89174	1659.09059	2124.28766	1
23324	H	90.26700	78.62680	78.90290	-1445.60582	-1853.86634	-2097.26055	1
23325	C	91.54100	81.64680	78.45690	-35.51050	-446.29956	-797.09137	1
23326	H	91.23900	81.98780	79.43590	1750.19217	-1805.57020	-1886.28395	1
23327	C	92.73700	80.82480	78.49790	-848.62530	148.03671	-322.99370	1
23328	H	93.63600	81.30280	78.94390	409.67599	-1805.76782	2534.63577	1
23329	H	93.12400	80.48380	77.51490	9.85446	-2364.30124	-2076.16703	1
23330	C	92.24000	79.53580	79.14890	-352.98667	-208.46490	810.58332	1
23331	H	92.99800	78.74380	78.96890	-2033.07651	2406.98548	-117.87916	1
23332	H	92.10900	79.69280	80.24090	1902.48921	922.23929	-2331.91371	1
23333	C	91.62700	82.88080	77.58990	241.68839	693.14751	-547.06959	1
23334	O	92.02600	83.95080	78.05690	142.54234	-167.16372	752.56465	1
23335	N	91.29900	82.78080	76.30590	-338.32292	600.73457	-501.42521	1
23336	H	91.10600	81.91780	75.84690	1438.75264	2796.77989	-111.68873	1
23337	C	91.14300	83.99380	75.47590	604.84887	-314.06511	-599.28591	1
23338	H	92.02900	84.60980	75.52090	334.23111	2840.27751	1316.20242	1
23339	C	90.89300	83.53080	73.98690	509.73219	-493.75844	-564.53696	1
23340	H	89.88900	83.05780	73.93690	2121.13629	1642.17408	1635.43948	1
23341	H	90.85600	84.47980	73.41090	-1264.53322	2233.67949	-1834.86309	1
23342	C	92.01000	82.69580	73.39690	-555.24922	498.95382	532.79230	1
23343	C	93.29400	83.19280	73.34590	778.46609	-194.97186	411.19007	1
23344	H	93.55400	84.19180	73.66590	2074.07972	1136.03738	-2074.33098	1
23345	C	94.39900	82.58680	72.68290	-626.48512	-283.79687	599.05816	1
23346	H	95.32400	83.13780	72.59590	647.85034	2028.50396	2314.26611	1
23347	C	94.10100	81.35380	72.07090	592.07914	415.31278	546.14982	1
23348	H	94.80900	80.81280	71.46190	2036.91765	-1251.39844	-2038.75525	1
23349	C	91.83500	81.41480	72.88390	-378.45493	-309.66484	-775.77502	1
23350	H	90.85900	80.95880	72.95990	2813.11635	1343.27426	-394.31620	1
23351	C	92.82900	80.73080	72.21990	270.21419	874.56722	-11.72674	1
23352	H	92.53500	79.82280	71.71490	658.77731	-2796.46782	1258.59595	1
23353	C	90.05300	84.85580	75.95490	645.34379	569.61098	-296.01316	1
23354	O	90.00193	86.08866	75.60760	337.34823	-129.52687	251.20160	1
23355	N	88.89800	84.23980	76.38290	-75.79354	-682.36849	483.68959	1
23356	H	88.83200	83.24980	76.48090	1524.22391	545.33974	-2697.71222	1
23357	C	87.77100	84.95680	77.05290	-798.32742	72.99855	445.70217	1
23358	H	87.71756	85.67552	76.22152	-1060.27454	1262.66127	-407.40534	1
23359	C	86.55800	84.09580	77.20590	163.11260	499.92033	743.42924	1
23360	H	85.74200	84.75480	77.57290	-20.07454	1991.78310	2436.18207	1
23361	H	86.63600	83.28580	77.96190	-1446.34277	-2244.98917	1662.08304	1
23362	C	85.94200	83.48480	75.94290	-442.36402	-529.88417	-600.01367	1
23363	C	86.43200	82.68380	74.93490	-345.72223	783.60156	328.51514	1
23364	H	87.49000	82.51880	74.79890	2677.19712	-1072.20530	1234.45955	1

23365	N	85.42800	82.11980	74.20990	-293.13340	724.27691	333.44806	1
23366	H	85.59200	81.26780	73.76190	-663.36023	1787.42280	-2511.06987	1
23367	C	84.25200	82.63580	74.59690	741.17339	-445.24619	-264.77802	1
23368	C	84.51500	83.48880	75.69290	560.58922	477.19987	531.73216	1
23369	C	83.41000	84.02980	76.41090	-688.33602	150.84721	586.55691	1
23370	H	83.66700	84.57280	77.30890	-3142.46524	-240.51300	-90.32763	1
23371	C	82.13800	83.76480	75.96090	-662.36626	-462.18708	429.54334	1
23372	H	81.32000	84.18880	76.52390	2392.24601	-856.60585	1843.58505	1
23373	C	82.96000	82.40980	74.11690	-624.28084	-652.82006	137.63412	1
23374	H	82.82800	81.82880	73.21690	3096.63441	-413.09320	291.94873	1
23375	C	81.86200	82.98280	74.83290	-50.54226	657.72889	632.56363	1
23376	H	80.85600	82.74780	74.51690	1524.34316	-1262.00261	2437.87261	1
23377	C	88.12699	85.67412	78.49015	-208.64380	-101.52265	-272.00850	1
23378	O	87.66764	86.76850	78.74311	-578.34744	401.96513	-286.06470	1
23379	N	88.88700	84.89880	79.22090	-44.81963	143.63465	-834.12364	1
23380	H	89.17100	83.95280	79.08290	-2214.68935	-2227.88938	-214.22198	1
23381	C	89.50176	85.44813	80.39190	-67.38272	228.71086	-704.05245	1
23382	H	88.63617	85.88516	80.89334	2764.15157	65.26324	1615.71942	1
23383	C	90.14400	84.27080	81.25390	374.41713	-501.42978	654.79595	1
23384	H	90.98300	83.74980	80.74590	2218.12834	1542.30109	-1610.19931	1
23385	H	89.46800	83.42280	81.49390	-1283.70864	884.49750	-2739.49382	1
23386	H	90.53800	84.71780	82.19190	-2546.37681	-1852.66993	-59.18317	1
23387	C	90.53947	86.70081	80.12791	-82.06572	-126.85675	244.75601	1
23388	O	90.90881	87.34953	81.08910	-121.37559	-189.59287	-261.25433	1
23389	N	90.78390	86.82588	78.83762	176.43769	700.10779	-261.95793	1
23390	H	90.36930	86.22902	78.13071	3286.55615	-708.91395	2427.61056	1
23391	C	91.28825	88.13800	78.50455	-706.65550	-965.86474	488.71906	1
23392	H	91.63102	88.48688	79.50673	266.52264	2796.99745	-1400.27475	1
23393	C	92.40557	87.88929	77.37398	-20.06760	-183.87894	-235.77041	1
23394	H	91.82718	87.66977	76.47439	-868.25630	3842.63729	80.28332	1
23395	C	93.29509	89.12236	76.95802	164.51971	-125.15333	385.61966	1
23396	H	94.18660	88.86391	76.37494	-844.23671	1765.88659	114.49386	1
23397	H	92.70566	89.89394	76.28295	-157.26374	-1505.91395	-1933.64468	1
23398	H	93.64277	89.69874	77.80746	-440.24576	-4312.79007	1674.99986	1
23399	C	93.24625	86.67135	77.84851	1000.78128	362.60233	-62.70973	1
23400	H	92.70926	85.72495	78.04577	-1238.79795	1819.38255	-1225.32931	1
23401	H	93.88709	86.80570	78.80846	-95.16985	-6.24474	929.32470	1
23402	H	94.11906	86.41710	77.14579	150.44420	2666.10970	2249.58614	1
23403	C	90.22325	89.21896	77.92990	267.09422	-1062.71100	-301.94898	1
23404	O	90.12713	90.34488	78.41136	-269.29974	-827.43290	-453.50166	1
23405	N	89.42168	88.56868	77.02180	-259.94389	-481.51267	-140.93322	1
23406	H	89.86256	87.67799	76.78170	-1791.39483	-2123.38730	993.01446	1
23407	C	88.62184	89.23356	76.00893	-712.42923	-285.68489	814.13643	1
23408	H	89.19406	89.77823	75.33328	-218.61087	3788.19828	-3699.33274	1
23409	C	87.79609	88.21148	75.18380	-372.36208	1541.98924	-185.45407	1
23410	H	88.51369	87.38086	75.08714	-324.35869	249.26553	-4648.56329	1
23411	H	86.94895	87.85277	75.80557	323.28492	-971.37853	1511.88394	1
23412	C	87.16003	88.92555	73.87822	228.73336	-20.42101	-773.70147	1
23413	O	87.10401	88.23647	72.82810	-83.70649	489.34000	473.44572	1
23414	O	86.72972	90.08170	73.95065	-570.98471	543.76992	220.56079	1
23415	C	87.59098	90.16021	76.85722	-240.73736	457.50960	-391.32451	1
23416	O	87.44030	91.31511	76.57607	-428.70658	-797.78799	-707.55054	1
23417	N	86.87346	89.45057	77.78753	73.30362	-484.49802	178.30214	1
23418	H	87.36294	88.52825	77.97505	3342.03899	-170.41063	-465.99740	1
23419	C	85.84546	90.10617	78.48087	-241.92387	-70.56751	-424.19917	1
23420	H	85.33722	90.57800	77.63433	889.92703	-1645.25680	706.99993	1
23421	C	84.86212	89.20818	79.35912	1294.46035	141.33184	969.65779	1
23422	H	84.01519	89.81494	79.72169	-1616.96449	1347.87514	970.13386	1
23423	H	84.40066	88.45927	78.71013	1335.62910	-1380.02187	-358.35365	1
23424	H	85.47720	88.74363	80.17845	1158.50600	2204.17768	295.18206	1
23425	C	86.41337	91.22817	79.52044	-13.22771	-629.42420	-548.56344	1
23426	O	85.60034	92.06726	79.90354	273.47626	-114.82161	85.83453	1

23427	N	87.70511	91.13769	79.82549	-381.95942	-332.01065	-423.37521	1
23428	H	88.16557	90.37760	79.23035	-3232.77983	-2299.71305	-1767.33678	1
23429	C	88.18446	91.66741	81.12689	427.20853	-165.51392	988.51398	1
23430	H	87.39523	91.89679	81.83498	-2812.42390	393.10582	-1037.28220	1
23431	C	89.18174	90.72300	81.63779	559.14595	-896.15431	-505.05762	1
23432	H	89.98524	90.63796	80.87013	440.63774	-2387.63200	-1601.88730	1
23433	C	89.65741	91.22523	82.99341	-544.90095	-479.22659	-506.63992	1
23434	H	90.54011	90.66028	83.32577	658.59058	2773.78161	-778.55597	1
23435	H	89.80377	92.34368	82.97097	-2337.85831	1538.77077	1499.56196	1
23436	H	88.88106	91.02055	83.71268	1835.48531	-2319.56930	-3703.87732	1
23437	C	88.84352	89.22020	81.76136	95.50460	-429.70802	-1126.31535	1
23438	H	88.67195	88.73867	80.78273	1149.73499	950.39969	-471.79717	1
23439	H	87.86458	89.13160	82.35493	754.71885	310.62335	1119.32858	1
23440	H	89.60000	88.58012	82.30876	-262.41822	2283.13169	-866.21194	1
23441	C	88.97797	93.01546	80.57618	-581.31368	682.35957	1042.15535	1
23442	O	89.00360	93.95903	81.31709	-428.17351	83.13330	231.63147	1
23443	N	89.67882	92.88718	79.42968	244.72024	88.71871	-882.18916	1
23444	H	89.59483	92.04534	78.86612	-2767.57190	289.97427	-609.72137	1
23445	C	90.82587	93.65488	79.08026	-1091.96739	-443.89634	232.92184	1
23446	H	90.70951	94.54511	79.76571	2313.67320	633.83049	-1292.07503	1
23447	C	92.16610	92.83760	79.13988	281.96814	-437.72066	859.54978	1
23448	H	92.86688	93.08186	78.24096	-1434.71195	-2012.58078	458.03448	1
23449	H	92.74227	93.13997	80.04301	-1215.95728	-1846.75414	987.59510	1
23450	H	91.94855	91.73617	79.05530	76.42483	2966.49272	364.11703	1
23451	C	90.65088	94.22089	77.51826	-630.18266	309.64727	-1069.98940	1
23452	O	90.14050	95.29667	77.34364	104.65630	-284.92157	424.96611	1
23453	N	90.86088	93.29738	76.57945	752.77674	-135.86827	-110.38845	1
23454	H	91.07378	92.44260	77.09091	-170.12559	-3255.47857	-737.55632	1
23455	C	90.84540	93.43008	75.16428	-746.78582	-587.69686	-538.41940	1
23456	H	90.03466	94.03674	74.77690	4857.44944	2671.97180	1974.69535	1
23457	C	92.10920	94.19537	74.62622	-29.03121	-630.95288	477.62795	1
23458	H	92.82308	94.30534	75.55697	3239.92520	1471.06742	-1234.42451	1
23459	H	92.67301	93.67292	73.75546	-778.34267	-939.28767	168.97337	1
23460	C	91.83816	95.64635	73.98993	584.28075	278.45369	454.43081	1
23461	O	91.42846	95.68826	72.84200	-328.37220	-175.56056	234.25936	1
23462	N	92.18112	96.68192	74.74818	-337.57197	-76.66999	742.01083	1
23463	H	92.45103	96.56193	75.73225	349.09609	-2291.88638	614.35724	1
23464	H	92.28776	97.66597	74.51639	1676.13607	19.44101	2650.70800	1
23465	C	90.97936	91.88793	74.59546	913.55547	-1203.46257	-402.24008	1
23466	O	91.69158	91.10671	75.22201	702.03599	-310.12349	595.45035	1
23467	N	90.40098	91.66312	73.41440	46.91848	123.70708	441.07978	1
23468	H	89.94461	92.41802	72.92030	-881.68064	-2406.97004	-2605.38124	1
23469	C	90.94230	90.54189	72.72237	-28.02226	239.63819	-233.69184	1
23470	H	91.27269	89.83768	73.47312	1156.52609	-1117.27577	-1759.37587	1
23471	C	89.67579	89.80678	72.05468	214.04855	-314.55163	-489.67460	1
23472	H	89.06437	90.52134	71.51635	-751.39072	-2113.81405	221.15989	1
23473	H	89.02265	89.53453	72.93841	3123.31354	-14.81066	-675.83228	1
23474	C	89.97529	88.64906	71.15543	-25.44129	849.83635	1008.06904	1
23475	C	90.36564	88.95311	69.77413	142.05167	211.26172	459.98111	1
23476	H	90.66111	89.90917	69.35463	3770.05526	-2145.28146	-932.85673	1
23477	N	90.46592	87.90879	68.99204	-687.73520	246.81056	-91.56040	1
23478	H	90.77090	87.78926	68.02033	-4435.92910	466.00575	-234.21996	1
23479	C	89.96257	86.81377	69.75477	113.82426	435.97361	1163.29358	1
23480	C	89.58182	87.26988	71.12886	-45.31952	265.09193	-251.85044	1
23481	C	88.99496	86.30347	72.02280	296.63585	616.43259	164.92201	1
23482	H	88.57361	86.48319	72.98724	201.93273	3089.87336	-347.06161	1
23483	C	88.99296	85.00436	71.56484	-697.46523	515.68177	-602.54120	1
23484	H	88.61042	84.14475	72.19979	-3443.38331	-934.84468	1664.96782	1
23485	C	89.73728	85.47870	69.27203	-837.50812	826.56766	95.08439	1
23486	H	89.92255	85.21171	68.23026	-13.66327	-588.60964	1249.56235	1
23487	C	89.32055	84.54624	70.21352	-384.49973	-1038.88386	40.32834	1
23488	H	89.15225	83.52049	69.88457	-520.94292	2658.35434	-1876.98236	1

23489	C	92.15317	91.11921	71.77012	77.64626	-190.98720	-736.80025	1
23490	O	91.96733	92.06135	71.02324	936.05994	590.13604	552.54770	1
23491	N	93.18235	90.29112	71.90356	432.64559	52.82990	513.74611	1
23492	H	92.98061	89.51467	72.49810	152.50950	-2690.96932	831.21358	1
23493	C	94.51351	90.62335	71.59327	-11.00214	-550.79999	99.77932	1
23494	H	94.45743	91.63876	71.17838	4023.19617	-883.69370	2696.85373	1
23495	C	95.56240	90.38682	72.77687	-903.99337	-299.55186	246.85214	1
23496	H	95.05905	89.44842	73.20763	418.82625	2105.16744	-2604.86540	1
23497	H	96.54189	90.30633	72.46084	322.46716	-2614.95262	-290.30286	1
23498	C	95.38595	91.50816	73.80734	-633.45659	256.86694	170.16637	1
23499	C	95.41737	91.20978	75.19109	-232.78580	595.61205	-40.22483	1
23500	H	95.63278	90.16557	75.49186	-1007.21725	-1976.49618	-2203.96692	1
23501	C	95.19530	92.21158	76.14630	-304.11881	1113.93860	1049.98503	1
23502	H	95.16170	91.83725	77.19438	117.14307	3762.64123	-358.13858	1
23503	C	94.92404	93.59869	75.82726	570.67605	508.06664	-431.13236	1
23504	O	94.56544	94.62562	76.76474	168.74434	219.37268	51.95342	1
23505	H	95.27216	94.54069	77.42407	-3085.24401	1051.65233	-1099.11056	1
23506	C	95.16528	92.83343	73.39727	-996.84082	-41.71472	438.62840	1
23507	H	95.14339	93.12665	72.34711	237.99315	-1471.51389	-1256.98805	1
23508	C	94.96775	93.75038	74.41095	1015.17465	120.80608	200.14562	1
23509	H	94.81208	94.80243	74.13567	1291.42493	350.67593	-2450.75431	1
23510	C	95.04039	89.57439	70.43652	-392.94485	-490.92946	-418.58436	1
23511	O	96.22321	89.47846	70.14062	-18.43964	356.19119	223.55161	1
23512	N	94.05088	88.93508	69.77883	-942.82487	539.02617	-242.42519	1
23513	H	93.12296	89.23905	69.96061	-284.48135	890.59405	2467.95621	1
23514	C	94.14858	87.61994	69.31933	-641.98515	-2.63238	219.09525	1
23515	H	95.19157	87.38449	69.61447	380.63000	-1515.11188	-3261.26246	1
23516	C	93.16010	86.64875	70.18353	550.89294	-272.71642	-844.46611	1
23517	H	93.38868	85.60484	69.83754	1087.21247	701.28098	-2099.99613	1
23518	H	92.17067	86.83661	69.91214	-1221.32844	81.73042	-687.23027	1
23519	C	93.31501	86.63713	71.68570	-688.29891	-586.49175	112.63655	1
23520	C	94.48273	86.87592	72.39868	617.55706	-187.95006	-44.31132	1
23521	H	95.38899	87.14128	71.81840	-2101.93159	364.60971	-659.91911	1
23522	C	94.56539	86.79824	73.82378	-390.73545	-906.94489	-822.23815	1
23523	H	95.53428	86.82857	74.33274	2436.72222	2306.16453	1821.96690	1
23524	C	93.34533	86.70927	74.50617	-312.08853	-596.14629	94.48858	1
23525	H	93.32606	86.57400	75.57474	-105.24581	-1472.26011	-1012.37032	1
23526	C	92.08304	86.29937	72.38803	828.83907	555.05850	-756.99720	1
23527	H	91.14236	86.02324	71.83925	-2243.50576	1522.59101	58.11483	1
23528	C	92.18523	86.45058	73.76362	854.83406	-183.70972	733.52167	1
23529	H	91.28022	86.34297	74.39087	2060.50125	-1785.72503	-482.47856	1
23530	C	93.77747	87.49479	67.68364	-601.40407	-442.21333	-457.75572	1
23531	O	94.20445	86.47304	67.21173	-965.11089	-110.36346	-476.72600	1
23532	N	92.97079	88.38958	67.20503	-24.55287	-505.82539	33.30133	1
23533	H	92.64997	89.11867	67.83213	703.13472	2245.16830	1863.06457	1
23534	C	92.76062	88.56096	65.79221	21.70476	-477.08957	787.30791	1
23535	H	93.68427	88.07871	65.26392	4370.39724	-1217.36335	-654.71441	1
23536	H	92.72932	89.74140	65.73220	-856.02817	3635.15941	-882.42076	1
23537	C	91.44396	87.86683	65.19134	46.94521	-586.89125	956.52637	1
23538	O	91.10842	86.80797	65.73350	108.54665	-24.46720	62.04596	1
23539	N	91.16154	88.37901	64.02693	-247.98547	-174.49821	408.98837	1
23540	H	91.61435	89.27185	63.74389	2484.54846	150.30835	-681.75130	1
23541	C	89.99845	87.97577	63.29645	-21.03500	239.37149	615.85949	1
23542	H	89.37117	87.67893	64.15408	-1168.55638	3566.64245	101.33557	1
23543	C	89.30669	89.16727	62.46225	126.60421	87.37702	-124.64196	1
23544	H	89.64913	89.29715	61.40028	62.30466	-432.27242	-129.46042	1
23545	H	89.57112	90.11717	62.90934	1077.66609	-809.31376	-466.39438	1
23546	C	87.74885	89.12477	62.29148	469.82175	-281.77130	-76.44593	1
23547	O	87.07881	90.12346	62.08146	1334.43960	-202.44487	-499.17704	1
23548	N	87.30593	87.85525	62.38123	728.73417	-193.95387	-49.78392	1
23549	H	87.86640	86.98047	62.40729	2284.19035	2284.71477	938.15901	1
23550	H	86.30653	87.70402	62.30338	1452.22665	2237.80651	-51.69253	1

23551	C	90.16057	86.56959	62.56523	278.19718	234.17339	-315.13445	1
23552	O	89.28083	86.05934	61.88678	-282.80650	227.20442	73.63119	1
23553	N	91.39087	86.02741	62.79273	697.98823	-315.23181	708.41241	1
23554	H	91.79990	86.40279	63.64083	-1021.53296	-580.83372	-50.32905	1
23555	C	91.51800	84.51480	62.52590	-314.84111	337.70502	-798.14484	1
23556	H	90.87200	84.13680	61.74790	641.95804	1485.71105	-2704.10817	1
23557	C	92.98800	84.28580	62.01190	-249.79702	379.53540	794.81225	1
23558	H	93.08100	84.82880	61.04690	1073.81968	-2912.30676	-425.43246	1
23559	H	93.75600	84.78580	62.63890	1117.56010	-2194.36978	1936.55402	1
23560	C	93.37900	82.83780	61.76390	597.74732	-543.57805	-397.25737	1
23561	C	93.09300	82.24380	60.53090	-480.21480	-645.51123	-430.08698	1
23562	H	92.55800	82.73080	59.72890	-1619.03187	-1765.70741	-2043.45513	1
23563	C	93.42400	80.89180	60.32490	-636.94378	-642.80439	106.87966	1
23564	H	93.07600	80.44380	59.40590	-1056.96770	1154.29294	2732.81864	1
23565	C	94.15700	80.14080	61.27890	568.92686	676.62414	-233.26303	1
23566	H	94.35300	79.09980	61.07090	1114.18823	-362.83730	2908.08357	1
23567	C	94.09900	82.07280	62.66490	451.91417	-767.14491	-121.50679	1
23568	H	94.24300	82.65980	63.55990	-96.34455	-3117.79203	326.51976	1
23569	C	94.50800	80.76380	62.47290	665.14410	116.30930	-608.71441	1
23570	H	94.97700	80.15980	63.23490	1550.20926	-1609.03405	-2206.55935	1
23571	C	91.15900	83.68080	63.73290	-522.29095	30.86254	750.72521	1
23572	O	90.49700	82.62580	63.60990	154.76027	367.78046	-687.79781	1
23573	N	91.54500	84.08880	64.97890	400.53455	-696.54886	211.82646	1
23574	H	92.25500	84.78180	65.07190	2438.77680	-1682.31607	1016.28561	1
23575	C	91.05900	83.46380	66.12890	-642.19439	227.29730	-623.13309	1
23576	H	90.97300	82.39880	65.96990	-1288.21407	-1114.91791	-2650.26536	1
23577	C	91.97900	83.68480	67.32190	669.53350	299.83802	530.00399	1
23578	H	92.00800	84.76880	67.56390	96.10404	2286.26177	2163.52663	1
23579	H	91.54900	83.17080	68.20790	2781.77159	1233.65436	-781.71507	1
23580	C	93.41300	83.09980	67.07090	454.38664	790.96032	54.79291	1
23581	H	93.86800	83.56380	66.16990	26.52113	2141.86721	2307.74682	1
23582	C	94.41000	83.62580	68.14990	-610.04034	-662.66560	-149.17717	1
23583	H	94.13600	83.23380	69.15290	1332.97300	-1097.92060	-2626.69494	1
23584	H	94.50000	84.72780	68.25790	-2094.18134	2354.61193	-216.93472	1
23585	H	95.41400	83.22980	67.88390	-2823.45447	-41.15834	-1410.96679	1
23586	C	93.41700	81.60480	66.91190	-596.73741	-409.09612	553.78820	1
23587	H	92.78300	81.17580	66.10690	59.99094	-2200.39947	2234.15968	1
23588	H	93.12900	81.18280	67.89790	-696.67920	1514.11090	-2680.35504	1
23589	H	94.45700	81.21880	66.84390	-1165.69871	-2818.67335	748.54857	1
23590	C	89.61400	83.83780	66.42890	-561.39294	-566.52995	-447.25423	1
23591	O	88.85000	83.03980	67.01290	266.17139	-622.83922	384.07104	1
23592	N	89.25001	85.05581	65.91918	-106.25737	-730.64882	-114.21601	1
23593	H	89.91786	85.70923	65.42524	732.19118	-2077.33553	-1268.87134	1
23594	C	87.82832	85.43484	66.16757	-357.92650	-630.46570	500.59327	1
23595	H	87.91585	85.21197	67.26820	605.92261	2480.86372	-1061.39250	1
23596	C	87.63834	86.98165	66.00021	-283.44298	559.09090	-826.81111	1
23597	H	87.32616	87.18130	64.89774	-3494.38744	-1351.27099	-3093.99707	1
23598	H	88.55126	87.58384	66.32520	-2532.63611	379.50443	1427.15616	1
23599	S	86.20541	87.25131	67.07443	226.20858	100.30766	41.54520	1
23600	C	86.67300	84.54580	65.53490	458.36775	-770.12205	-82.92837	1
23601	O	85.70400	84.06480	66.09490	-64.90151	-663.61914	410.33736	1
23602	N	86.85900	84.23180	64.25690	55.67696	-761.21625	338.14673	1
23603	H	87.68800	84.53680	63.79390	-146.28953	1077.07121	-2958.50408	1
23604	C	86.09400	83.32380	63.49490	119.92114	-821.73656	-355.84907	1
23605	H	85.03600	83.53880	63.49790	2357.78813	-1141.46710	-1724.44075	1
23606	C	86.54900	83.31080	62.03090	101.84808	645.82823	-645.61129	1
23607	H	86.13700	82.48080	61.41790	-315.49305	-3112.58887	-244.61584	1
23608	H	87.65600	83.22380	61.99490	2926.10362	-908.70079	652.02878	1
23609	C	86.19500	84.62180	61.36690	-508.67508	-278.28508	-709.99166	1
23610	H	86.44753	85.58236	61.96966	-1151.47896	3583.99607	-1469.53297	1
23611	H	85.09100	84.55380	61.26190	-2310.29808	-1774.91651	1193.84131	1
23612	C	86.79500	84.65480	59.96290	648.57340	313.57678	-552.93060	1

23613	H	86.34400	83.82380	59.38090	2415.00305	-1982.36036	-199.03186	1
23614	H	87.86800	84.41480	60.12190	-1399.02018	-1530.92573	-2368.60539	1
23615	C	86.37858	85.99619	59.26612	-366.00288	-343.87065	79.62239	1
23616	H	86.74988	86.04445	58.24483	-1192.71165	-179.54523	-3325.90490	1
23617	H	86.60041	86.91048	59.82654	1507.93265	1135.59571	1972.03219	1
23618	N	84.87434	86.09918	59.30726	-15.88492	-125.60069	398.23839	1
23619	H	84.49379	86.59132	58.41759	-2442.32254	-3372.26143	2714.47131	1
23620	H	84.53208	86.57728	60.23301	3832.45911	-3649.11059	2418.97324	1
23621	H	84.33045	85.09830	59.38533	-682.86993	-711.19678	988.35204	1
23622	C	86.02200	81.92880	64.05690	-35.45080	-722.53953	541.57784	1
23623	O	84.99900	81.30480	64.09590	-679.75656	-136.97610	389.71304	1
23624	N	87.20100	81.39480	64.42590	654.38963	332.12546	-411.37386	1
23625	H	88.05400	81.83980	64.16690	1864.48288	1579.56828	-1982.41481	1
23626	C	87.36500	80.09380	65.00890	-816.41882	414.29532	-129.89564	1
23627	H	86.88200	79.29380	64.46790	-850.08403	751.30029	-2943.60695	1
23628	C	88.86800	79.76980	65.00690	374.43435	420.87789	712.23849	1
23629	H	89.28500	79.59280	63.99190	232.44788	2849.84611	-1334.48981	1
23630	H	88.98400	78.87080	65.64790	-2632.33675	1517.72547	855.23828	1
23631	H	89.43500	80.62280	65.43790	-680.75503	322.01465	-3062.06516	1
23632	C	86.72700	79.92780	66.35090	438.45055	-658.59246	428.58437	1
23633	O	85.95200	79.01880	66.54290	8.87594	-526.44235	577.54551	1
23634	N	86.90000	80.80780	67.33590	43.02836	5.85719	-846.19593	1
23635	H	87.40500	81.66380	67.25290	-644.90563	3081.96811	-206.46889	1
23636	C	86.19000	80.52680	68.62890	-54.01345	-739.30871	518.84194	1
23637	H	86.32400	79.48480	68.87990	2480.69677	-1406.45585	-1309.59407	1
23638	C	86.84000	81.26180	69.83390	889.04089	-103.67968	-119.95892	1
23639	H	86.44200	80.90480	70.80790	1399.88128	2480.91490	1334.30405	1
23640	C	88.33400	81.07680	69.72290	-591.05031	639.38682	-306.80738	1
23641	H	88.48300	79.98080	69.82890	-1218.63648	2656.01997	1184.73515	1
23642	H	88.82500	81.27280	68.74590	-2168.56829	-2201.90570	591.68513	1
23643	H	88.77100	81.69980	70.53290	-2083.93822	-2098.25710	1073.92859	1
23644	C	86.58200	82.78080	69.82590	-592.30484	-475.06658	506.39840	1
23645	H	86.96400	83.25980	70.75290	2204.88349	-173.52341	-2231.24693	1
23646	H	85.55100	83.08380	69.54390	615.76563	2761.99008	1381.09233	1
23647	H	87.13100	83.11580	68.91990	-253.69985	3131.74586	-272.20067	1
23648	C	84.70900	80.73080	68.63990	-632.93376	-114.55297	650.64257	1
23649	O	84.02200	80.17280	69.49290	-246.99726	577.78224	486.75900	1
23650	N	84.24600	81.55880	67.65790	-160.86550	-803.22477	180.42175	1
23651	H	84.91200	81.97480	67.04290	1968.06047	1880.40704	1571.70651	1
23652	C	82.80800	81.69580	67.40890	490.44376	-241.22522	719.07705	1
23653	H	82.37200	81.78180	68.39290	-357.39592	-212.66674	-3121.15642	1
23654	C	82.41500	82.92780	66.52990	732.99075	-24.01000	526.49050	1
23655	H	81.41600	82.87480	66.04590	886.31487	-2277.04131	-1970.62278	1
23656	H	83.13300	83.04280	65.69090	-1156.73282	1814.86041	2303.95039	1
23657	N	82.99464	85.41785	67.33251	-137.06055	167.54972	-819.29057	1
23658	H	83.62783	85.85587	66.66844	45.51384	-634.55461	-1076.91690	1
23659	C	82.39900	84.15480	67.43290	892.37825	-118.13890	-48.73980	1
23660	C	82.63684	86.27936	68.29401	129.76532	-668.58627	-334.71898	1
23661	H	82.93134	87.37271	68.54639	864.61219	-3143.44012	1415.54353	1
23662	N	81.76267	85.61744	69.11117	-402.34330	802.57911	-1.55330	1
23663	C	81.65600	84.41580	68.51590	136.32421	-477.04237	-760.27294	1
23664	H	80.87200	83.84280	68.99590	-3030.68003	352.89241	-805.98543	1
23665	C	82.16700	80.46780	66.77990	716.29937	117.56263	-543.46946	1
23666	O	81.09700	80.01880	67.19390	469.88919	-448.28960	430.34229	1
23667	N	82.89000	79.89280	65.78590	178.60863	742.30407	-373.20411	1
23668	H	83.69400	80.36680	65.43590	1905.14723	-541.57481	2432.25945	1
23669	C	82.59700	78.59880	65.20790	44.61787	777.20444	-489.23877	1
23670	H	81.57800	78.58580	64.84890	-1058.63008	2434.04493	1702.79436	1
23671	C	83.57500	78.33080	64.01290	587.18264	-678.89911	51.86181	1
23672	H	84.59400	78.72480	64.21390	-506.67878	2046.68760	-2348.09777	1
23673	C	83.59900	76.78780	63.77490	222.56906	-872.16790	-53.80558	1
23674	H	84.31500	76.28780	64.46290	237.29848	210.01570	-3134.58664	1

23675	H	83.98300	76.51480	62.76890	-2347.76777	290.43070	2081.95348	1
23676	H	82.64600	76.27180	64.01990	-2677.18266	270.47322	-1651.28823	1
23677	C	83.00400	79.04680	62.75690	-688.89411	267.30127	548.01628	1
23678	H	81.91100	78.88580	62.63890	3109.59648	-300.41890	-266.69542	1
23679	H	83.47200	78.73680	61.79890	-202.07650	3031.12063	-856.68925	1
23680	H	83.14800	80.14080	62.88390	1761.75991	-2401.73212	-976.90497	1
23681	C	82.54300	77.54080	66.30590	-640.20002	152.33778	638.21347	1
23682	O	81.51500	76.91780	66.54690	-139.00049	587.41302	515.67853	1
23683	N	83.59100	77.46180	67.16990	118.05853	-110.46016	822.31414	1
23684	H	84.39600	78.01380	66.96890	1947.99311	-1109.82332	-2199.69674	1
23685	C	83.61000	76.47880	68.21290	164.42156	-878.69462	-138.38041	1
23686	H	83.48300	75.48980	67.79590	1992.96545	-2184.51893	-1049.43428	1
23687	C	85.03500	76.38780	68.80890	-556.68581	-700.11344	-181.95602	1
23688	H	85.44800	77.41780	68.87090	-1712.21024	1687.22724	2037.63034	1
23689	C	85.07400	75.72080	70.18590	-547.45866	-533.84552	493.75497	1
23690	H	86.10000	75.62280	70.60190	-2619.49490	1746.09905	-225.49320	1
23691	H	84.55100	76.30080	70.97590	-504.51032	-1165.57100	2872.75286	1
23692	H	84.66100	74.69080	70.12890	2360.72387	-2050.74295	237.51182	1
23693	C	85.97700	75.72480	67.76590	-98.18311	-238.41847	868.29468	1
23694	H	85.69100	74.65480	67.67490	-1516.47071	2275.84290	-1579.19068	1
23695	H	85.74100	76.16480	66.77290	1462.57973	1874.99856	2055.33318	1
23696	C	87.47200	75.97180	67.95890	390.06594	406.60744	710.68259	1
23697	H	88.05300	75.45780	67.16290	1576.13022	-2592.13432	-798.95125	1
23698	H	87.73000	75.66880	68.99590	1400.72879	3.39213	2807.28553	1
23699	H	87.69600	77.04780	67.79490	1752.71508	-1723.16113	-1955.06933	1
23700	C	82.51700	76.61280	69.28290	-620.28303	86.79355	-675.01447	1
23701	O	81.96700	75.61980	69.76790	-708.37877	241.28089	274.05532	1
23702	N	82.13600	77.82380	69.67790	-405.37820	-492.03869	550.69439	1
23703	H	82.59400	78.62980	69.31090	643.48411	2523.32227	1767.65899	1
23704	C	81.05000	78.07380	70.56590	646.20240	-585.12291	-237.33088	1
23705	H	81.27600	77.50580	71.45590	-385.17836	-3111.51755	-210.90985	1
23706	C	81.05200	79.58980	71.00790	-122.45321	868.02473	269.13565	1
23707	H	80.98000	80.15680	70.05590	934.85597	-567.14802	-2948.55670	1
23708	H	82.02300	79.80180	71.50490	-1756.22962	661.79516	-2534.59089	1
23709	C	79.92200	80.03280	71.97990	444.64135	532.81259	587.62017	1
23710	C	79.38500	79.12780	72.88490	747.08396	204.11898	-473.48387	1
23711	H	79.82100	78.13980	72.84190	2337.29381	-2085.87072	175.96666	1
23712	C	78.46300	79.55580	73.85390	-200.60253	802.41742	-397.01121	1
23713	H	78.13700	78.88380	74.63390	502.81930	2846.76741	1244.38230	1
23714	C	77.98700	80.85580	73.88990	702.32145	193.96661	-541.05088	1
23715	O	76.96700	81.12580	74.81990	326.91092	-635.25500	-323.92512	1
23716	H	77.08100	82.02380	75.14090	1599.39933	-1707.94424	2094.54542	1
23717	C	79.47200	81.38480	72.01490	-512.08454	743.42893	175.91709	1
23718	H	79.94600	82.09480	71.35290	1997.37048	-795.13771	2286.85788	1
23719	C	78.48900	81.79280	72.93090	683.63573	409.78497	-435.38856	1
23720	H	78.06400	82.77980	73.03490	43.21796	761.38660	-3053.68203	1
23721	C	79.67300	77.54080	70.07190	-599.60519	-266.32678	-641.46102	1
23722	O	78.96500	76.79380	70.76590	472.86070	-467.85158	-414.18717	1
23723	N	79.39400	77.68380	68.75890	-750.56784	-396.55506	3.18549	1
23724	H	79.95300	78.19680	68.11190	-1161.45304	-979.47494	2753.69883	1
23725	C	78.20500	77.02080	68.19390	53.36784	801.68309	438.01833	1
23726	H	77.43900	76.92980	68.94890	2948.95071	317.17172	1024.98411	1
23727	C	77.48800	77.80880	67.07390	356.32206	-635.43654	-537.39957	1
23728	H	76.97700	77.12180	66.36490	1480.23108	-2369.63446	1424.18386	1
23729	O	78.48200	78.54080	66.33890	-438.91983	-396.49627	-528.04442	1
23730	H	77.96600	79.06380	65.71990	-583.51300	2171.64280	2207.61326	1
23731	C	76.51200	78.84980	67.67590	688.63003	564.42455	179.79774	1
23732	H	76.14500	79.53180	66.87990	2240.35661	-1711.13794	-1375.63757	1
23733	H	77.06600	79.47580	68.40790	2625.80217	-1595.41141	626.26001	1
23734	H	75.64300	78.39980	68.20290	-722.19249	1855.38658	2441.24259	1
23735	C	78.36700	75.56380	67.75190	-15.45537	-791.20725	439.20027	1
23736	O	77.49200	74.70580	67.73790	231.74486	731.95887	-200.53705	1

23737	N	79.64800	75.13880	67.41590	-417.04813	729.58663	146.55234	1
23738	H	80.37000	75.81880	67.31490	481.84237	-2724.87400	-1486.18360	1
23739	C	79.99100	73.68980	67.21490	88.61976	910.31216	-75.63605	1
23740	H	79.38000	73.32380	66.40290	1627.53249	86.60163	2681.67877	1
23741	C	81.38900	73.44280	66.61790	744.85556	-136.45899	488.45660	1
23742	H	82.10200	74.18380	67.03690	-7.17878	-3122.37513	321.67498	1
23743	C	81.96200	72.04380	66.97190	581.85838	170.24355	670.09217	1
23744	H	82.88300	71.83080	66.38890	1726.18988	-1900.91977	-1808.47207	1
23745	H	81.18600	71.31880	66.64490	2495.23235	-876.93291	-1693.93308	1
23746	H	82.34400	71.99180	68.01390	417.09881	-1852.17733	-2508.37003	1
23747	C	81.32400	73.80080	65.10990	462.85643	442.26735	643.13038	1
23748	H	80.97800	74.84980	64.98990	2737.92801	-1509.59695	-229.85742	1
23749	H	82.37400	73.66580	64.77390	-1760.96601	1443.80697	-2188.29896	1
23750	H	80.63300	73.08980	64.60990	673.90006	-2975.76099	724.53691	1
23751	C	79.75400	72.79980	68.47990	-619.47648	625.62151	-275.61530	1
23752	O	79.20000	71.70380	68.33390	532.05505	395.53368	419.73852	1
23753	N	80.08100	73.22380	69.70090	172.91307	-496.29476	649.76621	1
23754	H	80.50800	74.12280	69.76890	-630.92253	-2683.67019	-1513.74082	1
23755	C	79.61600	72.58280	70.91190	-765.40476	82.82988	-505.29216	1
23756	H	79.83700	71.53080	70.80090	-2395.78744	-662.87450	1930.26743	1
23757	C	80.32000	73.15880	72.15090	166.68697	890.87963	121.05007	1
23758	H	80.52000	74.24680	72.04990	-494.45600	2922.19678	-1076.19734	1
23759	H	81.33400	72.70680	72.18690	-1949.49855	-1099.58608	-2219.90203	1
23760	C	79.57500	73.06880	73.50490	-6.02462	-706.39997	567.06380	1
23761	O	78.59100	73.73680	73.79790	496.58987	-66.62512	-608.64221	1
23762	N	80.05400	72.13480	74.36090	390.92450	-699.02938	242.07280	1
23763	H	80.91400	71.64380	74.22290	2437.24680	1923.59509	-498.06818	1
23764	H	79.62900	72.06180	75.26290	-1609.93060	-1822.22870	1993.21624	1
23765	C	78.06400	72.62880	71.06090	-130.35900	906.99412	-51.15619	1
23766	O	77.44500	71.63380	71.38190	-394.11678	287.39302	622.90152	1
23767	N	77.42000	73.74480	70.75490	-514.51697	-662.82992	-102.80784	1
23768	H	77.98600	74.52280	70.49790	-2042.12336	-2302.99929	653.81551	1
23769	C	76.00300	73.97580	70.88590	-853.49326	104.48439	-328.17675	1
23770	H	75.75900	73.92180	71.93690	1775.83032	-2456.36118	812.57362	1
23771	C	75.56400	75.38480	70.54190	-260.84233	-866.59548	88.80442	1
23772	H	75.41200	75.53680	69.45190	2139.40063	1429.51646	1802.39704	1
23773	H	76.35700	76.10880	70.82590	2119.95453	-2284.69824	-363.89328	1
23774	C	74.25900	75.91580	71.28290	-532.63391	548.48908	507.24060	1
23775	H	73.50300	75.10180	71.26190	-1673.71938	-2296.31594	1350.56780	1
23776	C	74.54200	76.24980	72.74990	-625.08393	-481.67277	460.69830	1
23777	H	74.82100	75.38380	73.38690	-358.26018	2868.99237	-1252.75363	1
23778	H	73.69400	76.78080	73.23390	-1927.88942	2245.74079	1084.89629	1
23779	H	75.40100	76.95280	72.71390	-596.90663	-2944.67558	923.91443	1
23780	C	73.71700	77.15380	70.58690	-95.59545	485.33462	768.21288	1
23781	H	72.74800	77.35680	71.09090	-1284.05773	2229.85564	1819.58436	1
23782	H	73.66100	76.90080	69.50690	-2211.89881	939.00296	2040.21554	1
23783	H	74.31300	78.05480	70.84590	-1242.66947	-2559.58921	1340.34148	1
23784	C	75.09600	73.04480	70.08690	-830.67000	391.40814	-68.73387	1
23785	O	74.19500	72.43780	70.57690	519.18896	459.19864	-377.07439	1
23786	N	75.58000	72.79280	68.84390	436.15886	-707.58737	-89.98110	1
23787	H	76.37800	73.29880	68.52390	593.94315	1451.42222	-2732.23636	1
23788	C	75.03800	71.79380	67.92590	32.93483	-544.63417	-729.87678	1
23789	H	73.97500	71.68380	68.08490	-951.47697	2270.49321	1965.34726	1
23790	C	75.21300	72.27780	66.44590	-7.92597	-905.10498	-37.37704	1
23791	H	74.68000	71.57580	65.76990	-399.32974	2225.39817	2191.84349	1
23792	H	76.30400	72.25780	66.23490	1244.19765	1670.42319	-2361.98875	1
23793	C	74.58800	73.64280	66.30190	17.91820	867.05587	296.10125	1
23794	C	73.40500	74.05580	66.90090	-629.94929	172.76706	-648.54161	1
23795	H	72.87400	73.31580	67.48090	2137.53221	2092.16844	-971.97083	1
23796	C	72.89700	75.36980	66.79290	-866.40716	249.81499	-191.97272	1
23797	H	72.03100	75.61380	67.39190	1594.61666	2179.29777	1611.49213	1
23798	C	73.59500	76.30480	66.07290	-548.19151	458.28481	-581.56154	1

23799	O	73.11000	77.58880	66.04690	451.16441	-249.30900	587.55699	1
23800	H	73.77800	78.08480	65.56790	2097.73861	-2261.07488	562.46490	1
23801	C	75.25300	74.59480	65.48390	-693.82110	87.46767	-599.33160	1
23802	H	76.17700	74.26580	65.03190	43.90296	-2922.94761	1142.27067	1
23803	C	74.76400	75.91180	65.39090	326.51314	472.42453	706.07737	1
23804	H	75.26000	76.67480	64.80990	2038.03290	-728.82327	-2274.80383	1
23805	C	75.55000	70.36280	68.08790	-738.36483	231.49811	-500.99192	1
23806	O	74.98700	69.48580	67.47890	484.80912	-461.66460	-407.98912	1
23807	N	76.64500	70.10980	68.85690	324.60309	-569.45571	-526.45440	1
23808	H	77.20900	70.81580	69.27890	-339.70625	-1607.88736	2675.75720	1
23809	C	77.21400	68.74780	68.93090	-690.73412	-61.80774	-605.38966	1
23810	H	76.76200	68.11280	68.18290	-2607.33324	1615.93048	732.73339	1
23811	C	78.76800	68.59680	68.72990	596.02643	453.96324	510.22043	1
23812	H	78.91700	68.76980	67.64290	2138.28278	-2293.65718	60.69739	1
23813	H	79.12100	67.55780	68.90390	-2646.86455	-693.10762	1555.95790	1
23814	O	79.43400	69.45380	69.61290	753.72654	216.49744	7.30554	1
23815	H	79.36600	70.29480	69.15390	-3054.98067	-659.25907	404.56468	1
23816	C	76.83600	68.12980	70.21990	498.71611	598.64270	-478.33864	1
23817	O	76.31600	67.01880	70.22490	-312.07694	534.42851	-505.87461	1
23818	N	76.90800	68.88580	71.39690	76.33347	474.55010	-701.74167	1
23819	H	77.09200	69.86380	71.34290	-1873.04815	2138.99858	1358.29924	1
23820	C	76.65900	68.29280	72.72790	493.82183	466.96369	-611.47836	1
23821	H	77.37300	67.49480	72.86990	-357.76700	-43.84511	-3132.16884	1
23822	C	76.99100	69.27280	73.89690	719.73008	76.41368	-552.60761	1
23823	H	78.08900	69.43780	73.90890	361.06741	3126.67842	-106.55854	1
23824	H	76.72300	68.86880	74.89590	2924.45232	81.36901	1137.66210	1
23825	O	76.37400	70.60180	73.75590	273.61857	523.50887	-528.99627	1
23826	H	76.99100	71.20580	73.33690	528.11915	2600.07205	-1699.16572	1
23827	C	75.22200	67.71180	72.98090	196.28844	-546.19085	693.27251	1
23828	O	75.04700	66.54180	73.22690	538.98853	-305.48630	-486.85253	1
23829	N	74.23400	68.54880	72.77190	-758.33135	-378.09186	-40.27274	1
23830	H	74.49300	69.49780	72.60890	1261.70224	2610.83105	1217.32485	1
23831	C	72.81700	68.20780	72.84690	703.93705	-424.81460	-384.02028	1
23832	H	72.69700	67.79180	73.83690	-692.38117	-1497.57152	-2683.39721	1
23833	C	71.92400	69.42580	72.75590	202.77923	-32.89934	882.88937	1
23834	H	72.28100	70.22380	73.44090	-2091.53959	2287.16702	572.96627	1
23835	C	71.88500	70.06880	71.32090	493.00725	-488.95624	-585.77024	1
23836	H	72.95400	70.30580	71.12690	2772.48877	743.89161	1271.35317	1
23837	H	71.46800	69.35080	70.58190	1517.77981	-1884.46883	-2005.61431	1
23838	H	71.31100	71.01980	71.33190	2630.76383	-1626.74725	-534.69420	1
23839	C	70.59100	69.04780	73.37790	-378.88912	-732.89266	385.00383	1
23840	H	69.91400	69.92780	73.42990	1618.89530	2264.70550	1460.04092	1
23841	H	70.01500	68.20180	72.94690	-870.29212	-2004.25216	2259.40314	1
23842	H	70.85600	68.68180	74.39290	-475.23382	2022.86710	2361.68283	1
23843	C	72.36900	67.11980	71.85690	623.20020	362.10758	-558.81193	1
23844	O	71.52900	66.26080	72.13090	-595.74733	366.56695	-384.55340	1
23845	N	72.91100	67.09180	70.61690	-455.97143	172.27515	-699.66837	1
23846	H	73.50900	67.85780	70.39290	1958.03657	-650.46098	-2373.29850	1
23847	C	72.45400	66.06380	69.71790	461.99671	-457.81713	625.57484	1
23848	H	71.39000	65.90280	69.80790	2184.99381	1250.03941	-1887.47170	1
23849	C	72.66000	66.54280	68.23090	-177.42518	-608.43741	647.48733	1
23850	H	72.52100	65.61380	67.63890	-2069.03808	-952.19184	2169.35455	1
23851	H	73.68700	66.96680	68.24990	1998.35153	413.78573	-2394.70920	1
23852	C	71.72500	67.59780	67.72090	121.19142	-722.64103	529.47482	1
23853	C	71.74100	68.95780	67.92090	886.99513	-24.53604	170.31397	1
23854	H	72.58600	69.44280	68.38690	2022.75025	2063.16446	1237.10149	1
23855	N	70.70500	69.55680	67.31790	719.53588	426.09331	-84.48278	1
23856	H	70.35400	70.42880	67.57890	-1981.56115	-1646.90024	1806.18484	1
23857	C	69.94900	68.58180	66.73890	235.53366	-58.03303	-880.19701	1
23858	C	70.55000	67.30580	66.99790	-198.50399	178.07977	870.36562	1
23859	C	69.90800	66.17080	66.61990	-101.37054	-655.12410	616.99733	1
23860	H	70.39900	65.26380	66.93990	2041.65126	-2011.44243	1272.68526	1

23861	C	68.76100	66.27480	65.85090	-384.86010	-612.26075	550.34397	1
23862	H	68.26800	65.37480	65.51390	1723.02216	-2323.15690	1212.00617	1
23863	C	68.83000	68.69180	65.97190	722.53225	-298.96665	-456.21608	1
23864	H	68.33200	69.62280	65.74690	-2328.63348	1344.50900	1646.60985	1
23865	C	68.20200	67.49880	65.54590	-252.48188	-636.25672	596.14240	1
23866	H	67.29300	67.52580	64.96390	-1273.79055	2123.00722	-1956.12699	1
23867	C	73.19300	64.74780	69.88990	-489.30772	-406.56480	-661.24204	1
23868	O	72.67800	63.69780	69.58190	-233.60774	521.33148	-558.55381	1
23869	N	74.40600	64.73880	70.51790	300.33587	447.64090	-656.17288	1
23870	H	74.96100	65.55880	70.63090	534.99465	-2258.70916	-2123.53367	1
23871	C	74.94700	63.53980	71.09390	205.50117	672.67114	576.15143	1
23872	H	75.05800	62.74180	70.37490	1187.37735	-1522.03301	2471.27108	1
23873	C	76.44200	63.74480	71.56290	-170.28977	-873.13127	-192.98627	1
23874	H	76.37000	64.76080	72.00790	-1636.27212	2148.64190	1618.30073	1
23875	C	76.85300	62.73380	72.62490	-614.08486	-644.14417	194.61024	1
23876	H	77.96400	62.74180	72.63890	2690.82302	-1616.65571	-45.44834	1
23877	H	76.59800	61.68380	72.36590	1174.25606	2734.89555	1016.14241	1
23878	H	76.41300	62.97180	73.61690	-1483.48706	1608.29212	-2274.23664	1
23879	C	77.39100	63.63880	70.36590	2.02453	270.51159	864.67500	1
23880	H	76.79400	64.06380	69.53090	456.22267	-2929.35831	-1043.04055	1
23881	H	77.58600	62.57880	70.09590	-1522.33790	1473.88629	2324.72180	1
23882	C	78.55700	64.57680	70.48490	833.31547	-350.08014	-28.82711	1
23883	H	79.21500	64.35480	71.35190	-442.63608	-2981.14660	-897.69110	1
23884	H	78.21700	65.63480	70.49190	2169.61326	-1944.70136	1159.98261	1
23885	H	79.23400	64.48180	69.60890	-338.07991	2201.89939	2220.20129	1
23886	C	74.09700	62.96180	72.24090	643.98279	642.01619	39.32556	1
23887	O	73.82900	61.77480	72.30290	-143.84965	181.02449	-764.32075	1
23888	N	73.51000	63.84680	73.06590	350.91058	-533.48797	538.90566	1
23889	H	73.79600	64.80180	73.04790	598.83253	2819.82152	1259.03548	1
23890	C	72.53000	63.56280	74.09690	-372.74664	822.39106	150.88159	1
23891	H	72.92800	62.80480	74.75590	-2235.70465	-2201.25487	-260.62730	1
23892	C	72.31300	64.68880	75.09590	-718.61129	536.43211	-198.55836	1
23893	H	71.43000	64.41080	75.70990	733.09784	-1444.89752	2688.71754	1
23894	H	71.98400	65.56780	74.50090	982.98567	-2621.13423	1421.93926	1
23895	C	73.46500	64.97780	76.06990	310.77232	812.52691	-280.37822	1
23896	H	74.37300	65.14780	75.45290	-1412.77966	-146.27732	2803.47063	1
23897	C	73.19900	66.08480	77.11390	-690.87982	-495.35593	-342.32155	1
23898	H	74.07700	66.31080	77.75590	170.57592	-2542.35200	-1848.37104	1
23899	H	72.87400	67.00380	76.57990	-2614.76317	-1499.93874	906.71710	1
23900	H	72.38300	65.70780	77.76590	1611.42585	-2453.78058	-1127.49665	1
23901	C	73.79100	63.67480	76.88490	647.00214	175.89547	-620.46536	1
23902	H	74.66400	63.90280	77.53190	1925.89868	-2009.14973	1452.19707	1
23903	H	72.87900	63.35080	77.43090	-542.02898	2886.01368	1129.03557	1
23904	H	74.16100	62.87780	76.20390	839.19187	-2802.67704	-1155.33045	1
23905	C	71.22700	62.91880	73.51690	182.50807	-386.97716	-808.81667	1
23906	O	70.71800	61.98380	74.14690	572.32794	-40.76907	530.69074	1
23907	N	70.70300	63.40180	72.34790	122.58244	635.50850	538.66868	1
23908	H	71.10300	64.26580	72.05290	181.07960	101.74061	-3144.70988	1
23909	C	69.73400	62.58180	71.58590	648.34332	-575.12251	-268.42957	1
23910	H	68.87900	62.38480	72.21590	1292.68007	-2809.95447	-553.13786	1
23911	C	69.26800	63.38280	70.33890	-415.98133	458.27721	670.51897	1
23912	H	68.28800	62.96680	70.02090	2100.01921	-2274.49337	515.39410	1
23913	H	69.96100	63.29480	69.47590	-2169.74637	29.44790	-2289.89062	1
23914	H	69.03900	64.45180	70.53990	1001.19022	952.27062	-2830.56755	1
23915	C	70.21000	61.21680	71.12590	485.52598	601.92988	-488.54126	1
23916	O	69.50700	60.27980	71.39790	-538.20560	-399.96629	-427.50780	1
23917	N	71.39700	61.10080	70.48690	-231.10616	-772.99183	234.04033	1
23918	H	71.96500	61.91780	70.43290	2161.00328	696.11652	-2180.21176	1
23919	C	71.91600	59.80780	70.10590	-131.76248	580.05229	688.18706	1
23920	H	71.21400	59.26580	69.48990	-696.12998	-1785.35097	-2501.25870	1
23921	C	73.26300	60.01580	69.27590	218.20334	189.20292	-872.24376	1
23922	H	73.86400	59.08180	69.30890	-1625.27937	-2118.81823	-1671.43583	1

23923	H	73.85400	60.81780	69.76790	1907.54809	-1736.68707	-1797.76264	1
23924	C	73.07700	60.37180	67.86290	-628.60216	-258.40322	604.55473	1
23925	C	71.99300	61.12680	67.38390	-160.61150	-687.47958	-579.58518	1
23926	H	71.19200	61.52980	67.98490	-1058.16331	-1862.78307	2296.25158	1
23927	C	71.80300	61.37380	66.02090	-115.57533	-454.91596	-786.29457	1
23928	H	70.93800	61.91180	65.66190	-2704.05929	573.98030	-1523.91824	1
23929	C	72.70500	60.88880	65.10690	551.44707	-580.45346	411.01262	1
23930	H	72.48900	61.01780	64.05590	-1401.12217	1805.65015	-2179.77737	1
23931	C	73.97600	59.87980	66.90290	-675.00621	-286.58379	-555.12678	1
23932	H	74.74700	59.17780	67.18090	-526.20559	-1943.58855	-2422.71101	1
23933	C	73.75000	60.08480	65.52790	338.21879	-758.88555	348.12355	1
23934	H	74.35200	59.44180	64.90390	1609.41313	-2422.45396	1168.43439	1
23935	C	72.12500	58.72180	71.18490	-309.08295	859.87109	-88.78740	1
23936	O	71.74000	57.56280	70.96290	-450.74789	521.30109	-405.22988	1
23937	N	72.61100	59.07480	72.37390	619.37944	-38.21568	558.54478	1
23938	H	72.89000	60.02280	72.50490	-2039.37977	-299.12877	-2388.61338	1
23939	C	72.68100	58.14080	73.49390	708.97810	-430.88606	357.45936	1
23940	H	73.09600	57.19180	73.18990	-1638.31849	657.59144	-2616.76016	1
23941	C	73.64600	58.74880	74.51190	255.77426	-15.45086	865.29395	1
23942	H	74.62300	58.87080	73.99490	-2072.23954	-1940.68312	-1366.77572	1
23943	C	73.16700	60.07580	75.15390	435.61198	-540.05119	-593.80901	1
23944	H	72.36900	59.90880	75.90790	-1739.45405	-1836.82695	-1879.90486	1
23945	H	72.74200	60.71680	74.35090	2071.55604	1148.21861	-2075.11122	1
23946	H	73.98700	60.55380	75.73090	56.95115	-2000.80573	-2433.02826	1
23947	C	74.00800	57.66680	75.58290	-411.79847	567.39218	-597.19857	1
23948	H	74.22300	56.72280	75.03790	-1798.06929	1570.17343	-2064.29712	1
23949	H	73.10600	57.48480	76.20490	-1529.55720	1841.99986	-2054.55968	1
23950	C	75.17000	58.18180	76.40990	761.30637	232.02322	-448.62555	1
23951	H	76.07100	58.47080	75.82890	2382.84635	-200.87051	2030.30033	1
23952	H	74.83000	59.07680	76.97390	-1841.75455	2220.25220	-1273.48893	1
23953	H	75.49500	57.43180	77.16290	2555.24984	732.06459	1669.21487	1
23954	C	71.27200	57.86480	74.12990	-478.07483	548.98183	-563.71422	1
23955	O	71.00500	56.75880	74.66690	-273.65406	341.08985	652.05306	1
23956	N	70.33700	58.79980	73.99790	641.71210	537.06900	89.08113	1
23957	H	70.55600	59.61580	73.46790	776.24324	-2095.15863	-2217.82991	1
23958	C	68.93700	58.59380	74.35490	588.89804	570.71732	-402.55005	1
23959	H	68.88800	58.26980	75.38390	203.23721	2079.24169	-2361.03565	1
23960	C	68.03700	59.88580	74.21290	-222.12311	-814.89646	334.76139	1
23961	H	66.94500	59.71580	74.32590	-663.69994	-2533.94876	1735.14646	1
23962	H	68.26200	60.32580	73.21790	-1038.34843	-2153.58984	-2051.15742	1
23963	O	68.38100	60.83480	75.21390	-258.51343	747.89098	44.86106	1
23964	H	69.14200	61.29780	74.85590	798.65678	3023.22937	-361.03401	1
23965	C	68.26600	57.55280	73.49690	-34.64225	-623.44795	-669.78394	1
23966	O	67.62400	56.66180	74.00890	-151.56733	766.53488	-141.11515	1
23967	N	68.41900	57.71580	72.14690	-292.81708	-25.95530	-800.49424	1
23968	H	68.91000	58.48880	71.75390	1140.43721	-2419.80352	1640.31736	1
23969	C	68.00800	56.73880	71.10290	154.59126	-400.43724	-809.47162	1
23970	H	66.93000	56.69380	71.05990	-2634.46903	1719.21771	-207.97587	1
23971	C	68.42200	57.32980	69.74790	-565.77673	-684.20661	-217.27932	1
23972	H	68.40100	56.60980	68.90190	699.79321	2174.96144	-2173.20039	1
23973	H	69.46400	57.71380	69.75790	-2182.27260	983.25788	2042.04955	1
23974	C	67.53700	58.48480	69.21390	-509.04354	81.57893	749.55058	1
23975	H	67.35400	59.16180	70.07590	1497.21856	-2759.38451	62.57491	1
23976	C	68.30300	59.44180	68.21290	-895.61475	92.00868	-187.77756	1
23977	H	67.50000	60.12880	67.86990	-473.68580	2720.45063	-1524.11903	1
23978	H	68.58400	58.83980	67.32290	3132.79836	-194.67120	-69.94405	1
23979	H	69.13000	60.00380	68.69590	-2156.15281	630.44582	-2216.70720	1
23980	C	66.27600	58.00980	68.50990	-861.56866	272.50213	-172.18448	1
23981	H	66.46300	57.26280	67.70990	-2988.03930	-565.76506	818.08468	1
23982	H	65.65900	58.82780	68.07890	796.64720	-1276.57705	-2765.46102	1
23983	H	65.59800	57.65380	69.31590	1204.62388	2489.99411	-1507.39327	1
23984	C	68.65300	55.42080	71.41890	386.38309	-377.78527	-738.50772	1

23985	O	67.96100	54.39280	71.36790	450.99383	548.47046	-353.16586	1
23986	N	69.99700	55.34680	71.65690	346.71945	566.61872	512.77007	1
23987	H	70.50300	56.19780	71.54090	-1984.42164	-2337.97912	696.34487	1
23988	C	70.66600	54.11680	71.95390	431.14343	177.04636	-791.38270	1
23989	H	70.37400	53.43580	71.16790	858.97596	2362.43786	-1903.96474	1
23990	C	72.21100	54.42880	71.99990	386.65291	680.85764	-478.46943	1
23991	H	72.41300	55.16980	72.80390	347.39631	-483.57060	-3097.72771	1
23992	H	72.52700	54.79380	70.99990	-2879.08386	-486.36130	-1191.42693	1
23993	C	72.99600	53.16680	72.28990	-162.36433	901.00101	23.58668	1
23994	O	73.09800	52.74080	73.45190	-323.81024	-33.74805	710.50385	1
23995	O	73.42800	52.48280	71.30890	17.19265	-568.35196	532.86874	1
23996	C	70.16900	53.41580	73.19190	742.77876	14.57817	513.42717	1
23997	O	70.09800	52.19680	73.28190	-326.03462	-298.40892	645.09130	1
23998	N	69.80300	54.19280	74.24790	-538.52781	-441.30656	470.39086	1
23999	H	69.85400	55.18780	74.23790	-102.52100	2182.23573	2257.74734	1
24000	C	69.17300	53.66180	75.45390	485.67326	636.36060	426.27044	1
24001	H	69.73600	52.83980	75.86990	-2532.61294	-1778.37191	-585.60540	1
24002	C	69.09800	54.71380	76.61790	-511.92869	605.20728	-465.13399	1
24003	H	69.19700	55.75280	76.23590	-2709.95308	521.74877	-1526.03547	1
24004	H	68.12200	54.60580	77.13890	1666.07427	1345.95866	-2311.39773	1
24005	C	70.26100	54.47080	77.66490	625.76425	-234.80350	607.57599	1
24006	H	70.11000	55.20080	78.48890	-1949.05624	1914.79601	1555.66742	1
24007	H	70.18700	53.40880	77.98390	-1772.06706	-2204.40894	1370.24183	1
24008	C	71.68300	54.73580	77.10590	319.95907	729.92053	433.92246	1
24009	H	72.30700	54.92680	78.00490	1722.79218	1880.79349	1830.99462	1
24010	H	71.52300	55.67780	76.53890	1227.31225	-704.41588	2798.91778	1
24011	N	72.29500	53.58780	76.26790	-649.48269	-479.90054	240.73562	1
24012	H	72.33300	53.71780	75.27790	-2300.91377	1213.15076	-1786.09770	1
24013	C	72.51900	52.36480	76.67390	658.79524	239.81014	569.80737	1
24014	N	72.45100	51.90980	77.92390	520.40839	588.43220	296.66953	1
24015	H	72.43900	52.51280	78.72190	-1789.89220	2470.46668	767.75309	1
24016	H	72.53400	50.92280	78.06190	616.86770	37.44322	3073.25972	1
24017	N	72.86300	51.48580	75.77490	-502.92684	367.77036	562.87129	1
24018	H	72.93300	51.87680	74.85690	425.10840	-2756.69158	-1460.24775	1
24019	H	73.24600	50.61580	76.08390	2885.34443	27.61262	-1258.51722	1
24020	C	67.78400	53.02580	75.23090	415.89836	-700.06882	394.58431	1
24021	O	67.57600	51.90080	75.66890	736.34238	-6.12107	-286.14530	1
24022	N	66.94800	53.66880	74.42790	268.38440	-524.78883	-609.45730	1
24023	H	67.26800	54.51680	74.01190	-118.71029	572.50983	3083.56521	1
24024	C	65.70600	53.17180	73.94890	798.57576	-340.13837	-273.85681	1
24025	H	65.24000	52.91680	74.88890	-777.19848	2936.86036	818.69882	1
24026	C	65.01600	54.39180	73.21590	-518.41563	-571.16632	-495.91629	1
24027	H	65.75700	55.08780	72.76690	581.60943	-1169.21922	-2868.10925	1
24028	H	64.48300	54.96280	74.00590	-1922.49656	-1948.20523	-1561.50398	1
24029	C	63.96000	54.00580	72.20890	585.02317	-648.56867	-252.85794	1
24030	C	62.81500	53.27380	72.56890	77.90767	-899.83397	97.58132	1
24031	H	62.64500	52.99980	73.59990	-1371.72827	-1994.38578	2002.98816	1
24032	C	61.86200	53.00680	71.55590	-404.11114	297.81288	757.07708	1
24033	H	60.98800	52.51080	71.95090	-297.05407	-3087.18672	-525.41814	1
24034	C	62.07000	53.38380	70.23690	-278.41132	82.26813	858.85904	1
24035	O	61.17200	53.02380	69.23190	490.50998	-71.58155	-617.49853	1
24036	H	61.57000	53.06280	68.35890	846.26218	-2243.81213	2022.91976	1
24037	C	64.22300	54.25280	70.86090	645.44227	-302.93341	-568.85148	1
24038	H	65.19200	54.70680	70.71490	1344.70304	2776.59144	-628.17127	1
24039	C	63.28000	53.95980	69.85490	-282.88346	538.36387	676.59364	1
24040	H	63.50300	54.29180	68.85190	1269.87847	-1225.09801	-2607.79956	1
24041	C	65.83400	51.91380	73.11590	570.09357	144.67543	-702.98137	1
24042	O	65.14200	50.94680	73.39390	548.59067	522.52322	-227.76100	1
24043	N	66.72600	51.85580	72.13990	417.84106	577.38608	-461.39207	1
24044	H	67.18100	52.70080	71.86790	1198.78391	-1027.58146	2709.18606	1
24045	C	67.06100	50.73780	71.34590	785.97495	427.23626	-174.59115	1
24046	H	66.18800	50.37980	70.82090	-2266.40685	-448.14061	-2149.12831	1

24047	C	68.18900	50.95680	70.27890	608.44143	649.53353	186.62614	1
24048	H	68.49600	49.97580	69.85790	1443.40853	1578.25930	2296.81528	1
24049	H	69.07300	51.42780	70.75990	-526.79684	3104.55861	89.92415	1
24050	C	67.74500	51.90280	69.18490	-396.14694	-811.61088	104.76430	1
24051	H	67.22000	52.78380	69.61290	-1781.41989	1365.21645	2202.18508	1
24052	C	68.90400	52.46280	68.26490	504.95426	644.93313	-410.88927	1
24053	H	69.21300	51.65180	67.57190	-820.20035	2424.67766	1828.26751	1
24054	H	69.81900	52.69180	68.85290	2302.05945	-1571.81411	-1455.44090	1
24055	H	68.67000	53.44480	67.79890	-518.40019	2264.39172	2119.08616	1
24056	C	66.79800	51.18780	68.16290	108.46188	249.95829	-880.23372	1
24057	H	67.28100	50.33580	67.63890	-1966.22193	-2095.88910	-1290.70459	1
24058	H	66.50300	51.92080	67.38290	-1871.88238	482.04052	-2496.44150	1
24059	H	65.90400	50.68680	68.59190	-1254.86745	1248.48020	-2614.70789	1
24060	C	67.57100	49.59980	72.22890	-514.05196	-752.71970	2.31411	1
24061	O	67.16500	48.45580	72.05690	166.26395	-392.52137	-672.66968	1
24062	N	68.39700	49.92080	73.24090	640.73237	411.91259	-370.88811	1
24063	H	68.72700	50.85680	73.34190	1475.57266	-44.98565	2766.14541	1
24064	C	69.08400	48.91580	74.02090	-274.21480	-764.85011	400.53276	1
24065	H	69.46000	48.13080	73.38090	1794.28436	437.75446	2533.73362	1
24066	C	70.26000	49.50580	74.88190	465.07817	-768.30340	124.75253	1
24067	H	69.96200	50.21280	75.68490	2051.24820	1368.97422	1941.07548	1
24068	H	70.89000	50.10780	74.19090	-2150.13984	1285.24650	-1920.06528	1
24069	H	70.83600	48.64580	75.28590	1456.55190	2742.13972	-522.23648	1
24070	C	68.12500	48.26380	75.04290	753.21694	507.98283	-70.86154	1
24071	O	68.45400	47.23480	75.64590	293.57383	-701.59669	191.54468	1
24072	N	66.89700	48.82080	75.37790	94.64898	401.19529	726.83615	1
24073	H	66.81100	49.74780	75.01990	-1514.42229	30.16907	-2769.26699	1
24074	C	65.93700	48.35880	76.39690	-627.14102	502.16741	-446.60511	1
24075	H	66.38800	47.45080	76.76890	-1513.50443	-1839.57855	2045.13431	1
24076	C	65.75500	49.42180	77.42890	-344.14157	-695.69183	469.41871	1
24077	H	65.76800	50.45180	77.01090	-1465.47371	1154.16753	2525.96007	1
24078	C	64.37800	49.29580	78.19190	-251.04184	762.97568	-442.89049	1
24079	H	64.35700	50.15180	78.89890	1470.24948	2763.43617	296.69239	1
24080	H	63.54600	49.42280	77.46690	1385.14424	-2562.76816	-1193.71654	1
24081	H	64.34900	48.32980	78.73890	2103.66702	-2040.30616	1130.96503	1
24082	C	66.94300	49.36980	78.37390	599.71160	-537.10553	414.22148	1
24083	H	67.87300	49.13980	77.81290	1555.79173	2342.06569	-1420.94173	1
24084	H	66.93800	48.50780	79.07490	1412.68826	694.68681	-2733.56706	1
24085	C	67.20200	50.71380	79.14890	-597.67340	367.43867	575.03284	1
24086	H	68.24400	50.65780	79.52990	-1749.71494	853.07562	-2483.22628	1
24087	H	66.39500	50.70680	79.91290	1659.23905	-1989.56077	1773.96148	1
24088	H	67.23000	51.56080	78.43090	2690.47753	-1447.46889	731.92960	1
24089	C	64.68400	47.94480	75.66090	9.81646	-907.09297	68.63304	1
24090	O	64.12400	46.89680	75.93190	-371.73781	-538.55501	-453.22230	1
24091	N	64.12500	48.67480	74.69190	85.34776	128.86434	820.13647	1
24092	H	64.58500	49.51780	74.42290	1218.80747	2315.48748	-1756.27576	1
24093	C	62.87300	48.23880	73.93890	697.46491	576.46033	-109.99669	1
24094	H	62.32800	47.76380	74.74190	1623.45023	-734.73399	2581.04448	1
24095	C	62.19700	49.49980	73.38790	-829.28761	66.25522	372.49021	1
24096	H	62.95800	50.04680	72.79190	26.82580	2228.65577	2213.69601	1
24097	C	61.03600	49.08980	72.50190	-502.56488	-241.24068	-732.22460	1
24098	H	61.35600	48.76480	71.48890	-2530.07179	1856.54130	-290.26858	1
24099	H	60.40500	48.31080	72.98290	-2246.08123	-1793.82772	1273.75598	1
24100	H	60.31000	49.90180	72.28490	2309.59696	-1445.39379	-1573.83196	1
24101	C	61.82500	50.37880	74.60090	-594.71770	-660.66756	200.20246	1
24102	H	61.06500	51.09380	74.21890	1952.00322	-430.70463	2418.44399	1
24103	H	62.72800	50.86480	75.02890	1186.82737	-2492.58644	1495.72972	1
24104	H	61.21500	49.71080	75.24590	-2262.35212	2111.20102	-592.28096	1
24105	C	63.20100	47.23580	72.87290	414.41401	309.52256	739.92325	1
24106	O	62.38700	46.38080	72.49590	-496.09719	597.62076	-172.21620	1
24107	N	64.47400	47.13380	72.43890	-197.18453	675.10461	-482.28510	1
24108	H	65.23300	47.65180	72.82590	467.54532	-1157.14390	-2896.88759	1

24109	C	64.77200	46.31680	71.22390	-613.62625	217.85179	-653.63917	1
24110	H	64.08400	45.51580	70.99690	-2483.82574	1234.52887	-1504.29886	1
24111	C	64.96500	47.11680	69.95990	-651.03536	643.52027	47.00296	1
24112	H	65.19000	46.42980	69.11690	785.79507	-2383.23414	-1901.89063	1
24113	H	65.80000	47.84180	70.06290	-2000.84926	-1790.43591	-1651.63719	1
24114	N	62.80000	47.30780	68.67190	243.65230	-156.86633	-800.63788	1
24115	H	62.85700	46.39880	68.25890	-1776.63609	2279.77499	1245.90447	1
24116	C	63.74700	47.92880	69.43990	-682.11039	608.36415	69.41078	1
24117	C	61.90700	48.23880	68.29190	393.99747	-518.63584	622.88364	1
24118	H	61.02100	47.93880	67.73390	-690.00605	490.98112	-3040.89364	1
24119	N	62.23400	49.43580	68.75890	409.66570	-664.77070	-315.91329	1
24120	C	63.35500	49.21480	69.53490	-534.13582	701.63540	-261.19813	1
24121	H	63.91700	50.02480	69.98390	-1324.76358	1004.83821	2665.20732	1
24122	C	66.09300	45.60480	71.41390	744.75796	-199.38263	-491.48612	1
24123	O	67.00800	45.60980	70.60490	546.19526	-562.54509	16.14102	1
24124	N	66.26200	44.96680	72.58690	-405.10445	-338.90929	647.45977	1
24125	H	65.54000	44.88280	73.26990	-1653.59558	1010.28629	2469.92102	1
24126	C	67.55100	44.53680	72.97490	-447.40240	539.27468	-600.41090	1
24127	H	68.36100	45.24380	72.87890	2745.12062	-1447.39523	480.12539	1
24128	C	67.54100	44.11380	74.52790	681.89240	132.54495	-600.55265	1
24129	H	67.20500	45.01580	75.08290	1849.54689	-1065.76317	-2320.26434	1
24130	H	66.79700	43.31280	74.72290	2407.82067	597.48768	-1944.91855	1
24131	H	68.52800	43.74880	74.88590	-1385.48577	-909.36494	-2687.57381	1
24132	C	68.08100	43.25480	72.25790	-401.21713	103.56178	801.29027	1
24133	O	69.24900	42.90780	72.37290	633.50709	-460.24013	-75.39025	1
24134	N	67.23100	42.50780	71.53190	1.17026	601.62127	582.50236	1
24135	H	66.32800	42.91980	71.44090	2909.38184	-472.00592	1078.07351	1
24136	C	67.54800	41.26580	70.93090	-338.44930	262.00579	794.11714	1
24137	H	68.32300	40.86780	71.56890	-2013.24624	1755.77455	-1682.79321	1
24138	C	66.43900	40.21380	70.95290	655.32282	516.87371	-379.97912	1
24139	H	66.01200	40.24680	71.97790	-1855.66420	1358.63043	-2164.37354	1
24140	O	66.96200	38.92080	70.87490	548.00677	85.71075	545.65181	1
24141	H	67.72100	38.72880	71.43090	-1579.23912	-1207.89929	2423.94821	1
24142	C	65.34400	40.37980	69.88590	746.57363	-32.05747	-530.74692	1
24143	H	64.40400	39.92280	70.26290	1712.84568	2073.29222	-1646.69109	1
24144	H	65.72800	39.97280	68.92590	-222.11109	-3063.65086	650.10859	1
24145	H	65.10900	41.45680	69.74290	1930.58464	1989.37299	-1500.71192	1
24146	C	68.04700	41.39180	69.50990	-682.22827	-594.28687	99.84075	1
24147	O	68.49600	40.41480	68.88190	289.42357	-339.70757	-661.64733	1
24148	N	67.97800	42.58880	68.90590	-102.57670	-222.98859	793.97315	1
24149	H	67.40400	43.31080	69.28390	1227.16811	1521.91003	2452.90968	1
24150	C	68.25700	42.84080	67.50690	-686.22325	477.14325	365.48814	1
24151	H	69.24300	42.47480	67.26390	1559.56426	-1926.96112	-1942.17554	1
24152	C	67.21300	42.10680	66.52190	752.89058	501.05338	96.04710	1
24153	H	67.50300	42.52180	65.53290	-2127.67054	372.28641	2279.83436	1
24154	H	67.39400	41.01280	66.44490	1700.38691	-128.77776	-2654.38843	1
24155	C	65.73100	42.38580	66.82990	-611.01660	-666.37811	-126.74558	1
24156	O	65.28300	43.17080	67.69590	696.32674	205.17871	292.00715	1
24157	N	64.85100	41.84280	65.95390	-475.25658	149.03727	673.32057	1
24158	H	65.23300	41.18080	65.30890	1893.29674	-1549.48730	-1982.33454	1
24159	H	63.87600	42.02380	66.07990	-980.91644	-1774.67666	-2416.00243	1
24160	C	68.28700	44.37280	67.28890	599.02635	256.65407	622.99842	1
24161	O	67.32600	45.05080	66.84790	-287.83890	76.28086	-745.68891	1
24162	N	69.42800	45.01480	67.51390	-514.37875	444.22513	497.16592	1
24163	H	70.29900	44.54280	67.62790	3068.96976	101.45686	652.67547	1
24164	C	69.59800	46.39680	67.30590	-255.33356	-745.87011	-464.56225	1
24165	H	69.34300	46.64780	66.28690	2375.14555	533.17972	1976.64375	1
24166	C	68.81800	47.28080	68.35890	-755.86137	373.39015	-373.47589	1
24167	H	67.74200	47.08880	68.15690	-1139.96449	1167.34942	2682.60577	1
24168	H	68.95200	48.36380	68.15390	2616.99703	1603.60439	672.81059	1
24169	O	69.09100	46.87480	69.72790	78.78937	581.43306	-544.07698	1
24170	H	68.34100	46.30280	69.90690	-998.35527	-1705.25099	2435.37657	1

24171	C	71.05900	46.81080	67.33990	-603.39884	-241.06350	-654.52919	1
24172	O	71.31200	47.99080	67.04890	-124.93277	-411.25865	648.15512	1
24173	N	72.08300	46.00080	67.59690	-240.12044	192.00784	-801.75217	1
24174	H	71.88000	45.04780	67.80590	-1945.99244	372.17189	2435.09883	1
24175	C	73.48600	46.44780	67.59790	-122.01471	813.53038	392.76429	1
24176	H	73.52400	47.26880	68.29890	-98.77291	560.75476	-3108.03626	1
24177	C	74.37500	45.29980	68.15590	344.83797	-689.17323	462.82236	1
24178	H	74.02300	44.33880	67.72490	2183.16678	1739.96521	-1464.64439	1
24179	H	74.17000	45.24680	69.24690	-466.31978	-670.60991	3024.09815	1
24180	C	75.92100	45.26480	67.94090	-692.79726	-182.89493	-581.70156	1
24181	H	76.30900	44.56380	68.70990	896.48900	2488.63148	1694.43600	1
24182	H	76.31100	46.28280	68.15790	2718.26765	922.81864	1268.03305	1
24183	C	76.47700	44.90180	66.52690	-699.18889	68.25363	573.26474	1
24184	O	77.48800	45.40880	66.06490	-588.36333	-396.41601	-362.25008	1
24185	N	75.84000	43.91380	65.89590	672.99079	-408.03938	-300.08580	1
24186	H	75.05300	43.46880	66.32490	1596.68199	2246.03387	1507.48763	1
24187	H	76.20200	43.57880	65.02690	1903.00392	-174.10758	-2509.86880	1
24188	C	74.06300	47.03080	66.32090	516.96651	-569.60057	-490.01852	1
24189	O	74.69700	48.06380	66.27790	239.25143	-340.95713	653.09351	1
24190	N	73.75600	46.55480	65.10790	-762.97200	150.92084	-356.39819	1
24191	H	73.25200	45.70380	64.98290	-489.56238	494.52513	3056.80764	1
24192	C	74.08400	47.23980	63.86290	-167.33684	-743.48236	479.22659	1
24193	H	75.12800	47.51180	63.92690	-1070.95554	-2925.27309	393.28814	1
24194	C	74.06800	46.20880	62.72890	-737.26254	-462.33586	262.44693	1
24195	H	73.13500	45.60880	62.79690	-2014.95128	-1591.83512	1804.63613	1
24196	H	74.85700	45.42680	62.72790	-422.45800	-521.30722	3059.46218	1
24197	C	74.06200	46.76480	61.27790	-783.39815	-428.49391	180.08899	1
24198	H	73.11700	47.30680	61.06290	1410.75592	2745.79577	-639.75603	1
24199	H	74.90400	47.46680	61.10090	-1653.65977	876.11261	-2549.17887	1
24200	C	74.25100	45.71380	60.15490	781.08808	-423.87682	-168.94738	1
24201	H	75.13100	45.04580	60.27290	-2347.46345	1042.99132	1815.65100	1
24202	H	73.41700	44.99080	60.02890	-282.91913	2911.76533	1166.15965	1
24203	N	74.37500	46.45680	58.85890	-549.00922	-475.50562	416.01853	1
24204	H	73.83000	47.27780	58.68890	432.48442	2685.84398	1580.50816	1
24205	C	74.66200	45.80580	57.73890	405.23041	612.07520	-559.53666	1
24206	N	75.21300	44.60980	57.67290	336.16035	-474.57223	586.23416	1
24207	H	75.14000	43.94180	58.41390	1059.80701	1711.21555	-2435.92192	1
24208	H	75.29600	44.15880	56.78390	-2748.92980	601.32314	-1439.84142	1
24209	N	74.43800	46.41980	56.59390	-660.42550	451.27371	-316.01628	1
24210	H	74.35200	47.41580	56.55990	-373.93637	-824.26229	-3024.33804	1
24211	H	74.81700	46.00380	55.76690	-2097.32999	-2341.91090	-25.13575	1
24212	C	73.45900	48.66280	63.65890	361.32950	-642.02644	512.49571	1
24213	O	74.22500	49.62080	63.25590	585.44956	-298.37823	-436.45338	1
24214	N	72.19600	48.93680	63.88290	-575.89993	564.60104	-288.63468	1
24215	C	71.15200	47.91380	63.64390	548.94581	321.19184	639.73344	1
24216	H	71.01200	47.26380	64.53490	-413.84573	-2501.49060	1843.33151	1
24217	H	71.30300	47.24080	62.77290	2308.10647	-2078.90596	425.61972	1
24218	C	71.58800	50.28980	63.86990	217.23388	-565.55243	662.80544	1
24219	H	71.84300	50.86080	62.98890	2437.44045	-1871.98459	617.37501	1
24220	C	70.07700	50.06480	63.96190	-445.95951	-565.58922	546.76390	1
24221	H	69.46100	50.84980	63.47390	-2711.42939	798.66443	1387.32466	1
24222	H	69.73700	49.93580	65.01190	-1622.03770	-405.29586	-2678.51147	1
24223	C	69.87000	48.68880	63.34890	-613.21563	-673.42588	10.38788	1
24224	H	69.82900	48.81780	62.24590	1995.17600	2198.29174	-1055.23047	1
24225	H	68.94600	48.19980	63.72390	-1186.91566	-2500.82987	1478.01520	1
24226	C	72.06400	51.10980	65.08690	412.53173	-609.17385	-537.78032	1
24227	O	72.36800	52.25980	64.91690	-317.02332	-681.59418	221.31612	1
24228	N	72.14200	50.58980	66.34490	-294.89778	-590.75016	511.50242	1
24229	H	71.85400	49.64680	66.48990	1358.25410	2598.70764	-1158.03879	1
24230	C	72.81900	51.31980	67.35990	351.91091	633.91148	544.68531	1
24231	H	72.31400	52.25080	67.56990	2497.19955	1403.22538	1285.89274	1
24232	C	72.89600	50.49980	68.67390	-262.44793	-477.52780	-740.98348	1

24233	H	73.60400	51.00680	69.36290	-2488.28117	1677.30182	954.74163	1
24234	H	73.30500	49.50780	68.38590	-1682.51852	2352.04220	1243.44402	1
24235	C	71.62900	50.31280	69.43890	-168.37168	-586.08073	-686.27707	1
24236	H	70.76200	49.92680	68.86190	-559.65797	2994.19767	-818.97110	1
24237	H	71.29200	51.26680	69.89990	476.39114	-1471.94550	-2746.97423	1
24238	C	71.72500	49.24180	70.58390	442.49825	-770.19268	-191.37206	1
24239	H	70.75000	48.93880	71.02290	1482.53120	-1567.26582	2273.32451	1
24240	H	72.23500	48.32680	70.21490	-1812.15875	1957.55504	1665.61453	1
24241	N	72.53600	49.96180	71.58390	-297.14036	790.41810	-101.18643	1
24242	H	72.73100	50.93480	71.46790	-1198.30436	2652.10244	-1219.21024	1
24243	C	73.24800	49.36280	72.44790	806.90231	-413.38071	7.94799	1
24244	N	73.02000	48.12780	72.87290	-790.92055	-156.60550	246.63520	1
24245	H	72.19900	47.67380	72.52690	-2517.18007	-423.28480	1831.04580	1
24246	H	73.73800	47.68480	73.40890	1841.69352	1765.33507	1828.36066	1
24247	N	74.05500	50.13280	73.16390	-15.04288	845.36897	48.60781	1
24248	H	74.03900	51.12880	73.07790	-994.43650	-2633.28870	1390.20117	1
24249	H	74.58500	49.72780	73.90890	-1580.20108	1004.53104	2519.55615	1
24250	C	74.26400	51.75680	67.03390	485.27188	-82.81479	-774.61144	1
24251	O	74.70400	52.87880	67.34290	-103.24079	-776.13933	42.07046	1
24252	N	74.99000	50.84080	66.43790	385.87259	-410.16592	-633.22636	1
24253	H	74.53700	50.00780	66.12990	-2440.43973	1269.25506	-1552.81444	1
24254	C	76.32900	51.05180	65.91890	750.00473	431.44780	270.18258	1
24255	H	76.92000	51.30980	66.78590	2377.60066	981.56217	1795.48304	1
24256	C	76.94900	49.70280	65.47390	-132.79331	456.55058	-795.66158	1
24257	H	76.30500	49.24080	64.69590	-1467.85942	-770.05688	2662.50296	1
24258	H	76.96900	49.10280	66.40990	2345.99452	2045.00219	-474.78415	1
24259	C	78.38400	49.85180	64.90690	501.27405	436.58084	611.26410	1
24260	H	78.99800	50.42380	65.63490	1533.51034	2184.92047	-1681.92621	1
24261	H	78.48000	50.46080	63.98190	491.62756	1593.39586	-2684.06982	1
24262	C	79.08600	48.50880	64.76090	-471.22170	-572.24939	-541.93719	1
24263	H	80.13800	48.65880	64.43590	-1804.39904	2105.93179	-1517.35324	1
24264	H	79.13800	48.00180	65.74790	-1717.84197	2023.05771	1689.18624	1
24265	C	78.42400	47.54480	63.73590	-282.71738	-453.98516	722.09007	1
24266	H	77.43900	47.19580	64.11290	2057.04869	-893.43939	2184.30410	1
24267	H	78.43800	48.07180	62.75690	-587.98097	-1288.61506	2793.13125	1
24268	N	79.19100	46.31480	63.58490	663.03911	-41.16655	498.17751	1
24269	H	79.15700	45.54480	64.28290	-1460.83311	2741.40663	-567.74920	1
24270	H	78.84600	45.88880	62.70090	2796.33516	704.04280	-1264.11311	1
24271	H	80.20700	46.41180	63.38790	-1400.97448	175.46195	-2829.79287	1
24272	C	76.45600	52.09780	64.76190	-346.83726	385.92933	-767.86486	1
24273	O	77.33400	53.00380	64.73790	474.52158	281.17854	-574.87307	1
24274	N	75.49900	52.07180	63.80890	468.21756	170.61529	-690.17931	1
24275	H	74.82500	51.33980	63.87890	-1350.05438	-1821.86440	-2190.50158	1
24276	C	75.37200	53.05880	62.72290	498.99985	-637.04090	-411.13316	1
24277	H	76.24900	53.07880	62.09390	1989.27152	-1787.29559	1628.91077	1
24278	C	74.08200	52.69580	61.93290	459.99495	-628.05981	-468.20702	1
24279	H	73.19500	52.54980	62.58490	2985.21577	-690.76197	666.48193	1
24280	H	74.18000	51.73280	61.38690	-2650.71923	-1370.19298	993.79664	1
24281	C	73.59900	53.60380	60.75090	738.94847	-140.03042	492.00150	1
24282	H	73.51200	54.61580	61.20090	-2267.06883	2008.63595	878.54273	1
24283	C	74.75200	53.70080	59.70190	385.10775	826.78280	-98.44269	1
24284	H	75.73100	53.99880	60.13390	966.29002	-2222.42708	-2003.84499	1
24285	H	74.40100	54.35980	58.87990	-2815.63690	-601.89582	-1291.99105	1
24286	H	74.77600	52.72380	59.17190	453.24426	-2957.84310	929.50604	1
24287	C	72.26900	52.99980	60.24790	138.30100	-603.52171	-670.64694	1
24288	H	72.31900	51.91280	60.01990	-2685.30396	725.39069	-1498.25548	1
24289	H	71.53100	53.17380	61.05890	2803.73150	724.06968	-1227.75871	1
24290	H	71.90400	53.53280	59.34390	-589.89200	1823.06455	-2513.22049	1
24291	C	75.26700	54.48680	63.29190	857.46373	-203.01132	-210.72295	1
24292	O	75.99400	55.39780	62.81990	-730.11267	-57.51772	-321.30755	1
24293	N	74.42500	54.77980	64.32690	49.60680	668.92250	-530.84638	1
24294	H	73.71000	54.13580	64.58490	1475.19613	2730.42400	-542.84923	1

24295	C	74.40000	55.99780	65.09690	128.71191	895.37080	142.24922	1
24296	H	74.15100	56.75380	64.36690	1809.47997	-1652.55803	1951.69755	1
24297	C	73.31000	55.86980	66.17990	141.09321	808.97746	-415.52063	1
24298	H	73.30000	56.73880	66.87090	-1885.75583	563.97614	2451.36681	1
24299	H	73.61800	54.94780	66.71790	-130.39787	1128.27826	2926.58921	1
24300	C	71.87600	55.65080	65.62390	-298.99488	-453.06640	-740.65503	1
24301	H	71.83700	54.60480	65.25090	847.23306	-45.83255	-3037.20758	1
24302	C	70.97400	55.48080	66.86590	-268.31261	281.79241	-837.38622	1
24303	H	71.23100	54.55980	67.43290	-41.66374	1344.65351	-2855.93313	1
24304	H	71.08600	56.36480	67.52890	684.15038	-2296.87017	2021.74742	1
24305	H	69.94100	55.32880	66.48690	782.90579	-2493.64858	1732.03370	1
24306	C	71.25800	56.61480	64.56090	500.24046	567.01962	-518.45106	1
24307	H	70.17700	56.37880	64.46190	-1753.33254	-1854.42977	1831.68873	1
24308	H	71.83700	56.72880	63.61990	1428.70709	2806.10593	8.29230	1
24309	H	71.32500	57.64680	64.96790	-609.20163	-2181.51549	-2187.55219	1
24310	C	75.73500	56.27280	65.77590	442.77175	697.00924	-400.76698	1
24311	O	76.34600	57.33580	65.63190	91.38162	-730.89108	-274.59935	1
24312	N	76.31200	55.24680	66.49890	467.86672	701.95531	52.50885	1
24313	H	75.88100	54.35180	66.58390	-2134.34327	2175.76858	802.37847	1
24314	C	77.48200	55.40080	67.33590	-194.85262	690.52994	-582.81457	1
24315	H	77.32600	56.29280	67.92390	-2254.29297	1530.60254	-1597.16347	1
24316	C	77.62100	54.17580	68.29490	651.18316	-245.72227	569.25506	1
24317	H	78.49700	54.34580	68.95590	-1360.61252	2562.72275	1222.50909	1
24318	H	76.75900	54.12480	68.99390	-191.70204	-694.55094	-3072.66743	1
24319	H	77.70900	53.20180	67.76690	758.40050	-1521.56714	2630.59552	1
24320	C	78.78300	55.65680	66.64290	-510.71876	524.13799	544.80839	1
24321	O	79.62000	56.37780	67.15490	-526.47782	-549.71917	197.75963	1
24322	N	78.96700	55.15180	65.41590	-176.63391	790.11408	-276.58616	1
24323	H	78.26300	54.58880	64.98890	-2836.84021	302.58266	-1352.82670	1
24324	C	80.24300	55.01480	64.81890	-749.27072	-312.40969	-433.00281	1
24325	H	80.93500	55.54480	65.45490	-1290.53626	1413.88268	2492.52386	1
24326	C	80.74100	53.60680	64.68090	363.21828	-782.78577	-277.39084	1
24327	H	81.54200	53.50280	63.91790	1360.46863	2837.76882	-157.94459	1
24328	H	79.93900	52.99380	64.21490	-1237.18088	-440.35238	-2872.88940	1
24329	C	81.19200	53.07180	66.00590	-445.80418	438.14582	659.81821	1
24330	H	80.21400	52.97080	66.52290	816.48576	-2070.56846	2202.74617	1
24331	H	81.98500	53.67880	66.49090	2419.78114	1972.54137	-400.75966	1
24332	C	81.80000	51.67080	65.81990	-200.72994	649.06205	-630.96281	1
24333	O	82.54700	51.38680	64.86090	484.43785	518.88131	335.20637	1
24334	O	81.46400	50.77080	66.62690	581.34300	104.41494	505.76077	1
24335	C	80.24800	55.64180	63.46990	-400.60600	-291.88705	754.54583	1
24336	O	81.28400	56.18180	63.05390	178.28896	-755.60998	-87.90331	1
24337	N	79.10300	55.73680	62.73990	-6.02370	628.30108	-583.69403	1
24338	H	78.21300	55.39680	63.03490	-2998.36955	-315.60248	908.76507	1
24339	C	79.08500	56.37380	61.44790	449.18781	-543.41871	553.23660	1
24340	H	80.07800	56.57180	61.07090	2073.18563	-149.35995	2343.34040	1
24341	C	78.41800	55.43180	60.43790	587.60089	-254.02333	-649.63633	1
24342	H	77.80000	55.86380	59.62190	-1209.28454	1925.82846	-2197.24391	1
24343	H	77.61800	54.90880	61.00490	-2347.29435	2088.79092	-321.19380	1
24344	C	79.39200	54.30580	59.96390	516.14872	559.38488	-515.81585	1
24345	H	80.20100	54.78780	59.37390	1624.40086	621.50424	2607.25318	1
24346	H	79.81400	53.79280	60.85490	3074.89944	-621.35754	-23.82686	1
24347	C	78.69400	53.25980	59.05890	527.44625	-544.60194	-499.72818	1
24348	H	78.18300	53.69880	58.17490	-2904.62717	-1218.45469	-34.80698	1
24349	H	77.89200	52.86580	59.71890	567.14931	-3059.47331	-401.96550	1
24350	C	79.52300	52.08780	58.64990	112.08407	-207.76697	-889.93133	1
24351	H	78.88900	51.18480	58.52290	1543.22358	-127.34759	2721.13691	1
24352	H	80.17100	51.87080	59.52690	-1843.37379	85.47762	-2566.67083	1
24353	N	80.41500	52.29680	57.45590	-348.93292	-228.42309	721.88373	1
24354	H	81.01600	53.14280	57.39090	2069.20691	1720.94978	1617.13397	1
24355	H	80.99800	51.45480	57.27390	2028.83707	-1669.01547	-1724.54868	1
24356	H	79.79000	52.30380	56.62490	-145.24844	-2222.30847	2199.78620	1

24357	C	78.36900	57.66680	61.44790	-443.85329	503.46723	-639.59044	1
24358	O	78.89200	58.71780	61.08490	-95.56371	-603.51848	481.31239	1
24359	N	77.09500	57.58980	61.86190	599.82624	535.38486	-265.87578	1
24360	H	76.77100	56.72180	62.22990	1451.04393	-1989.28140	-1954.82403	1
24361	C	76.09900	58.66480	61.66090	125.40718	-776.41859	436.18634	1
24362	H	76.35500	59.15680	60.73390	-2983.52435	-984.63203	234.76565	1
24363	C	74.63500	58.10880	61.42090	-243.53900	694.76222	-560.48350	1
24364	H	74.40700	57.32080	62.17090	-2600.34443	293.95016	-1768.08687	1
24365	C	73.63900	59.25180	61.53490	404.56248	75.43875	802.11199	1
24366	H	73.66300	59.64980	62.57190	1116.90884	1038.27498	-2759.57414	1
24367	H	72.61900	58.85480	61.34290	-2450.60433	-1677.98237	1036.03466	1
24368	H	73.85800	60.07080	60.81690	1047.57058	-1523.09928	2529.50736	1
24369	C	74.54200	57.54180	59.97590	-330.85686	394.38267	751.39924	1
24370	H	75.40900	56.88280	59.75790	1212.42514	-2094.84714	1986.27471	1
24371	H	73.71200	56.81880	59.81990	2006.98204	1375.03937	1983.28321	1
24372	H	74.61300	58.32480	59.19190	292.93704	-2506.89357	1856.27013	1
24373	C	76.21100	59.84480	62.65990	-20.19817	14.46279	-920.43837	1
24374	O	75.93300	60.98580	62.30390	568.43492	220.81106	-504.14863	1
24375	N	76.85000	59.71980	63.88290	-402.51819	467.08611	-596.43216	1
24376	H	76.85700	58.81880	64.30890	-1752.78236	-2608.11605	-116.81619	1
24377	C	77.20900	60.88380	64.76190	675.24898	-359.06390	472.58917	1
24378	H	76.28000	61.42980	64.83790	-1976.32822	1643.79874	1819.96294	1
24379	C	77.73400	60.39280	66.08790	-534.94606	-101.37022	-744.42155	1
24380	H	77.00500	59.71580	66.58190	2067.39703	1549.87069	1783.72348	1
24381	C	79.03700	59.53180	65.95890	-165.90729	-553.14012	-711.45673	1
24382	H	79.91700	60.21080	65.96790	3074.96229	-7.27957	622.91396	1
24383	H	79.30200	58.94780	65.05190	-1126.62849	-2545.24816	-1469.26867	1
24384	H	79.18400	58.75480	66.73890	-2405.44286	592.49887	-1959.28981	1
24385	C	77.96200	61.63780	66.98490	230.87880	-722.08789	485.91949	1
24386	H	78.82900	62.29580	66.75890	2523.65181	1761.93189	-650.71781	1
24387	H	78.00300	61.31880	68.04790	-1572.75740	1841.02619	2010.59348	1
24388	H	77.05900	62.28480	66.98290	-1202.01580	2428.19398	-1621.59416	1
24389	C	78.17500	61.78680	63.99590	583.78685	304.43068	-635.74563	1
24390	O	78.09900	62.98780	64.12390	-687.77655	408.88809	-10.25757	1
24391	N	79.04000	61.27880	63.15690	453.72176	230.57172	-679.78649	1
24392	H	79.21600	60.30180	63.07090	-359.18443	1960.50849	2432.39110	1
24393	C	79.83300	62.16880	62.23990	-751.46667	-443.26194	265.15522	1
24394	H	80.38500	62.91080	62.79690	-575.58032	2265.57573	2108.01287	1
24395	C	80.87800	61.35180	61.53590	239.37329	885.59131	-44.18072	1
24396	H	81.46900	62.00780	60.86190	1659.63450	-2653.30173	156.23329	1
24397	H	80.48200	60.49880	60.94490	3023.96529	329.25121	765.58974	1
24398	C	81.78800	60.76180	62.55890	-550.21739	460.85781	-586.63005	1
24399	C	81.47900	59.48980	63.13990	602.84787	88.41092	-682.85346	1
24400	H	80.54500	58.99280	62.92390	2086.51558	-2299.50166	-443.53573	1
24401	C	82.33100	58.99680	64.14690	-635.09973	-277.82176	585.66247	1
24402	H	82.11600	58.00880	64.52490	1281.83923	-2491.63988	-1421.73036	1
24403	C	83.50600	59.67180	64.52090	590.08671	566.42652	-414.11907	1
24404	O	84.34300	59.10380	65.48790	777.92006	-8.50792	-97.28425	1
24405	H	85.16400	59.59980	65.50190	1982.35277	2347.75954	-693.28586	1
24406	C	82.96400	61.42180	62.94590	-751.60863	-219.21431	-485.84314	1
24407	H	83.22800	62.37680	62.51590	-1609.56871	-1945.08154	-1884.88264	1
24408	C	83.79600	60.81880	63.85490	-654.16529	651.01902	-22.72083	1
24409	H	84.68400	61.36680	64.13590	-1085.03970	1769.54483	2363.40748	1
24410	C	79.07200	63.01480	61.18490	747.41413	-495.49191	68.05880	1
24411	O	79.35300	64.19780	61.05590	296.52150	541.63349	488.49945	1
24412	N	78.11400	62.42880	60.51990	-339.15127	761.69630	-199.30970	1
24413	H	77.89300	61.46280	60.63090	-1809.25602	-2409.61269	-907.14035	1
24414	C	77.45200	63.00280	59.37490	-180.07709	896.37031	114.34817	1
24415	H	77.88600	63.93180	59.03590	1736.02504	-283.85762	-2608.81330	1
24416	C	77.51400	62.02580	58.15990	487.04969	433.28826	-645.09008	1
24417	H	78.58700	61.74980	58.07590	-1996.81996	1603.89019	1837.01622	1
24418	C	76.64800	60.74380	58.20490	-847.15506	68.48776	345.88648	1

24419	H	76.89000	60.04880	57.37290	1940.83473	-923.95083	-2294.36115	1
24420	H	75.57900	61.03780	58.26890	-1404.42562	2697.07929	844.51504	1
24421	H	76.88300	60.24480	59.16990	-864.46497	693.05221	2940.52911	1
24422	C	77.07000	62.83080	56.90790	-580.46090	-599.63346	358.32039	1
24423	H	77.53500	63.83980	56.88090	466.82891	-673.48808	3026.23040	1
24424	H	77.24600	62.12980	56.06390	-2198.97686	-1800.79180	1343.07341	1
24425	H	75.98500	63.07180	56.90790	-1340.37592	-1408.04660	2465.87345	1
24426	C	75.96700	63.43180	59.71690	-281.24034	-583.33562	-645.05832	1
24427	O	75.23100	63.95280	58.88690	-92.80887	419.57774	-676.26520	1
24428	N	75.55600	63.14580	60.96990	-159.21374	833.73552	85.19709	1
24429	H	76.07500	62.48980	61.51290	495.75025	2423.88883	1943.74229	1
24430	C	74.24300	63.52480	61.53090	-532.45093	369.55641	-659.57635	1
24431	H	73.64800	62.66780	61.80990	-1290.94369	2678.37987	1051.58848	1
24432	H	73.74100	64.17580	60.82990	-2172.98733	-661.90614	-2189.45440	1
24433	C	74.39400	64.47380	62.76890	659.07886	-586.40855	-189.23257	1
24434	O	73.38900	65.08080	63.16490	205.13911	500.01744	572.93663	1
24435	N	75.62000	64.65580	63.34290	399.56257	-520.73957	510.51012	1
24436	H	76.40600	64.05980	63.19790	-1573.61474	-717.40465	2623.82629	1
24437	C	75.80700	65.65780	64.37690	240.49383	567.21993	668.73841	1
24438	H	74.96800	66.32780	64.49790	-143.08701	2862.38767	-1319.58968	1
24439	C	76.01200	64.93380	65.67590	271.00381	-364.05890	778.45565	1
24440	H	76.89500	64.26080	65.65490	2086.07268	-2297.06148	-463.35788	1
24441	C	76.30800	65.94080	66.83790	652.38309	-147.19577	-616.82951	1
24442	H	77.32300	66.35880	66.66890	2596.77436	1424.28181	-1057.80538	1
24443	H	76.23100	65.35680	67.77990	1835.78682	1281.32310	2201.29192	1
24444	H	75.48500	66.68680	66.80890	2549.49239	-1822.59998	-132.55930	1
24445	C	74.73100	64.15080	66.04990	-268.25646	596.39359	-650.94474	1
24446	H	73.85200	64.82480	66.13390	-1567.36498	-2584.04256	-875.87048	1
24447	H	74.86500	63.63880	67.02690	-1590.28974	896.18077	-2575.75427	1
24448	H	74.49800	63.28680	65.39090	-1485.33817	-1557.27222	-2302.37301	1
24449	C	76.98200	66.54980	64.00090	-319.62905	-656.65072	535.58414	1
24450	O	76.81300	67.75280	63.82890	484.62355	-560.74831	234.53268	1
24451	N	78.17500	65.95380	63.88490	661.23506	330.10514	-407.42313	1
24452	H	78.34800	64.98480	64.04090	-1960.31912	-1894.52189	1564.12119	1
24453	C	79.38000	66.79380	63.80390	266.98529	277.29598	-833.31883	1
24454	H	79.33300	67.52180	64.60090	427.35846	-1558.06577	-2700.69354	1
24455	C	80.72500	65.95580	63.88190	775.73837	-400.65193	-231.25890	1
24456	H	81.57500	66.47980	63.39390	944.14519	2553.79953	1576.74243	1
24457	H	80.62700	65.05980	63.23190	-943.89031	-1353.39837	-2685.48031	1
24458	C	81.07600	65.46380	65.23690	748.79857	-494.74360	-91.17663	1
24459	C	81.17800	64.13780	65.68490	-800.26077	-344.33405	-290.24381	1
24460	H	81.15400	63.23580	65.09090	401.89647	1628.37139	-2673.89716	1
24461	N	81.54500	64.11680	67.03990	-635.21560	256.01380	-514.51776	1
24462	H	81.89000	63.41080	67.61890	-806.42737	1859.05762	-2422.82009	1
24463	C	81.67300	65.44380	67.41590	792.62484	-392.56919	-188.04299	1
24464	C	81.36600	66.28480	66.35090	-269.13274	-596.15425	624.27452	1
24465	C	81.43800	67.69780	66.49390	442.17669	-618.22955	-495.22018	1
24466	H	81.35400	68.36680	65.64990	2129.29498	1833.70266	1405.18937	1
24467	C	81.95200	68.19480	67.67890	788.14822	-395.96127	183.75422	1
24468	H	82.20600	69.23880	67.78590	-1107.60105	2901.37586	548.19788	1
24469	C	81.95100	65.96580	68.65390	-483.74781	770.68565	132.03154	1
24470	H	82.12500	65.34080	69.51690	2145.51891	779.86574	2152.19918	1
24471	C	82.16800	67.36880	68.71590	105.15084	-685.59158	-590.83826	1
24472	H	82.68500	67.67280	69.61390	-1258.30837	-1413.83318	2505.82014	1
24473	C	79.54100	67.60780	62.56990	-670.83785	-390.62879	-490.51508	1
24474	O	79.68900	68.83180	62.62190	-81.63037	691.29861	383.18344	1
24475	N	79.43900	66.98780	61.39490	225.08745	-467.31575	-663.66519	1
24476	H	79.52900	65.99580	61.36090	-1667.41157	-135.09976	2662.36747	1
24477	C	79.40100	67.72880	60.09790	655.25659	-578.23167	204.79411	1
24478	H	80.27400	68.36380	60.06790	807.40031	610.16136	-2984.75803	1
24479	C	79.57800	66.71580	58.97690	-99.15614	139.28121	891.10475	1
24480	H	79.06400	65.76680	59.23990	1511.07981	1989.27557	1907.48586	1

24481	C	79.02300	67.18080	57.59490	-576.33391	596.49450	401.70896	1
24482	H	79.08700	66.33780	56.87390	-755.60676	-1558.36590	2616.33608	1
24483	H	77.97200	67.53780	57.64990	2918.22463	1094.17986	-390.03962	1
24484	H	79.57700	68.09680	57.29790	2033.50425	-2074.78549	-1178.76925	1
24485	C	81.08100	66.50980	58.92390	378.81266	704.92986	436.65804	1
24486	H	81.56100	66.51280	59.92590	2712.55304	-1224.27163	975.98595	1
24487	H	81.53800	67.31980	58.31590	1789.47265	2411.54523	937.78298	1
24488	C	81.48100	65.22680	58.17990	544.95429	-304.88049	-659.74369	1
24489	H	82.58100	65.23080	58.01990	-558.70171	-2323.65979	-2045.43343	1
24490	H	81.14600	64.38880	58.82690	-1072.10281	1855.55210	2307.27899	1
24491	H	81.07500	65.34680	57.15190	-2536.71703	-1834.85846	-337.60796	1
24492	C	78.20300	68.68480	59.97390	-178.68822	518.11313	731.42557	1
24493	O	78.39300	69.81780	59.50690	-740.86036	-154.03873	244.86235	1
24494	N	76.94300	68.38580	60.25590	372.83429	-441.77333	597.30598	1
24495	C	76.40600	67.04980	60.23790	92.20920	48.26332	-911.32467	1
24496	H	76.84500	66.50280	61.09990	-44.30372	-2356.41240	-2081.16667	1
24497	H	76.61900	66.55080	59.26890	-2225.02899	1840.83087	-1284.66671	1
24498	C	75.89100	69.36780	60.47890	-513.29334	-374.50043	-661.55612	1
24499	H	75.63800	69.83980	59.54090	2400.43543	1727.70564	-1069.60121	1
24500	C	74.79500	68.58480	61.07990	313.33841	-414.71185	735.65127	1
24501	H	74.84900	68.53780	62.18890	-1049.71664	-1893.96860	-2285.14776	1
24502	H	73.81200	69.09380	60.98690	2232.63141	-2140.04970	-511.85871	1
24503	C	74.91000	67.23780	60.38990	-334.73327	-647.86420	-548.61103	1
24504	H	74.48000	66.36180	60.92190	2396.04926	206.03947	2012.75875	1
24505	H	74.36300	67.34880	59.42990	-66.09527	854.67675	3024.37293	1
24506	C	76.27700	70.60180	61.32290	693.50925	-38.42021	-583.46927	1
24507	O	75.93900	71.65980	60.85690	-733.48608	-193.64087	-247.19952	1
24508	N	76.98300	70.49280	62.53090	432.56564	359.12845	622.92414	1
24509	H	77.22900	69.59880	62.89790	-1007.53313	-2119.55950	2086.55158	1
24510	C	77.34300	71.60280	63.34590	42.68293	715.22039	-577.25576	1
24511	H	76.43300	72.10680	63.63490	2889.05142	-1164.87975	-357.57866	1
24512	C	78.07100	71.11780	64.56590	-261.82031	666.29798	-581.96253	1
24513	H	77.40400	70.42680	65.12390	-1419.62469	-2307.54121	-1601.95493	1
24514	H	78.32800	71.98480	65.21090	-2718.39690	374.82847	1551.02186	1
24515	H	79.06500	70.67980	64.33290	-3075.84667	144.86915	-692.39826	1
24516	C	78.26200	72.58380	62.57290	673.06652	455.16243	402.60916	1
24517	O	77.99600	73.79480	62.52490	-487.85868	558.35324	299.36893	1
24518	N	79.28600	72.04380	61.88190	-199.61111	-622.86003	-532.24627	1
24519	H	79.45000	71.06180	61.82190	1704.70720	1957.20149	-1783.57001	1
24520	C	80.16600	72.83480	60.97290	-491.35076	-358.93419	676.62999	1
24521	H	80.56600	73.62780	61.58790	-7.90732	3150.20417	-174.53145	1
24522	C	81.26100	71.99780	60.26490	-652.21970	-591.55684	235.40881	1
24523	H	80.87300	71.21680	59.57690	1243.84230	-2868.22342	-217.61628	1
24524	H	81.86300	72.79880	59.78490	1341.72893	-2400.91828	-1508.75716	1
24525	C	82.21600	71.17680	61.14290	27.57144	707.86204	578.53810	1
24526	H	81.67600	70.33280	61.62390	-1345.08475	-1070.71383	-2642.25981	1
24527	C	83.30900	70.67280	60.22790	-657.48643	-283.50665	564.55440	1
24528	H	82.82200	70.02180	59.46990	-344.33767	1921.21255	2469.81018	1
24529	H	83.81700	71.51980	59.71990	-1104.56714	2160.81211	2011.93571	1
24530	H	84.03400	70.09680	60.84190	2159.85173	-2222.86834	-463.94355	1
24531	C	82.83200	72.00880	62.34890	-743.72962	-21.00980	-545.64023	1
24532	H	81.97800	72.18080	63.03890	1609.20860	2650.04229	542.06596	1
24533	H	83.61500	71.40980	62.85990	1025.72647	1227.48140	-2715.80249	1
24534	H	83.28400	72.93580	61.93590	894.41993	2728.43596	1292.38142	1
24535	C	79.39800	73.56380	59.85490	-423.18297	820.77333	-51.76486	1
24536	O	79.60700	74.74080	59.58190	-275.78072	696.10315	281.59806	1
24537	N	78.44400	72.86480	59.19490	620.08219	465.31907	-331.82323	1
24538	H	78.25100	71.91980	59.44990	-2238.48934	1247.22921	1839.25719	1
24539	C	77.51900	73.42580	58.26290	455.83227	-592.20465	497.82511	1
24540	H	78.15500	73.93980	57.55690	1326.29671	-2712.76738	-838.88686	1
24541	C	76.60000	72.37380	57.56490	299.20902	440.60336	-745.45259	1
24542	H	75.90000	72.97980	56.94990	331.41798	-2236.12979	2172.76913	1

24543	H	76.05600	71.96080	58.44090	1074.20211	938.16104	-2807.43600	1
24544	C	77.41200	71.39580	56.68990	855.61287	262.90448	124.86789	1
24545	H	78.23700	70.92380	57.26490	-1880.98495	-1582.98942	1960.26724	1
24546	C	76.51500	70.32580	56.03890	-590.39960	-514.86965	464.11298	1
24547	H	75.79800	70.79480	55.33190	1937.84676	-2439.93705	304.53988	1
24548	H	77.06300	69.52180	55.50390	924.90167	-2825.90107	983.28528	1
24549	H	76.02800	69.82180	56.90090	-2214.64161	1007.78362	-2015.97120	1
24550	C	78.08700	72.20080	55.55590	-559.93978	-205.27941	691.03286	1
24551	H	78.93000	72.84180	55.89090	2435.28200	-879.84844	-1770.78919	1
24552	H	77.35600	72.90380	55.10290	-30.90421	-3069.61804	-643.98096	1
24553	H	78.47800	71.55980	54.73690	-1983.70216	-1439.32854	1971.20232	1
24554	C	76.65800	74.51080	58.81890	221.29771	571.52990	-682.53442	1
24555	O	76.44500	75.53780	58.13990	703.06541	-30.75151	-337.65438	1
24556	N	76.13800	74.39180	60.04090	607.02510	295.28631	-502.53976	1
24557	H	76.10800	73.55980	60.58990	2155.50746	-1845.03157	-1335.01778	1
24558	C	75.18900	75.41980	60.53390	690.78667	-516.69752	250.82729	1
24559	H	74.52600	75.63580	59.70990	932.19047	-2935.52705	582.20902	1
24560	C	74.32700	74.98880	61.72290	-459.75931	-335.68086	-717.41210	1
24561	H	73.68700	75.85480	61.99690	2625.00466	195.92129	1706.69283	1
24562	H	75.08200	74.73680	62.49790	-2845.95063	1129.51046	768.86118	1
24563	C	73.43400	73.79580	61.37990	-410.20594	374.71992	729.85548	1
24564	H	73.87200	73.05280	60.67990	-2491.98032	-1104.49096	1578.09738	1
24565	C	73.20600	72.96180	62.64590	515.10632	380.91286	-648.43760	1
24566	H	72.47500	72.15780	62.41390	-144.61805	1456.87451	-2792.05397	1
24567	H	72.89900	73.58880	63.51090	-228.98401	-1194.04164	2896.99241	1
24568	H	74.09900	72.35780	62.91390	1555.56595	1588.09768	-2228.36189	1
24569	C	72.04600	74.18280	60.80190	-283.80572	423.88915	761.69400	1
24570	H	71.38500	73.30880	60.62390	739.94229	-2798.41693	1206.30418	1
24571	H	71.56400	75.00680	61.36990	1616.80317	-1965.59983	-1834.22272	1
24572	H	72.15400	74.59180	59.77490	-2167.82668	-588.68824	-2212.80742	1
24573	C	75.85100	76.71480	60.91390	411.64184	-380.48005	-710.84916	1
24574	O	75.24100	77.76980	61.06290	-546.80566	155.80816	558.90441	1
24575	N	77.17700	76.61080	61.06990	424.90511	434.81303	-586.89528	1
24576	H	77.61500	75.74080	60.85690	3066.35354	-164.76678	631.29385	1
24577	C	78.06900	77.62580	61.56690	-395.66455	631.77743	-544.95499	1
24578	H	77.44900	78.34180	62.08490	1208.89925	2261.74677	1823.53816	1
24579	C	79.05700	77.17280	62.62790	-219.67119	-668.53281	571.31625	1
24580	H	79.78300	77.96780	62.90290	-2056.90350	799.17527	2251.69792	1
24581	O	79.81600	75.99880	62.30490	-547.24314	495.65730	-315.63501	1
24582	H	79.18000	75.28680	62.20490	1716.32183	-1698.00638	1998.15508	1
24583	C	78.13500	76.76780	63.83490	234.66870	-852.99271	174.25984	1
24584	H	77.36500	77.55080	64.00490	-1796.53536	-1425.96404	-2158.93782	1
24585	H	78.74600	76.71880	64.76190	-1228.01056	2034.14866	2071.79134	1
24586	H	77.51500	75.84680	63.79690	-476.23723	-685.34452	3030.24867	1
24587	C	78.80100	78.28280	60.43990	-676.59126	465.67604	-425.97191	1
24588	O	79.82000	78.91780	60.65690	-563.04016	566.47697	85.51670	1
24589	N	78.35900	78.17880	59.20190	-173.33991	-565.20626	594.59712	1
24590	H	77.57900	77.59780	58.98190	-378.56668	-1892.55032	-2481.50634	1
24591	C	78.86300	79.05080	58.16390	-25.49605	-438.00347	-796.34859	1
24592	H	79.93700	78.96980	58.24790	-2004.09576	-1599.98681	1824.00637	1
24593	C	78.55500	78.55580	56.73090	644.18188	-519.17384	-349.94297	1
24594	H	77.45400	78.54380	56.58590	-2227.23334	2238.01908	-165.36703	1
24595	C	79.23400	79.47680	55.69190	-171.65359	513.14394	741.96704	1
24596	H	79.23300	79.06580	54.66090	2866.76385	-1255.69529	60.15515	1
24597	H	78.67300	80.41380	55.48890	3120.36933	-44.57245	-286.63545	1
24598	H	80.26600	79.78080	55.97290	-378.34591	-1145.79812	-2905.07384	1
24599	C	79.06900	77.10780	56.54390	-405.85815	631.47601	-541.68589	1
24600	H	79.00500	76.45980	57.44390	-2510.66162	-1540.86089	1113.19532	1
24601	H	80.15200	77.14780	56.29690	688.92150	2273.32972	-2073.80635	1
24602	C	78.26600	76.33080	55.51690	-577.77835	-622.99635	-334.07641	1
24603	H	78.23500	76.94280	54.59090	-1813.04525	-2234.03311	-1273.48904	1
24604	H	77.16900	76.27180	55.68190	2406.97194	-1953.39123	434.63609	1

24605	H	78.74700	75.33680	55.39290	655.53009	-2138.08350	2195.45950	1
24606	C	78.55300	80.52180	58.35990	629.90991	-3.45889	-649.37358	1
24607	O	79.45400	81.34280	58.28290	418.24404	-381.35659	-536.00691	1
24608	N	77.30800	80.94280	58.79090	-713.42213	119.54194	454.92666	1
24609	C	76.06600	80.31780	58.47990	-469.78434	453.44999	-652.15478	1
24610	H	75.80500	79.49080	59.17390	1823.25331	2553.98545	234.81074	1
24611	H	76.09400	79.92480	57.44090	-2300.77681	1690.10603	1353.45014	1
24612	C	77.11200	82.34380	59.28390	673.82307	597.16398	125.42642	1
24613	H	77.25900	83.06080	58.48990	-2815.54335	-1122.20710	-870.33359	1
24614	C	75.62100	82.35380	59.68890	253.60509	818.23424	-325.41372	1
24615	H	75.54600	82.00980	60.74290	-1981.99377	2012.65591	-1413.12877	1
24616	H	75.08500	83.32580	59.65190	-1987.15054	255.53046	2436.59504	1
24617	C	75.00600	81.34580	58.64290	-741.14373	520.31913	-194.76731	1
24618	H	74.62200	81.75380	57.68290	15.45380	2687.22712	1651.25763	1
24619	H	74.09500	80.94680	59.13790	-1453.85275	-2478.30331	-1277.72462	1
24620	C	78.03700	82.78180	60.40490	-299.72846	-855.83958	-27.40984	1
24621	O	78.48700	83.90380	60.44290	59.77811	-678.56130	-382.36546	1
24622	N	78.30300	81.91980	61.40090	187.74278	750.96759	348.15147	1
24623	H	77.87300	81.02280	61.32790	-2910.33825	1098.48771	549.29266	1
24624	C	79.25100	82.16380	62.47790	-733.68360	425.54731	-367.80906	1
24625	H	78.89200	83.09180	62.89790	1617.39444	-2315.57867	-1360.30646	1
24626	C	79.28600	81.04580	63.50590	809.27887	350.70485	203.86501	1
24627	H	80.16800	81.03780	64.18090	-2681.51260	1121.65418	-1234.87323	1
24628	H	79.41000	80.13580	62.87990	-1631.15399	-1174.18381	2421.68131	1
24629	C	78.00000	80.97680	64.30490	472.19911	644.29030	-440.60752	1
24630	O	77.75200	81.96580	65.02190	-557.31693	570.73410	78.28402	1
24631	O	77.25500	79.98480	64.24790	461.94657	-365.96450	510.21618	1
24632	C	80.65900	82.48880	61.91190	-617.26384	-452.08860	500.27815	1
24633	O	81.35100	83.42380	62.34390	415.14157	-531.52148	386.85445	1
24634	N	81.09300	81.65880	60.95190	211.36359	237.69372	779.85955	1
24635	H	80.60900	80.81980	60.71590	867.16627	-195.41891	-3016.10288	1
24636	C	82.35100	81.84880	60.18090	-77.06504	-898.92975	43.06637	1
24637	H	83.14500	81.81080	60.91190	949.26265	-2224.07508	-1999.29721	1
24638	C	82.61200	80.57680	59.36790	644.91732	-401.24233	-484.08751	1
24639	H	81.68500	80.38480	58.78690	2126.37805	265.94545	-2296.34994	1
24640	H	82.65500	79.66680	60.00390	1800.34278	2268.32361	1227.92084	1
24641	C	83.86900	80.51280	58.43890	580.55069	-537.01999	-428.72967	1
24642	C	85.11900	81.10280	58.74990	447.25002	-624.89947	-469.33615	1
24643	H	85.29600	81.67880	59.64590	-1980.58035	-1693.49139	1763.11402	1
24644	C	86.16200	81.10780	57.83790	-589.16118	-694.92187	-11.62482	1
24645	H	87.06200	81.63480	58.11890	905.39309	2220.76512	-2046.15688	1
24646	C	85.98200	80.43580	56.65890	-895.32717	219.29523	85.65220	1
24647	H	86.69700	80.46980	55.84990	-1077.47895	-973.01051	-2795.46777	1
24648	C	83.79600	79.72480	57.31990	451.11837	632.82890	-482.91563	1
24649	H	82.86100	79.25980	57.04390	-899.98930	1712.31678	-2495.85290	1
24650	C	84.80600	79.76980	56.36290	519.75540	-476.44951	-561.00796	1
24651	H	84.81800	79.17080	55.46490	-2254.09432	-1128.37504	-1893.84342	1
24652	C	82.49700	83.11280	59.39990	-16.22563	-664.20386	-615.75940	1
24653	O	83.51000	83.80280	59.50090	277.55415	-597.40090	412.23448	1
24654	N	81.49500	83.40680	58.56490	-495.86895	-623.10980	-279.97650	1
24655	H	80.75700	82.74780	58.43890	-2105.55753	-1996.84538	1218.49334	1
24656	C	81.46900	84.64280	57.71890	439.17989	-774.16144	110.39379	1
24657	H	82.41100	84.77380	57.20590	-1830.53945	-1519.83786	-2062.62189	1
24658	C	80.38000	84.70980	56.67890	578.84199	-251.72890	-642.96563	1
24659	H	79.41800	84.79380	57.22890	-1946.28735	-1004.26525	-2264.91847	1
24660	C	80.21701	85.96634	55.74970	-416.25983	-507.20293	-117.63548	1
24661	H	80.95553	85.95566	54.92777	3615.79431	-1747.54314	-871.99592	1
24662	H	80.30886	86.94940	56.26698	939.56182	1354.60270	-2831.01888	1
24663	H	79.13772	86.01775	55.27761	-2312.30406	435.33556	1701.23069	1
24664	C	80.27800	83.41680	55.77490	58.56899	-719.44325	540.53171	1
24665	H	80.08400	82.53880	56.42690	1868.93798	2013.48913	-1533.16754	1
24666	H	81.26700	83.29280	55.28390	573.91809	2104.30621	2273.18621	1

24667	C	79.15000	83.46480	54.79990	508.44956	-365.49591	-646.93054	1
24668	H	79.31000	82.70080	54.00990	-870.57016	1969.28971	2307.68831	1
24669	H	79.14200	84.43280	54.25390	1792.03248	-563.30942	-2511.98078	1
24670	H	78.13300	83.27280	55.20590	1486.23023	-2742.52218	-266.04005	1
24671	C	81.33358	85.96500	58.64478	418.71692	-143.96429	-1095.58700	1
24672	O	81.88722	87.02494	58.40788	-242.62750	-178.88317	89.78963	1
24673	N	80.39863	85.75436	59.62373	-189.63463	-1075.22293	-530.40353	1
24674	H	80.00489	84.80761	59.75935	-1734.91638	-2643.56824	1850.08596	1
24675	C	79.88575	86.91122	60.32627	324.14124	-118.24001	-1.71222	1
24676	H	80.31699	87.71263	59.77088	736.97878	1448.65622	-2379.48863	1
24677	C	78.34094	86.87030	60.58956	-128.95291	70.15703	-226.94378	1
24678	H	78.21013	85.98678	61.29655	925.23560	-2100.56014	965.96776	1
24679	H	77.98107	87.78624	61.04008	-252.59531	2873.45330	678.88752	1
24680	C	77.60790	86.64222	59.21654	737.88759	-834.78919	972.87875	1
24681	C	77.69454	87.53216	58.06730	578.01731	-274.77038	94.13042	1
24682	H	78.50472	88.28050	57.93559	-1861.49855	1102.96707	-2365.83685	1
24683	C	76.86955	87.26671	56.95544	828.62240	-202.47949	570.54389	1
24684	H	77.01038	87.91848	56.08992	1239.02468	4518.74316	1153.68789	1
24685	C	75.91072	86.23781	56.98281	1015.59924	43.00353	231.84692	1
24686	H	75.18135	86.13601	56.20488	-1515.58467	-1298.07997	-2104.47195	1
24687	C	76.57320	85.67526	59.27882	-309.62813	-418.64821	-1128.67631	1
24688	H	76.39214	85.11126	60.20651	833.22624	-912.89594	-2203.23163	1
24689	C	75.77952	85.42430	58.14542	-1107.95202	-401.83888	-156.40087	1
24690	H	74.98261	84.68003	58.16935	-386.83015	486.95893	-1164.22925	1
24691	C	80.47728	86.63586	61.80423	601.89717	953.12483	100.35715	1
24692	O	79.75153	86.62143	62.77887	882.73506	-589.36978	-84.76549	1
24693	N	81.78203	86.31159	61.80992	-259.82133	446.57546	262.00797	1
24694	H	82.21654	86.17379	60.92682	-341.48977	2759.73224	-735.93052	1
24695	C	82.47201	86.70255	63.01240	150.58090	7.20461	408.20393	1
24696	H	81.77102	87.19246	63.71355	-2465.02487	839.13481	1598.65829	1
24697	C	83.16441	85.48172	63.71156	-401.82932	-770.23886	75.18201	1
24698	H	83.96699	85.79261	64.40489	861.31737	-1710.97095	687.66988	1
24699	H	83.68000	84.87680	62.92990	-2808.11188	-1164.93592	833.61193	1
24700	H	82.44800	84.78880	64.16490	730.59968	1466.66037	-2688.08976	1
24701	C	83.67620	87.69220	62.52886	740.88366	-301.79003	856.35627	1
24702	O	84.59040	87.37034	61.72242	530.53651	546.72032	-843.96843	1
24703	N	83.70023	88.68125	63.40796	452.07202	424.86364	204.48846	1
24704	H	82.96069	88.50488	64.08087	-2084.02144	-122.76630	598.32965	1
24705	C	84.40406	89.93631	63.35868	-555.12253	-132.90106	-1172.22288	1
24706	H	85.34864	89.74474	62.70774	2946.37578	-3599.36482	422.72825	1
24707	C	83.44713	91.06824	62.84248	188.80121	179.08652	82.38335	1
24708	H	83.16795	90.78242	61.82601	-219.46276	2668.05719	-2532.70810	1
24709	H	84.09699	91.96272	62.87857	-4225.31399	2362.30352	575.48980	1
24710	C	82.17479	91.46776	63.69233	1229.08390	92.78318	742.91176	1
24711	O	81.24417	90.68049	63.77387	137.98383	-225.14508	-664.27149	1
24712	N	82.30314	92.63601	64.29081	-78.27937	-441.54725	418.10735	1
24713	H	83.11915	93.29233	64.27537	863.79206	-893.94824	-1656.97824	1
24714	H	81.72947	92.91315	65.12805	2313.44230	-1402.46171	353.53993	1
24715	C	84.78515	90.38984	64.85924	-530.16073	585.34745	-566.32933	1
24716	O	84.30560	89.85023	65.85537	-289.40495	-863.89253	-1124.21484	1
24717	N	85.81859	91.20458	64.70215	-37.74993	688.79707	134.76417	1
24718	H	86.09604	91.37535	63.75118	-1999.43726	1428.93402	255.06252	1
24719	C	86.19329	92.07477	65.80893	-381.35990	335.66660	-23.11330	1
24720	H	86.25891	91.33686	66.70988	-223.81517	1176.13333	-979.68310	1
24721	C	87.62873	92.69682	65.41440	-89.94040	-1543.75482	242.86150	1
24722	H	88.41327	91.87409	65.45912	-3089.40536	-1331.52464	-624.68968	1
24723	C	87.65007	93.30123	63.96311	-88.52127	937.11571	873.41216	1
24724	H	88.46996	94.05020	63.78019	375.56721	304.55938	409.19315	1
24725	H	86.77622	93.93872	63.66053	-470.18230	97.91303	3905.27812	1
24726	H	87.68768	92.57635	63.08062	-2453.85441	-2435.68125	641.41042	1
24727	C	88.06232	93.79315	66.42635	493.88223	183.28078	-343.98769	1
24728	H	89.12214	94.05681	66.30961	-88.29946	2495.99346	-1050.40380	1

24729	H	87.50920	94.76081	66.22809	1245.28485	-1553.99364	-1319.20388	1
24730	H	87.84348	93.50036	67.48195	2.11125	-78.68527	3432.90828	1
24731	C	85.18408	93.32138	65.81968	-629.32416	170.15686	748.87282	1
24732	O	84.80376	93.80971	64.74789	-386.40450	193.72746	-291.43043	1
24733	N	84.98054	93.86134	66.99016	-608.31249	582.41666	260.45104	1
24734	H	85.50299	93.41608	67.72923	202.13266	-1115.54567	3948.43001	1
24735	C	84.41312	95.14409	67.27263	33.85007	12.19263	-560.56819	1
24736	H	84.67775	95.81991	66.41563	-936.02605	928.41815	-1183.53665	1
24737	C	82.86753	94.90473	67.28369	313.94881	710.48814	-269.10414	1
24738	H	82.60413	94.00599	67.84134	-1601.35505	-447.85051	829.78872	1
24739	H	82.50906	94.68519	66.25027	2320.75010	1253.16757	581.09430	1
24740	O	82.04062	96.11245	67.84646	-108.49296	171.66894	-444.70528	1
24741	H	81.31155	95.62585	68.19586	1054.64991	-2410.81157	1696.29568	1
24742	C	85.05469	95.61994	68.72921	-645.33500	-164.30264	-210.57281	1
24743	O	86.23650	95.34861	68.92262	-16.79826	-179.56913	-160.36023	1
24744	N	84.25085	96.27377	69.48853	-1232.38276	-198.60885	69.19253	1
24745	H	83.28451	96.37821	69.10575	-4611.85008	1094.62009	-2032.51884	1
24746	C	84.65469	97.18815	70.53107	-427.36063	-50.63898	-457.82534	1
24747	H	85.62764	96.71673	70.76522	-556.52359	2270.27471	-1062.97709	1
24748	C	84.69120	98.60408	69.92481	527.34513	-271.06957	-36.92734	1
24749	H	84.61205	99.27826	70.83854	-907.21048	-910.46232	257.10693	1
24750	H	83.84443	98.96163	69.32682	1098.20456	-1872.64302	821.38095	1
24751	C	86.03992	98.89403	69.12064	-168.36471	-99.00088	-643.80490	1
24752	H	86.34806	99.94418	69.21657	321.79129	282.60104	489.62699	1
24753	H	86.87213	98.28566	69.59099	-837.08146	396.00491	617.27185	1
24754	C	85.82852	98.61851	67.54623	-84.64175	162.04658	-1431.14976	1
24755	O	84.67362	98.44199	67.14227	500.27622	866.57696	398.75339	1
24756	O	86.81648	98.66613	66.84552	136.97943	4.23255	70.65934	1
24757	C	83.55518	96.99048	71.76969	-521.47886	-167.56433	81.84468	1
24758	O	82.37615	96.97508	71.50816	521.18042	757.23057	178.65518	1
24759	N	84.15501	97.06842	72.95762	-840.30955	-360.46783	-752.11325	1
24760	H	85.14667	96.97967	72.91395	871.26855	-20.26995	-4995.50230	1
24761	C	83.43815	96.57688	74.08350	493.88774	-685.17096	-311.22280	1
24762	H	82.33282	96.74553	74.00689	-1049.36334	-1614.76254	292.14549	1
24763	C	83.88989	95.06926	74.09294	248.88522	-266.54356	-469.46294	1
24764	H	84.89656	94.88718	74.49054	1881.38429	1084.62162	-2652.29624	1
24765	H	83.85172	94.69527	73.00996	348.86629	-678.25124	3008.89853	1
24766	H	83.07396	94.60426	74.78175	-1588.53054	91.22863	1205.38619	1
24767	C	84.15856	97.23315	75.41722	746.58034	711.77777	-477.26267	1
24768	O	84.72741	96.54519	76.24488	-171.29950	716.16016	-170.18677	1
24769	N	83.92550	98.54883	75.42594	-279.05811	-749.69199	-285.25786	1
24770	H	83.15722	98.81577	74.78703	-947.35179	1696.83059	1103.48279	1
24771	C	84.40592	99.42606	76.43526	-252.25159	-813.73440	396.88724	1
24772	H	83.66255	100.19428	76.34467	-1758.16397	3465.90291	-1258.76412	1
24773	C	84.56354	98.71516	77.84925	71.74695	133.46763	682.48311	1
24774	H	85.31441	97.89711	77.73900	965.35100	1137.63993	-1090.91358	1
24775	H	84.96948	99.47144	78.52276	283.34773	-4589.82884	-1718.44803	1
24776	C	83.19105	98.18386	78.41165	-209.84094	-312.12072	1367.66511	1
24777	O	82.15172	98.84736	78.29498	-473.34792	-258.35673	-8.89002	1
24778	O	83.30216	97.14676	79.45872	503.00323	-312.10365	-207.49937	1
24779	C	85.86282	99.98384	75.89949	809.36718	-764.22699	-419.71097	1
24780	O	86.79502	99.97292	76.65200	-542.64274	444.73169	-323.36679	1
24781	N	85.75921	100.28943	74.60915	43.90189	-432.42764	390.67222	1
24782	H	84.77441	100.17322	74.25107	2673.68758	1110.76636	2170.07954	1
24783	C	86.76227	100.99277	73.89225	148.77352	-1411.91075	-27.03844	1
24784	H	86.34869	101.27028	72.91067	311.41124	43.39253	4823.57102	1
24785	C	86.98432	102.25435	74.74845	158.62151	-27.06878	-684.80702	1
24786	H	88.03873	102.63390	74.58910	-205.64082	-1930.91474	988.96253	1
24787	H	87.02375	101.99572	75.81669	4286.23361	-2404.45640	-1559.98546	1
24788	C	85.86435	103.38745	74.42991	-421.47606	352.63485	52.79263	1
24789	O	85.22111	103.23311	73.37236	82.15850	-759.38810	-131.82605	1
24790	O	85.79828	104.47309	75.04631	-510.28999	263.41815	311.23404	1

24791	C	88.15808	100.07268	73.69498	89.09056	-121.78424	-110.83657	1
24792	O	89.25787	100.57245	73.60021	-333.12111	-435.73311	516.89615	1
24793	N	87.77097	98.85708	73.48207	82.78348	542.39992	-292.60677	1
24794	H	86.75228	98.63664	73.47602	-1075.93436	-479.29434	-3561.63795	1
24795	C	88.74734	97.80148	73.34193	602.44749	-110.89379	10.37821	1
24796	H	89.70228	98.33051	73.03684	487.65978	-1250.21305	1765.82563	1
24797	C	88.99426	97.04589	74.72343	316.15916	-398.22236	116.85040	1
24798	H	89.40394	96.08270	74.40081	-237.02614	-1464.45746	2219.92948	1
24799	H	89.71586	97.60280	75.40968	2616.45976	-1949.79833	3460.01437	1
24800	C	87.51979	96.93142	75.28285	460.11943	827.31252	-162.50010	1
24801	H	86.79427	96.77286	74.44084	-3735.67443	1319.99815	4278.03912	1
24802	H	87.17717	97.81883	75.79539	-4176.58974	-671.90900	203.78685	1
24803	C	87.30623	95.66868	76.26244	-92.93629	90.67867	635.67549	1
24804	H	86.58674	95.75577	77.14511	217.48146	-1518.43268	1121.26594	1
24805	H	88.31318	95.46001	76.73263	-3222.46473	-1873.15723	1279.91666	1
24806	N	87.13622	94.51270	75.51587	-221.73454	152.22197	-411.39370	1
24807	H	87.79395	94.52357	74.72758	1604.70540	2082.71997	-541.84761	1
24808	C	86.34877	93.49729	75.63460	108.36620	234.65153	-933.05800	1
24809	N	86.69817	92.68083	74.56098	-20.84402	118.60348	-38.89007	1
24810	H	87.41262	92.90332	73.79441	-398.56872	-636.97660	216.25130	1
24811	H	86.28243	91.78086	74.52561	-1169.06704	-221.40510	331.91791	1
24812	N	85.46761	93.43188	76.71195	469.55619	283.80525	-591.78254	1
24813	H	85.39422	94.22220	77.36530	-435.17992	-341.28615	-292.52098	1
24814	H	84.58154	92.78584	76.92598	-2572.48991	-703.80328	1170.66155	1
24815	C	88.04733	96.85020	72.24930	-228.23382	622.03682	-289.05255	1
24816	O	86.83586	96.68929	72.23181	-1368.12803	864.20016	396.12230	1
24817	N	88.98119	96.27651	71.50619	-536.34497	-393.24340	495.95971	1
24818	H	89.97793	96.27203	71.83672	-3102.14933	1376.17992	-1370.98836	1
24819	C	88.58367	95.17665	70.66184	-678.13886	286.22221	-576.25203	1
24820	H	87.96120	95.58316	69.88220	1307.11131	-2074.43049	75.60070	1
24821	C	90.01870	94.63661	70.12512	1510.29024	267.19132	-499.75808	1
24822	H	90.60595	94.32915	71.04216	-3126.26078	-916.39570	-2274.17649	1
24823	H	90.51680	95.52017	69.70989	757.33453	1611.53398	1969.57330	1
24824	C	90.05223	93.42235	69.19800	-257.13430	-910.79834	621.16340	1
24825	C	89.05725	92.46193	69.07815	-8.75926	1074.11461	-292.10620	1
24826	H	88.19279	92.52531	69.78230	-255.21441	-692.53476	-1103.85088	1
24827	C	89.09550	91.45340	68.11256	787.63746	562.78230	-1106.54480	1
24828	H	88.31777	90.62198	68.09939	-1841.84155	-1536.46118	-1262.54535	1
24829	C	90.22602	91.36154	67.27258	-369.98778	-286.00612	-771.69417	1
24830	O	90.29569	90.43537	66.17583	107.02634	611.23432	-45.93095	1
24831	H	89.51517	89.94798	66.23430	-64.29579	2716.76303	-3170.25565	1
24832	C	91.25750	93.21663	68.45919	56.55276	-134.01876	-423.41002	1
24833	H	92.11068	93.93389	68.60321	-2301.77590	-282.77602	-501.43270	1
24834	C	91.29755	92.24830	67.50379	-124.88383	514.14400	-152.38830	1
24835	H	92.11699	92.15327	66.76216	2932.99925	-1011.12276	3391.54809	1
24836	C	87.89127	94.05817	71.51706	-942.15908	-528.75870	-147.29812	1
24837	O	88.27528	93.64785	72.61566	610.55925	540.60171	-862.93750	1
24838	N	86.85332	93.57529	70.81887	-1008.29984	24.67063	-177.66666	1
24839	H	86.60602	93.91982	69.91428	1708.62782	-362.70588	356.26475	1
24840	C	86.12181	92.39083	71.21671	-631.71180	357.74631	69.13962	1
24841	H	86.75704	91.83966	71.99087	1278.66596	166.79965	44.58386	1
24842	C	84.72349	92.77528	71.74802	-894.95765	-474.83470	466.72089	1
24843	H	84.88430	93.65001	72.41445	3260.69013	1900.69782	1892.43497	1
24844	C	83.74203	93.20352	70.68969	-857.73216	138.78449	80.27747	1
24845	H	84.17908	94.02017	69.98878	-1988.84056	-610.57486	-2152.45192	1
24846	H	83.35604	92.33528	70.08231	-2236.59295	5087.53493	943.47194	1
24847	H	82.83519	93.69530	71.10554	-577.17594	-569.82099	-395.51847	1
24848	C	84.17294	91.59975	72.55433	-81.65261	52.49783	94.63702	1
24849	H	85.02901	90.99877	72.95356	-477.16206	-2888.04965	-1650.23944	1
24850	H	83.62089	90.87049	71.83003	-169.40613	1440.99130	-106.60495	1
24851	C	83.19477	91.93012	73.73877	121.01447	-291.40758	332.83578	1
24852	H	82.38767	92.70278	73.54954	1693.86897	-872.63679	-2285.24244	1

24853	H	82.60587	90.97986	74.09244	-359.67066	546.62447	-2170.36583	1
24854	H	83.61998	92.32603	74.71721	96.56686	-63.08869	2103.63949	1
24855	C	85.98899	91.42228	69.89173	205.99228	-179.41299	97.56169	1
24856	O	85.96684	91.89871	68.79223	283.80397	-499.89350	63.00181	1
24857	N	85.94895	90.13457	70.32964	346.29173	80.76254	516.64040	1
24858	H	85.68919	90.01599	71.32033	-1510.80850	1179.47391	-2545.74571	1
24859	C	85.41269	89.11246	69.42629	-203.13320	79.96849	351.86032	1
24860	H	85.88453	89.44973	68.49322	-3387.75073	597.68117	3223.42729	1
24861	C	85.90492	87.74723	70.06796	108.26197	-810.89440	-94.44096	1
24862	H	86.35930	87.94483	71.09630	2493.69810	939.57964	-1429.03522	1
24863	H	85.07293	86.99125	70.32318	-648.86514	2495.19166	2551.33062	1
24864	S	87.17012	87.19982	68.93314	117.96865	457.98989	167.44470	1
24865	C	83.79631	89.24074	69.49339	-92.92086	-39.90106	-46.30539	1
24866	O	83.27846	89.49741	70.57031	-401.87244	-509.47378	-708.82703	1
24867	N	83.32714	89.33163	68.28765	924.85992	209.47457	139.40486	1
24868	H	83.92019	89.12328	67.41182	117.18413	211.36571	2004.72982	1
24869	C	81.96796	89.66228	68.04915	-170.26851	-893.10319	208.43721	1
24870	H	81.52188	89.85992	69.01679	657.12048	-78.24069	1041.23588	1
24871	C	82.04730	90.87608	67.04298	37.52221	725.02053	-36.57682	1
24872	H	81.98075	90.56794	65.93468	-988.05057	903.58751	938.64864	1
24873	H	83.09831	91.29099	67.10469	-1057.95758	238.97674	159.27193	1
24874	C	80.89040	91.92620	67.38178	-13.59396	89.07677	-261.89958	1
24875	O	80.15480	91.64512	68.34084	-120.60503	-293.66516	-567.26410	1
24876	O	80.75444	92.91864	66.64431	-625.39969	-102.56892	-592.66126	1
24877	C	81.16508	88.54538	67.14507	-104.89364	-433.83134	-189.19768	1
24878	O	81.73566	87.84845	66.32872	-0.63073	-17.19566	-142.58205	1
24879	N	79.88907	88.84947	67.35201	-295.16308	-736.55953	898.39510	1
24880	H	79.56502	89.48179	68.01672	-1741.10497	-10.44373	-17.45581	1
24881	C	78.94553	88.47099	66.33971	-276.65306	593.57902	-197.15251	1
24882	H	79.48030	88.01683	65.46531	-174.53325	98.43442	-2171.27857	1
24883	C	78.10887	87.48533	67.26084	203.21389	-56.70801	-764.18351	1
24884	H	77.07957	87.89401	67.42720	-1235.63476	-3712.46267	1765.35248	1
24885	H	78.60711	87.27746	68.22404	772.30944	2577.58568	-99.87484	1
24886	C	77.86499	86.07154	66.60319	-38.84233	280.89735	-429.38721	1
24887	H	77.45799	86.32368	65.63516	-3204.56282	1832.21205	144.15469	1
24888	H	77.04006	85.52410	67.12221	328.13406	245.92892	2057.43479	1
24889	C	79.21530	85.26550	66.59098	-628.21714	338.95696	420.08486	1
24890	H	79.86067	85.50393	65.67934	1372.95692	-96.75933	-1677.47540	1
24891	H	79.79509	85.49456	67.52432	-983.87971	1214.41607	-1451.92164	1
24892	N	78.71300	83.93980	66.64390	129.68470	638.74798	541.49376	1
24893	H	78.51800	83.39480	65.82790	1536.04414	1718.37737	-2140.13364	1
24894	C	78.40500	83.36480	67.75690	-669.71685	382.72445	-503.93154	1
24895	N	78.10900	83.97080	68.86490	775.37864	311.89971	-57.01942	1
24896	H	78.26600	84.95480	68.95690	-1726.74713	1644.23690	-2064.52110	1
24897	H	77.74400	83.35480	69.56290	-1361.87435	1940.68538	-2079.11843	1
24898	N	78.05200	82.10080	67.70790	-574.68861	534.41367	-338.04985	1
24899	H	78.04200	81.66580	66.80690	-1278.12271	2590.29701	1268.70153	1
24900	H	77.44800	81.87880	68.47390	-1860.96389	1828.68648	-1774.12020	1
24901	C	77.90741	89.63669	65.81687	-22.64975	38.39967	48.76358	1
24902	O	76.83790	89.86917	66.33817	-543.93142	126.61625	578.52904	1
24903	N	78.28326	90.01851	64.60860	759.55782	-59.01645	26.56256	1
24904	H	79.19123	89.63398	64.24030	-1123.96743	168.20772	-379.07684	1
24905	C	77.52988	90.99057	63.92146	-29.90646	269.89363	-854.79213	1
24906	H	76.60809	91.22685	64.59363	-3576.18801	-605.47142	-636.74709	1
24907	C	78.28343	92.45899	63.96460	-197.36090	-107.95219	-1068.64968	1
24908	H	78.84650	92.61685	64.90878	-1053.21516	-1901.87039	2411.14634	1
24909	H	78.95701	92.59082	63.08557	1458.82563	2103.75602	-206.78166	1
24910	C	77.01756	93.32013	63.91868	-618.48644	835.05600	-235.72673	1
24911	C	76.39615	93.79631	65.09393	212.16276	-1215.28310	-775.37474	1
24912	H	76.88664	93.35101	65.97461	1390.67285	396.35844	-146.50210	1
24913	C	75.30204	94.61152	65.12276	133.09450	-449.97077	19.50977	1
24914	H	74.89906	94.90247	66.14756	-1676.62523	122.84822	-630.50711	1

24915	C	74.75321	95.17561	63.92627	353.88133	-502.60696	-297.66569	1
24916	H	73.84053	95.76523	63.90902	469.67793	924.19218	-1582.83209	1
24917	C	76.49348	93.83583	62.68597	-363.62327	447.07565	-1363.91957	1
24918	H	77.03886	93.60965	61.76879	-905.95842	-1156.95261	1373.46410	1
24919	C	75.44111	94.79287	62.71855	288.11290	774.47463	512.45776	1
24920	H	75.16623	95.26046	61.75570	-1012.98599	1216.91603	2211.85445	1
24921	C	77.07320	90.46224	62.40178	4.47677	-462.28460	5.63949	1
24922	O	77.89569	89.92563	61.71106	220.79827	-98.19612	-413.18458	1
24923	N	75.88482	90.97073	62.09384	238.64885	211.57753	429.11073	1
24924	H	75.30449	91.44548	62.82889	856.16787	-888.25974	811.86170	1
24925	C	75.13036	90.32063	61.07649	956.97583	540.25022	247.91791	1
24926	H	75.93893	89.72020	60.58693	-1075.07462	574.34666	1818.16953	1
24927	C	73.89495	89.58225	61.74915	-424.68422	200.86958	623.88891	1
24928	H	73.22315	89.14115	60.99164	-2708.12384	-3472.82567	101.28437	1
24929	H	73.27466	90.35686	62.26516	-868.47459	651.89452	248.93421	1
24930	C	74.34503	88.53736	62.80534	-153.21347	550.98992	225.42354	1
24931	C	74.84332	87.28491	62.37350	84.02194	-225.69173	-21.32003	1
24932	H	75.06127	87.05520	61.33614	822.22397	3314.48923	-712.40352	1
24933	C	75.21416	86.30119	63.34284	545.93474	155.32222	25.83747	1
24934	H	75.55392	85.28085	63.02825	-1659.78878	-1068.30139	1731.91483	1
24935	C	75.05644	86.52182	64.77996	145.02516	904.61264	-1310.31990	1
24936	O	75.17769	85.47251	65.66695	-216.15581	18.86170	-253.51124	1
24937	H	75.54600	84.77580	64.99090	1.54280	-1167.25246	2919.82418	1
24938	C	74.46557	88.82343	64.20512	-382.78791	-39.77464	-244.36681	1
24939	H	74.24859	89.86997	64.54938	706.91751	-2701.41736	-227.32824	1
24940	C	74.75814	87.88370	65.16045	442.93763	-408.42667	896.87227	1
24941	H	74.85606	88.14868	66.25710	-563.29031	-1987.21027	922.91641	1
24942	C	74.40342	91.35609	60.08009	-741.83322	-599.34034	144.86183	1
24943	O	74.27800	92.58633	60.32979	116.69066	-728.97668	-281.43938	1
24944	N	73.98728	90.70386	58.98653	-254.93064	269.60583	213.60746	1
24945	C	74.55838	89.46267	58.51879	-257.15150	-852.37281	-131.53881	1
24946	H	75.66366	89.59399	58.23992	-11.48849	261.58902	968.68897	1
24947	H	74.53868	88.69599	59.33547	-2314.13929	-668.32019	-1394.00599	1
24948	C	73.45849	91.43252	57.84176	-286.69749	932.16304	-153.15244	1
24949	H	74.16201	92.24255	57.78401	-1197.72678	1916.47722	-1654.35031	1
24950	C	73.49675	90.47201	56.57855	-389.18072	-295.42545	152.07751	1
24951	H	72.56679	90.46774	55.95710	-1061.19890	-1105.41898	576.74431	1
24952	H	74.43713	90.87709	56.00172	-1217.34623	330.14705	1720.13468	1
24953	C	73.69348	89.08388	57.22802	-799.80882	-135.86201	490.04944	1
24954	H	72.72218	88.62921	57.57541	-2080.35406	390.60340	-1591.53084	1
24955	H	74.28816	88.40282	56.50549	2969.83704	-1211.39813	-192.10441	1
24956	C	71.94843	91.97883	58.10879	555.73414	235.37406	499.59807	1
24957	O	71.01614	91.46600	57.55949	158.23757	42.54129	-351.05321	1
24958	N	71.99290	93.00154	58.99612	31.02496	-451.36954	244.13307	1
24959	H	72.96439	93.16593	59.50623	-1517.01033	23.77152	3257.14375	1
24960	C	70.79864	93.19451	59.74431	158.88492	289.12183	822.95570	1
24961	H	71.16777	94.15143	60.17848	-120.15839	-4375.71760	1514.86001	1
24962	C	69.47950	93.19440	58.85618	-102.66503	-923.63658	306.70698	1
24963	H	69.76991	93.58811	57.85599	395.46871	-2961.86399	2507.77216	1
24964	H	69.11822	92.10986	58.81459	1406.10915	-362.18980	2284.49828	1
24965	C	68.37154	94.02992	59.59295	-472.08985	1012.71329	901.19137	1
24966	O	68.51069	94.82481	60.49812	546.32712	247.62512	32.30230	1
24967	N	67.20710	93.66941	58.99527	-31.79452	-494.12193	907.93810	1
24968	H	67.27496	93.02744	58.19819	-2251.97120	26.17991	-318.85877	1
24969	H	66.22321	94.04634	59.10264	-1495.30567	-1455.00854	-772.56149	1
24970	C	70.48608	92.02320	60.83088	544.00593	-428.78371	764.21155	1
24971	O	70.75841	90.81840	60.78391	362.71145	-285.80337	316.45532	1
24972	N	69.81047	92.58595	61.78556	560.06150	-414.50119	814.35163	1
24973	H	69.67457	93.55996	61.65491	2071.93697	2779.26116	-2380.92300	1
24974	C	69.37746	91.88135	62.98110	-201.69313	12.29596	526.97930	1
24975	H	69.94151	90.84659	62.93994	1601.36279	1182.18586	-685.02842	1
24976	C	69.39700	92.62181	64.34432	-350.87790	-596.92253	-173.50194	1

24977	H	68.76749	93.50320	64.20424	-894.48142	2464.12600	-3357.37718	1
24978	H	68.92547	92.00550	65.16294	938.37585	-328.62509	1736.04256	1
24979	C	70.98506	92.72885	64.56832	-328.61723	708.93460	1011.01591	1
24980	O	71.43306	93.73962	65.17765	-1142.64902	-337.99689	-249.75621	1
24981	O	71.72701	91.91172	63.95989	640.89935	699.58297	-517.56135	1
24982	C	67.81876	91.37204	62.77115	45.15955	297.04689	-553.49202	1
24983	O	67.16913	91.14925	63.74929	186.08900	154.05027	806.33324	1
24984	N	67.41404	91.34116	61.48969	-125.71694	-1020.36038	-602.37640	1
24985	H	68.07665	91.68843	60.78348	767.36817	631.53303	1933.50975	1
24986	C	66.56527	90.28005	60.97191	-672.87736	-47.32190	-1072.79479	1
24987	H	66.13890	90.08185	61.94698	-3647.83187	-1866.97648	-1002.86329	1
24988	C	65.56884	90.93096	59.85275	510.31125	253.46156	481.72888	1
24989	H	65.70596	92.02115	59.85899	2239.56828	2181.06251	-770.61962	1
24990	H	65.81867	90.59655	58.85176	1553.26143	-925.62823	1105.39057	1
24991	C	64.10866	90.60517	60.03640	75.47211	38.47832	-863.13199	1
24992	H	63.51132	91.08448	59.24884	5370.13521	2043.91012	1399.63160	1
24993	C	63.88070	89.12363	59.90666	-236.33255	-107.54915	60.33583	1
24994	H	64.48955	88.68111	59.10079	-3799.16279	-322.11829	-192.21839	1
24995	H	62.77789	88.95429	59.73718	-1664.56917	-4537.27164	-1484.04152	1
24996	H	64.14659	88.53610	60.80557	-386.11545	2051.27834	979.37313	1
24997	C	63.58913	91.20535	61.33528	252.31630	-688.55340	650.86519	1
24998	H	64.18660	90.84664	62.20446	2131.49483	3277.00631	1501.52347	1
24999	H	63.63100	92.35730	61.27490	-3083.37919	-1435.09954	1198.32659	1
25000	H	62.51213	90.95509	61.49804	2813.85152	97.47193	-3809.18671	1
25001	C	67.38730	89.08524	60.27885	510.44828	-781.49615	161.47800	1
25002	O	66.79171	88.06716	60.07357	131.63076	107.42844	-376.01934	1
25003	N	68.70361	89.30037	60.05067	-292.15711	-209.41641	523.66505	1
25004	H	69.23147	90.13890	60.35954	-758.05878	-617.51050	-340.59615	1
25005	C	69.40104	88.09212	59.76548	43.71413	-145.97826	-611.51831	1
25006	H	68.62155	87.51298	59.18324	944.79618	2048.53569	1606.15655	1
25007	C	70.73322	88.32977	58.85324	-482.43798	1108.02869	-66.61904	1
25008	H	71.46484	87.55475	59.14598	-1221.30234	-1716.44731	936.84183	1
25009	H	71.22327	89.28446	58.99755	1321.72676	1292.53116	4538.38354	1
25010	C	70.33843	88.11206	57.37072	880.93477	-662.85268	371.51252	1
25011	C	70.14027	88.95859	56.26323	635.05348	-278.25890	-198.38195	1
25012	H	70.32935	89.96540	56.14708	2579.29139	-347.52691	-2738.77966	1
25013	N	69.86351	88.25895	55.14592	-1008.84312	-208.62489	-680.01712	1
25014	H	69.79177	88.58138	54.15002	-9.90166	797.11259	224.89129	1
25015	C	69.74756	86.94450	55.42224	-820.90679	-785.07021	1469.50988	1
25016	C	70.01154	86.77551	56.88807	302.14574	-334.68803	355.75968	1
25017	C	69.96837	85.45161	57.41357	-275.13761	-613.41412	-1153.27079	1
25018	H	70.22015	85.21232	58.46737	-1075.31295	-1065.64839	-1434.59161	1
25019	C	69.68000	84.43180	56.55090	-261.75673	529.31251	708.63711	1
25020	H	69.73600	83.43380	56.95890	1497.44626	472.94824	2722.92890	1
25021	C	69.46473	85.82520	54.51541	329.26743	221.40896	-248.31267	1
25022	H	69.51892	85.79366	53.47496	-794.56357	1391.97709	383.41179	1
25023	C	69.46400	84.55980	55.13790	-738.99889	-507.25343	195.19978	1
25024	H	69.43900	83.61780	54.60990	-1250.26919	2891.48783	254.33855	1
25025	C	69.87819	87.38856	61.13867	455.99778	147.09879	47.91252	1
25026	O	69.79482	86.15934	61.30530	797.01102	-151.01026	311.26086	1
25027	N	70.34353	88.28523	61.98507	375.80401	-181.94776	130.83032	1
25028	H	70.46905	89.16974	61.58407	4486.79641	367.76602	-806.65606	1
25029	C	70.61305	87.95393	63.34518	759.40095	429.07201	313.02681	1
25030	H	71.49148	87.25506	63.16213	-3737.78759	-2071.96153	1210.18860	1
25031	C	71.06128	89.17533	64.31113	334.72246	1175.32266	46.02971	1
25032	H	71.51747	89.88902	63.57799	-1885.04848	-206.33370	1151.13748	1
25033	C	69.80978	89.79036	65.02019	-478.50638	-732.99229	-109.33139	1
25034	H	70.08321	90.61745	65.66954	303.26240	2280.69874	-169.88001	1
25035	H	69.34227	88.97563	65.64844	2597.76738	969.68951	-1927.79442	1
25036	H	69.01733	90.01854	64.23331	948.16402	2891.93415	2170.48414	1
25037	C	72.04731	88.75746	65.42813	-314.00503	-83.01808	182.17407	1
25038	H	71.58588	88.24874	66.32124	-4106.43361	-2260.56170	-1289.63162	1

25039	H	72.68933	88.02266	65.03690	-3252.16268	-1829.32280	2545.62073	1
25040	H	72.65366	89.65417	65.78353	-4421.96875	-1026.75638	-1747.09416	1
25041	C	69.36740	87.15281	64.05186	1068.40133	-845.43991	954.81371	1
25042	O	69.76546	86.51727	65.01506	344.61441	548.94696	-88.35861	1
25043	N	68.15259	87.43059	63.69198	169.86218	-259.57756	-93.65658	1
25044	H	67.87318	88.03273	62.91914	1488.47477	-1685.29312	-2197.60105	1
25045	C	67.05348	86.73960	64.29413	-724.45246	-365.84531	834.71454	1
25046	H	67.34979	86.45830	65.35273	3242.31978	-414.44789	2379.37603	1
25047	C	65.70477	87.55615	64.13592	-151.71993	994.53450	120.76950	1
25048	H	65.82516	88.64678	64.27146	-798.53533	-1197.96236	998.31384	1
25049	C	65.10843	87.34667	62.69676	-125.01312	229.15212	-80.98226	1
25050	H	64.00359	87.56166	62.57888	1176.46516	-1835.52826	-972.21654	1
25051	H	65.66192	87.88452	61.93153	824.94746	-2557.45690	-106.16972	1
25052	H	65.13783	86.22224	62.37060	-1528.44046	235.60424	418.67425	1
25053	C	64.77625	86.86874	65.19463	-358.93126	-48.21872	661.46957	1
25054	H	63.90260	87.47986	65.44623	874.59531	2436.40528	-726.09208	1
25055	H	64.19963	86.03606	64.71055	1139.60155	2274.14455	-53.72044	1
25056	H	65.24467	86.55294	66.15623	-1005.94824	-623.01737	296.40487	1
25057	C	66.82691	85.27779	63.57024	272.34747	960.91660	-1112.05843	1
25058	O	66.19800	84.42780	64.14390	-493.11914	598.47032	202.09267	1
25059	N	67.10475	85.39384	62.26354	284.32373	513.05167	156.99665	1
25060	H	67.72636	86.18653	62.01089	-2468.97986	-2194.57246	-1815.34076	1
25061	C	67.17300	83.92780	61.67790	674.54896	328.55623	510.61167	1
25062	H	66.24200	83.39480	61.79890	1638.57860	2263.41028	1446.62985	1
25063	C	67.57000	83.97580	60.15290	593.55725	-404.78203	546.19152	1
25064	H	68.48300	84.59580	60.02690	2092.95810	2025.78972	-1178.76287	1
25065	C	67.61400	82.57980	59.52390	-555.46018	461.17386	576.70484	1
25066	H	66.79600	81.88480	59.80990	1850.95937	-1436.48296	-2082.21162	1
25067	H	68.52000	82.02080	59.84090	2853.10552	1308.51358	-28.99859	1
25068	H	67.66500	82.68580	58.41990	-2623.79696	-1730.10003	-230.85054	1
25069	C	66.50700	84.79580	59.46790	822.57960	356.96003	-111.35045	1
25070	H	66.63300	84.77480	58.36390	-2518.88562	-463.89648	-1838.32479	1
25071	H	66.46421	85.87822	59.89081	2181.89468	1049.55511	-576.38688	1
25072	H	65.54000	84.29880	59.69790	-1709.77409	-2187.65009	-1478.61206	1
25073	C	68.20200	83.10680	62.39890	539.66221	596.06844	-423.27764	1
25074	O	68.02100	81.91380	62.76490	254.46358	-638.90999	-367.88389	1
25075	N	69.35700	83.66280	62.70190	600.68696	-446.16128	-363.29158	1
25076	H	69.64500	84.55180	62.35490	-1794.89989	-1009.30813	-2381.52954	1
25077	C	70.38900	83.01780	63.55090	-427.52719	400.57925	710.40315	1
25078	H	70.48900	81.98180	63.26390	-1082.04763	2674.05858	-1277.50920	1
25079	C	71.76000	83.63580	63.31290	-495.13612	714.33280	311.70241	1
25080	H	72.58800	82.97480	63.64590	-2649.12598	1678.41681	377.38975	1
25081	H	71.82400	84.63980	63.78390	-809.58490	3047.25306	123.96293	1
25082	C	72.03300	83.72280	61.79390	-226.37882	-514.53022	717.45198	1
25083	C	71.81600	82.59080	60.95990	268.69434	-710.11494	-486.53216	1
25084	H	71.47000	81.69580	61.45590	-2327.39246	1917.39177	941.36044	1
25085	C	72.08100	82.67680	59.54890	595.09723	107.47225	674.57000	1
25086	H	71.79200	81.91980	58.83390	-2140.52028	1676.37226	-1606.78140	1
25087	C	72.48800	83.89180	59.02390	184.09325	862.65264	-250.80159	1
25088	H	72.66000	83.92580	57.95890	-2550.20373	1504.79887	1105.49257	1
25089	C	72.42300	84.92880	61.19290	-61.69377	134.37953	-899.76818	1
25090	H	72.52969	85.84600	61.82238	-4695.73605	-408.38900	319.04503	1
25091	C	72.71085	85.04859	59.79912	441.31855	-81.68309	110.29012	1
25092	H	72.93175	85.95841	59.32850	-2933.65149	839.58364	-1967.53325	1
25093	C	70.05300	82.90880	64.99590	-713.76563	573.76150	119.90452	1
25094	O	70.29400	81.84380	65.59190	572.39985	-252.02142	-465.85988	1
25095	N	69.42700	83.89580	65.60790	-680.07231	-222.55687	-457.85248	1
25096	H	69.17200	84.72080	65.10890	-2608.54160	1221.67570	1294.60872	1
25097	C	68.97800	83.85380	67.00790	-793.53447	-174.45386	432.25232	1
25098	H	69.89000	83.70380	67.56490	336.69557	-2272.71660	-2140.46556	1
25099	C	68.23451	85.23710	67.35263	292.66140	108.89595	159.18020	1
25100	H	67.22545	85.14415	66.86510	-1340.85613	140.78298	-935.86479	1

25101	H	68.76238	86.10525	66.83338	2842.04627	112.91006	-2245.53171	1
25102	C	67.94843	85.35279	68.88401	381.13596	-457.09295	746.65493	1
25103	H	67.37700	84.47980	69.36990	-260.93854	459.34235	-3099.80111	1
25104	H	67.38887	86.23955	69.09882	1666.68923	-652.22513	602.63840	1
25105	C	69.35329	85.54875	69.67978	426.51266	-572.89895	662.14877	1
25106	O	69.85967	86.63124	69.64024	179.23493	89.93805	754.61947	1
25107	N	70.01700	84.39780	70.10590	421.94438	-470.16065	-547.39151	1
25108	H	69.81800	83.47480	69.77790	1622.55556	1466.17372	-2256.12547	1
25109	H	70.95200	84.61280	70.38790	-1626.88291	-2631.03011	582.28280	1
25110	C	68.01400	82.64180	67.17590	-691.47896	-70.35297	-598.42540	1
25111	O	68.15500	81.79780	68.04290	494.45132	295.38965	536.06006	1
25112	N	67.09000	82.50080	66.23490	-551.73207	104.93306	-637.14924	1
25113	H	67.03700	83.21580	65.54290	-1837.25908	1532.87338	2058.40188	1
25114	C	66.19800	81.42780	66.04390	-658.87063	636.21011	110.13260	1
25115	H	65.61500	81.36480	66.95090	-759.21271	2996.09497	624.74465	1
25116	C	65.20800	81.57280	64.87290	366.33712	-420.55116	-710.52024	1
25117	H	64.70000	82.55680	64.95890	702.59930	-2273.50156	-2045.72539	1
25118	H	65.78400	81.60080	63.92390	-2791.58441	1459.92500	-216.71896	1
25119	C	64.14300	80.54880	64.85190	187.84801	-873.43987	144.54341	1
25120	C	64.10100	79.51580	63.85590	-299.93141	-537.13496	674.88244	1
25121	H	64.80100	79.56380	63.03490	2737.37139	337.63242	1498.19734	1
25122	C	63.15900	78.47080	63.93090	606.96738	327.26839	591.34489	1
25123	H	63.17600	77.65880	63.21990	2075.93021	1599.28753	-1732.86698	1
25124	C	62.29400	78.35380	65.04990	324.67526	-801.51592	265.39230	1
25125	H	61.65200	77.48780	65.10490	-1204.67534	-2702.79375	1068.70587	1
25126	C	63.23200	80.41480	65.92290	645.76086	-202.91495	601.66398	1
25127	H	63.26300	81.05080	66.79490	-1816.94921	942.85338	2400.80517	1
25128	C	62.34100	79.34080	66.02690	-647.29577	632.72424	-170.73402	1
25129	H	61.57100	79.40480	66.78190	-2437.31887	825.01055	1827.11800	1
25130	C	66.93500	80.04880	65.78090	185.51737	-787.23867	-405.11360	1
25131	O	66.63200	79.06580	66.49690	43.02157	685.26939	-396.46884	1
25132	N	67.94200	79.96780	64.95690	-157.12304	-819.41831	101.50161	1
25133	H	68.28900	80.79880	64.52890	631.81715	-2943.34618	889.07764	1
25134	C	68.76200	78.73780	64.76490	-293.23029	419.11986	762.23257	1
25135	H	68.18600	77.88280	64.44390	883.51482	-325.42108	-2998.15999	1
25136	C	69.92700	79.06480	63.73590	-29.97833	743.23518	-536.57555	1
25137	H	70.79800	79.64880	64.10390	710.23353	-279.83598	-3048.93808	1
25138	H	69.47600	79.59580	62.87090	-1776.60285	2484.17863	800.90759	1
25139	C	70.63800	77.74080	63.25190	-577.75789	-688.99587	-158.42621	1
25140	H	69.81100	77.09780	62.88090	1459.71849	2646.72906	-877.34153	1
25141	H	71.15600	77.18480	64.06190	1320.76984	2329.68180	1651.82632	1
25142	C	71.61500	77.98280	62.06390	-183.57874	683.34146	-587.44140	1
25143	O	71.30400	77.62580	60.88590	242.65659	755.72354	-3.70144	1
25144	N	72.76000	78.65180	62.30290	-767.02497	255.55323	279.40772	1
25145	H	73.02500	78.74080	63.26290	-86.07817	1769.30667	2604.48148	1
25146	H	73.53400	78.74680	61.67590	-1140.38143	2031.38641	-2128.31023	1
25147	C	69.42700	78.31480	66.03490	-560.53207	-306.17687	656.15684	1
25148	O	69.49300	77.10380	66.30090	598.34213	158.15066	480.70878	1
25149	N	69.91900	79.24580	66.90290	435.18209	-379.81905	-605.43855	1
25150	H	69.86900	80.20080	66.61990	2586.19785	41.11701	-1776.96585	1
25151	C	70.55000	78.86580	68.12590	-792.89712	-47.72209	462.42339	1
25152	H	71.32000	78.13480	67.92590	-470.84950	-2694.18667	1548.35292	1
25153	C	71.25000	80.09480	68.80590	188.39862	894.86349	14.70330	1
25154	H	71.58700	79.73080	69.79990	2737.90395	307.94611	-1504.50617	1
25155	H	70.61000	80.97980	69.01290	-3106.40486	-542.35814	-61.66605	1
25156	N	73.40700	81.20880	68.59690	-218.00415	627.20489	531.09856	1
25157	H	73.43300	81.28880	69.59390	-2049.35763	1016.00048	2170.68230	1
25158	C	72.35200	80.62980	68.01290	-257.13638	569.33224	-671.77808	1
25159	C	74.26900	81.55580	67.58590	-164.56622	-892.94456	-4.45513	1
25160	H	75.19500	82.08080	67.81790	964.36751	-214.85061	2983.57918	1
25161	N	73.76200	81.31280	66.40590	153.90073	-146.19086	814.23736	1
25162	C	72.56300	80.67780	66.66290	675.42861	306.15047	-521.55498	1

25163	H	72.02400	80.25780	65.82290	1189.81656	-2020.43699	-2086.34960	1
25164	C	69.64000	78.25780	69.17190	-755.56318	359.94509	383.12254	1
25165	O	70.02400	77.39280	69.98090	-542.31828	-575.57332	46.31880	1
25166	N	68.39300	78.68480	69.17490	37.03482	-838.75477	6.91137	1
25167	H	68.03400	79.38880	68.56790	-2092.28871	1362.26491	-1926.01792	1
25168	C	67.34400	78.10680	69.99190	-494.55348	362.81404	683.20302	1
25169	H	67.88300	77.80780	70.87890	1815.76342	-2245.06283	-1231.15866	1
25170	C	66.26800	79.14380	70.38190	346.21217	-751.55797	-367.22305	1
25171	H	65.65100	79.44880	69.50990	-1693.58618	2212.05637	1478.65630	1
25172	C	65.27500	78.49980	71.45990	810.35051	372.83942	160.12749	1
25173	H	65.85400	78.09680	72.31790	-712.13120	2361.19444	1960.37271	1
25174	H	64.71300	77.63880	71.03790	-1930.22039	1063.31385	-2252.38262	1
25175	H	64.49100	79.19980	71.82090	958.24805	2014.32142	2219.50651	1
25176	C	66.88300	80.46080	70.88990	570.23939	-635.35497	299.77828	1
25177	H	67.63100	80.93980	70.22190	1952.82010	-583.24383	-2387.35068	1
25178	H	67.49200	80.42380	71.81890	-2319.38512	1816.46620	1127.13144	1
25179	C	65.83800	81.51180	71.27090	-837.47420	-341.87966	-155.34711	1
25180	H	65.02200	81.53180	70.51890	1138.12320	792.83102	-2818.84247	1
25181	H	65.46700	81.24480	72.28390	421.88059	-2162.87154	-2239.13990	1
25182	H	66.38100	82.47880	71.20490	-2339.64765	-1869.38214	-975.77161	1
25183	C	66.76900	76.84280	69.45490	-348.32388	614.17860	-585.60059	1
25184	O	66.63400	75.81380	70.12590	94.07323	-619.24440	474.58570	1
25185	N	66.31500	76.98580	68.18590	150.49793	832.75558	32.96124	1
25186	H	66.41500	77.87280	67.74190	-2625.27939	-320.82662	-1715.64358	1
25187	C	65.74200	75.94280	67.37790	143.03148	-218.12590	-870.92860	1
25188	H	64.79300	75.72480	67.84490	324.30234	2449.14976	1952.28320	1
25189	C	65.55500	76.47180	65.99690	507.46353	749.68793	101.41441	1
25190	H	65.01800	77.43680	65.87590	-2318.51205	-1644.79931	1358.65944	1
25191	H	66.57200	76.68280	65.60290	-2388.01253	1330.52391	1576.04284	1
25192	C	64.89500	75.49180	64.95890	689.88165	-81.96528	579.19872	1
25193	H	65.50600	74.59380	64.72490	1867.85014	-2493.78257	358.60383	1
25194	H	64.58300	76.09980	64.08290	-1223.06154	2904.21073	154.55697	1
25195	S	63.30800	74.83580	65.62490	407.32895	-312.54930	193.31094	1
25196	C	62.41500	74.52080	64.05090	-732.40188	539.76075	152.14615	1
25197	H	61.57500	73.84080	64.30990	1885.30766	-1394.65765	-2085.09637	1
25198	H	63.09600	74.03980	63.31690	1010.02979	2213.89121	1995.94345	1
25199	H	62.01300	75.46580	63.62590	-1991.76569	1155.70527	2156.46978	1
25200	C	66.62700	74.71180	67.33690	566.02024	-547.63433	-443.69196	1
25201	O	66.22400	73.62780	67.63590	480.69322	-603.67269	120.57797	1
25202	N	67.94400	74.80680	67.04190	404.31455	222.55930	702.67172	1
25203	H	68.38100	75.69680	66.93390	-1575.41415	1039.49512	2523.97734	1
25204	C	68.78100	73.65580	66.86890	-605.26123	88.09302	682.88605	1
25205	H	68.16600	72.78480	66.69290	1488.80437	731.21489	2668.47951	1
25206	C	69.72500	73.87980	65.70990	-184.38339	-815.74160	-356.41889	1
25207	H	70.51200	74.64080	65.89490	2162.54580	2261.53862	-309.31514	1
25208	C	70.49500	72.60180	65.37190	369.83477	57.93103	-830.26144	1
25209	H	71.16400	72.77680	64.50290	-1839.35718	-1920.56684	1681.26462	1
25210	H	71.16100	72.19280	66.16290	-1703.04796	-1030.51563	-2442.48400	1
25211	H	69.76400	71.82480	65.06090	1331.36376	2675.36942	-990.69164	1
25212	C	69.01400	74.34080	64.41390	-823.17850	-203.85299	-354.48575	1
25213	H	68.75000	75.40280	64.60590	-2516.38675	1881.30151	308.46887	1
25214	H	69.68600	74.31480	63.52990	-1954.85134	-2283.72458	-933.28185	1
25215	H	68.06000	73.80680	64.21390	2318.63136	2122.17780	38.83395	1
25216	C	69.60800	73.28180	68.10590	724.50327	-353.17356	406.48092	1
25217	O	69.97600	72.13480	68.30190	-6.48210	-546.09172	-568.24874	1
25218	N	69.88600	74.25980	68.99390	355.11130	-727.16783	212.01169	1
25219	H	69.62600	75.21180	68.84890	1747.25429	-2604.01094	-114.20069	1
25220	C	70.53000	73.95480	70.25190	890.15267	-98.99091	-124.15531	1
25221	H	70.92300	74.92080	70.53490	-44.29553	-2566.58964	-1815.10344	1
25222	H	71.34000	73.25280	70.12490	2699.65002	1506.22475	557.66958	1
25223	C	69.62700	73.38380	71.24690	-462.30739	567.03467	552.12983	1
25224	O	70.00600	72.62580	72.09890	-193.25623	-684.95282	337.23549	1

25225	N	68.35400	73.82580	71.22490	303.84146	607.84358	499.25097	1
25226	H	67.99000	74.44980	70.53890	1518.53857	633.74333	-2679.06692	1
25227	C	67.42000	73.44580	72.28490	481.95988	-659.95935	-392.42077	1
25228	H	67.91200	72.76780	72.96590	-209.37439	-173.82877	-3136.21574	1
25229	C	66.91300	74.68680	73.11490	277.41407	640.07114	586.05873	1
25230	H	66.12200	75.16780	72.50090	629.04919	1544.09082	-2668.03940	1
25231	H	67.73000	75.39380	73.37290	-1159.77067	-1007.18160	-2748.18601	1
25232	C	66.30000	74.35180	74.45690	522.88303	600.40511	-439.91228	1
25233	H	65.60900	73.48980	74.34190	-1410.89194	1895.47200	2082.55559	1
25234	C	67.30900	73.99080	75.58390	-362.58732	193.49428	-817.99640	1
25235	H	67.94500	74.88180	75.77790	-2892.61340	-571.10531	1112.20412	1
25236	H	67.87700	73.11080	75.21290	1548.61834	1909.14294	1958.98023	1
25237	H	66.84500	73.70680	76.55190	1694.49616	-1756.73421	1978.16583	1
25238	C	65.46100	75.57580	74.92890	-563.35646	-707.59131	135.68800	1
25239	H	66.10500	76.45080	75.16190	2758.03685	963.74418	1153.38843	1
25240	H	64.93300	75.42080	75.89390	-653.88616	-1901.84253	-2419.93456	1
25241	H	64.70300	75.83080	74.15790	-733.05921	964.69196	-2905.33347	1
25242	C	66.18200	72.68480	71.76890	-558.52970	148.18115	-712.57725	1
25243	O	65.92800	71.57280	72.17990	653.95009	-85.13834	422.08078	1
25244	N	65.43300	73.25880	70.81490	343.55608	-92.58705	-762.55901	1
25245	H	65.71600	74.14280	70.44990	-1163.42503	2422.63582	1645.51100	1
25246	C	64.18200	72.72380	70.30190	-374.46427	-586.85441	589.75481	1
25247	H	63.58800	72.69080	71.20390	-2352.18933	1347.05807	-1610.37968	1
25248	C	63.33000	73.64380	69.47090	-889.17524	-144.75981	-180.35622	1
25249	H	63.72500	73.82480	68.44790	-1271.23091	-2859.32624	-323.53179	1
25250	C	61.92300	73.14780	69.18390	-170.71055	892.82657	-116.98351	1
25251	H	61.36800	72.94880	70.12590	1861.32511	2276.00479	1113.35569	1
25252	H	61.30500	73.85280	68.58890	-2070.89136	1102.10971	-2105.49589	1
25253	H	61.96700	72.21880	68.57590	2155.72512	-1228.19024	-1923.78266	1
25254	C	63.22400	75.10980	70.05690	-718.62982	-198.66685	534.75858	1
25255	H	62.72800	74.93580	71.03590	-1730.32376	-2217.93762	-1413.04642	1
25256	H	64.20300	75.58080	70.29190	66.74507	-2988.46981	-970.29498	1
25257	C	62.38800	76.05980	69.16990	-910.04492	-86.37760	-98.35264	1
25258	H	62.69600	75.86280	68.12090	-2203.35371	-1315.82713	-1826.20805	1
25259	H	62.61200	77.12580	69.38790	-2967.06608	946.92023	504.47801	1
25260	H	61.29600	75.86780	69.23290	607.52105	231.86098	-3075.47318	1
25261	C	64.17900	71.32780	69.69790	608.41724	-497.19667	447.90782	1
25262	O	63.61300	70.39280	70.22690	665.77352	413.69124	-49.84050	1
25263	N	64.84000	71.21580	68.46890	23.26596	-686.29764	-486.31440	1
25264	H	65.25800	71.95580	67.94690	2826.50967	-1121.17158	771.95129	1
25265	C	64.86800	69.95580	67.69390	591.19307	-660.26052	174.57177	1
25266	H	63.81200	69.72680	67.68790	-2273.18201	-1201.80999	1818.09324	1
25267	C	65.36600	70.19380	66.22890	-483.83997	754.89336	204.77972	1
25268	H	66.39600	70.60980	66.18990	1939.75970	-2072.16207	1335.46095	1
25269	H	65.22500	69.21180	65.72890	-1111.15153	-1699.49992	2401.12144	1
25270	C	64.53200	71.18780	65.44590	637.31819	-520.43286	-373.01987	1
25271	H	64.74800	72.23680	65.73890	1025.98501	-427.56025	-2940.46084	1
25272	C	64.82900	71.16480	63.94490	-202.32466	501.12193	739.32363	1
25273	H	64.37600	72.06480	63.47790	1021.29033	-2824.30811	-910.15096	1
25274	H	64.51100	70.21780	63.45690	-1796.97869	1877.96864	-1789.41669	1
25275	H	65.92000	71.13280	63.73590	-2328.62841	435.95955	2079.76066	1
25276	C	63.01800	70.99680	65.50990	328.84530	468.07369	-710.26629	1
25277	H	62.67500	69.94880	65.36790	-2178.15872	-2094.92540	882.41572	1
25278	H	62.52000	71.27080	66.46390	1278.89592	-1968.60660	2084.62357	1
25279	H	62.58300	71.55980	64.65590	924.31313	2313.69340	-1923.70129	1
25280	C	65.59900	68.81180	68.33190	-494.70155	410.04553	-657.61829	1
25281	O	65.01500	67.77580	68.08990	44.43369	757.13622	-235.04732	1
25282	N	66.67700	68.82680	69.08290	709.14638	-412.54576	158.52437	1
25283	C	67.51000	69.99280	69.37990	-321.02388	-694.84543	492.07167	1
25284	H	67.00000	70.92280	69.70990	-1125.30740	2944.24355	44.27198	1
25285	H	68.07300	70.27080	68.46290	336.48408	2910.91108	-1156.77297	1
25286	C	67.20100	67.63480	69.73590	-541.32715	713.59851	201.67861	1

25287	H	67.07000	66.78880	69.07690	-864.49203	3027.86277	135.81839	1
25288	C	68.66500	68.04580	70.17490	474.53261	395.09626	664.78028	1
25289	H	69.12400	67.49880	71.02590	-2147.45487	-1999.86567	1136.60055	1
25290	H	69.38400	67.82280	69.35690	665.81493	2145.02501	2201.29420	1
25291	C	68.55100	69.51580	70.42490	-703.07688	-403.16392	-428.72291	1
25292	H	69.49600	70.06980	70.24090	-969.60565	2612.90599	1468.35788	1
25293	H	68.18300	69.79180	71.43690	-2268.10015	-1923.87449	-1037.29430	1
25294	C	66.39300	67.26680	71.00390	-460.22454	742.80488	277.12409	1
25295	O	66.32900	66.10480	71.31490	-143.79429	642.64690	438.70699	1
25296	N	65.84600	68.26680	71.68190	518.76376	647.47320	-148.97223	1
25297	H	65.99600	69.19580	71.35290	2323.79627	686.95939	-2002.31293	1
25298	C	64.95700	68.17180	72.79490	393.67741	-675.38736	458.18254	1
25299	H	64.63100	69.17880	73.00590	2050.39186	1122.31898	2098.92922	1
25300	H	65.55800	67.86280	73.63690	1727.63420	97.06101	-2626.58938	1
25301	C	63.76000	67.32980	72.57190	-16.15531	-836.72768	-359.42025	1
25302	O	63.42600	66.47880	73.44190	-442.74268	-215.22819	-623.63315	1
25303	N	63.06200	67.53680	71.42990	760.01015	163.12671	313.22686	1
25304	H	63.28600	68.31780	70.85290	-1868.34063	1372.32815	2132.69438	1
25305	C	61.89500	66.79280	71.11990	127.61219	-580.96582	685.46881	1
25306	H	61.24900	66.80980	71.98490	-1369.68121	-2720.16075	-794.36821	1
25307	C	61.08100	67.31480	69.93990	586.47292	-685.33796	-77.70395	1
25308	H	60.31700	66.55780	69.66190	1187.72408	2580.89911	-1353.08395	1
25309	C	60.20100	68.50380	70.43690	-68.98729	-705.54588	569.86940	1
25310	H	59.64400	68.05180	71.28490	1657.94306	1186.21215	2391.77831	1
25311	H	59.37700	68.71880	69.72290	-672.71707	3057.52386	-352.73998	1
25312	H	60.89200	69.32080	70.73390	1489.79135	-1900.50530	-2010.09223	1
25313	C	61.97000	67.64580	68.73790	-11.14916	824.00639	-399.73436	1
25314	H	62.59600	68.53580	68.96190	-12.33331	-233.10734	3135.47366	1
25315	H	62.67200	66.81080	68.52690	1504.73905	-444.53988	2720.01118	1
25316	C	61.18200	67.81180	67.43490	-836.13465	-316.02936	-207.71407	1
25317	H	61.83300	68.03080	66.56190	2978.93554	-733.17551	-660.43712	1
25318	H	60.42100	68.61980	67.48290	1463.84887	618.99150	2710.79834	1
25319	H	60.54100	66.91780	67.27590	1961.95166	-2309.78589	814.63559	1
25320	C	62.10100	65.27780	70.85890	536.24226	-408.84263	603.55484	1
25321	O	61.32600	64.41780	71.31790	-96.29828	-193.75489	-762.56759	1
25322	N	63.17400	64.90480	70.18990	-123.83526	378.17960	743.85218	1
25323	H	63.73500	65.66780	69.88090	727.85591	-2820.32900	-1180.35995	1
25324	C	63.66700	63.56780	70.06490	-596.17947	642.64117	-277.08099	1
25325	H	62.88200	62.91180	69.71890	1861.93921	2190.53873	-1278.30066	1
25326	C	64.85000	63.46980	69.11790	66.72759	-743.90270	512.52703	1
25327	H	65.76400	63.92480	69.55590	-67.35601	-1126.57123	-2939.82582	1
25328	C	65.11100	61.98380	68.79790	581.98930	-564.81118	-407.31289	1
25329	H	65.53400	61.39180	69.63790	2123.40360	1690.94945	1581.09418	1
25330	H	65.93800	61.98080	68.05590	862.69286	-2719.99370	1306.64822	1
25331	H	64.16200	61.56580	68.39990	-1390.04854	-1783.68373	-2193.03110	1
25332	C	64.66600	64.18280	67.82090	-518.92918	749.95530	110.93793	1
25333	H	64.71900	65.29080	67.87690	1580.94029	-184.48722	-2712.95926	1
25334	H	65.40800	63.84580	67.06590	1793.57735	-1931.01503	1701.33638	1
25335	H	63.66800	64.06080	67.34590	1340.76477	2036.46805	-1991.66304	1
25336	C	64.06000	63.02280	71.47490	-7.51084	754.87586	-519.77062	1
25337	O	63.68600	61.86980	71.71690	709.25250	-90.97897	-326.85921	1
25338	N	64.69800	63.81880	72.35490	545.63686	-395.88356	495.90340	1
25339	H	64.92200	64.75380	72.09190	1059.52783	2434.15084	-1692.27898	1
25340	C	64.99500	63.39580	73.70990	78.96657	857.57817	-308.32330	1
25341	H	65.58600	62.49180	73.72390	-1383.71628	-2171.90976	-1813.55464	1
25342	C	65.90700	64.41680	74.47290	-553.93910	-721.74333	77.72866	1
25343	H	65.40800	65.40280	74.35890	-804.24724	-3002.02377	482.90058	1
25344	C	65.96600	64.10380	75.97690	116.78843	469.48150	768.62941	1
25345	H	64.99500	64.04380	76.51390	1060.08381	1359.22657	-2634.66321	1
25346	H	66.52400	63.15380	76.11390	723.70093	-2506.91396	1749.17447	1
25347	H	66.62700	64.80880	76.52590	-2162.51048	217.29979	2275.06557	1
25348	C	67.28900	64.30380	73.77390	744.16528	-455.10374	-250.48438	1

25349	H	67.15200	64.24880	72.67190	-425.77974	-1906.07702	-2470.01860	1
25350	H	67.80800	63.36280	74.05590	1286.96860	-2511.08408	-1387.76591	1
25351	C	68.16400	65.49680	74.02690	-399.93473	465.53731	-683.56255	1
25352	H	67.70100	66.33980	73.47090	2080.81159	1739.17207	-1594.10860	1
25353	H	68.23500	65.67980	75.11990	2817.57021	-546.86014	1272.04864	1
25354	H	69.22100	65.29580	73.74790	1920.60780	-1483.18315	1990.46288	1
25355	C	63.73700	63.05580	74.48490	488.45607	-497.74511	-586.06088	1
25356	O	63.59500	61.94380	75.01890	-737.02026	92.16497	276.73800	1
25357	N	62.71100	63.97680	74.42690	-393.51217	-499.39871	-561.16694	1
25358	H	62.97700	64.85880	74.04390	1945.60809	-1150.36670	-2186.10609	1
25359	C	61.40000	63.89880	75.00690	-70.70251	688.68512	592.05453	1
25360	H	61.51400	63.67880	76.05790	-1955.87549	1538.79440	-1933.39315	1
25361	C	60.66100	65.21180	74.74190	517.43717	727.48888	-177.47926	1
25362	H	60.92700	65.60280	73.73690	-1880.25493	1773.58447	-1803.34982	1
25363	H	59.56300	65.07380	74.83190	-3112.41882	304.02274	-391.29498	1
25364	C	61.13800	66.33980	75.75290	-531.48320	-297.16207	680.15232	1
25365	H	62.24600	66.39680	75.69090	-1301.40630	1076.75184	-2659.62240	1
25366	C	60.60400	67.72780	75.32790	554.27240	572.37731	-439.24426	1
25367	H	60.92600	68.06380	74.31990	2171.18571	890.42568	2088.68801	1
25368	H	59.49500	67.79180	75.33190	-1723.26691	-2186.53689	-1471.95069	1
25369	H	60.93400	68.51280	76.04190	933.77526	2087.95228	-2159.88955	1
25370	C	60.79400	66.15080	77.20290	788.84956	-219.39317	-394.05462	1
25371	H	61.31900	65.24480	77.57390	-585.63575	1168.86331	-2865.25287	1
25372	H	60.95400	67.10180	77.75390	-2959.25444	506.47122	953.12281	1
25373	H	59.72800	65.90580	77.39990	1748.25453	232.66494	2600.24733	1
25374	C	60.68300	62.63780	74.55090	-427.75404	681.62713	431.98247	1
25375	O	60.15800	61.87580	75.38690	503.14428	598.19819	-97.94068	1
25376	N	60.66600	62.35580	73.27790	-577.70782	391.22150	479.29382	1
25377	H	61.20100	62.96480	72.69590	1744.47096	-2012.26006	-1670.52476	1
25378	C	60.10100	61.11180	72.65490	140.90697	301.04026	-852.75534	1
25379	H	59.04500	61.08180	72.87990	773.42778	-2128.58558	2176.82642	1
25380	C	60.12500	61.11180	71.07890	-87.20908	643.23334	639.62247	1
25381	H	59.92400	60.10280	70.65790	2235.18739	-2095.63068	684.66122	1
25382	H	61.15700	61.42380	70.81190	1729.03814	-2484.60271	-842.09458	1
25383	O	59.30200	62.05380	70.45490	-360.32839	-46.00652	700.71962	1
25384	H	58.40200	61.85880	70.72590	-977.88441	2987.43297	-209.18439	1
25385	C	60.70300	59.78680	73.11590	591.33585	-629.86168	272.96314	1
25386	O	59.91400	58.83680	73.29290	-342.32257	-9.17415	709.12639	1
25387	N	62.04400	59.67780	73.24190	210.26956	-353.23633	-740.02479	1
25388	H	62.55400	60.48180	72.94690	-1118.55459	-2281.51299	-1860.58936	1
25389	C	62.74300	58.45280	73.65390	-417.34587	-247.34127	768.36831	1
25390	H	62.41300	57.69680	72.95690	-622.77630	2900.95223	-1060.43901	1
25391	C	64.26900	58.73380	73.87290	-733.56851	261.43838	476.45738	1
25392	H	64.76100	57.78280	74.17290	897.14896	933.18841	-2873.12404	1
25393	H	64.35500	59.49580	74.67690	-1456.98083	-2620.25625	950.61363	1
25394	S	64.98900	59.21680	72.26490	-199.23621	-73.74322	511.45803	1
25395	H	64.69800	60.50780	72.31790	-686.62890	-1450.37428	2700.74460	1
25396	C	62.19100	57.92080	74.99590	112.65185	740.67851	-526.19692	1
25397	O	61.86400	56.75380	75.16990	178.67799	594.22236	482.25813	1
25398	N	62.14600	58.80680	76.01990	41.66216	805.73763	-255.60349	1
25399	H	62.48500	59.73680	75.89890	-679.08358	-2326.64101	-2011.41013	1
25400	C	61.69700	58.38880	77.38590	-744.60959	-479.04057	-234.94274	1
25401	H	62.07100	57.41880	77.67990	-2649.38099	1517.77581	764.80955	1
25402	C	62.30100	59.29480	78.44190	754.05497	468.38295	-200.48667	1
25403	H	61.96400	58.85080	79.40290	2402.98963	1320.73956	-1542.48239	1
25404	H	61.85500	60.29480	78.25690	2779.28262	1101.91177	964.42472	1
25405	C	63.83700	59.35180	78.28390	-806.64473	141.13776	402.51307	1
25406	C	64.38900	60.56680	77.83490	566.12223	536.25287	-473.78064	1
25407	H	63.80300	61.43580	77.57490	897.30392	2307.92115	1934.64121	1
25408	C	65.78200	60.60780	77.65190	-41.60776	-596.86470	-693.38240	1
25409	H	66.16600	61.51380	77.20790	-908.95382	1354.21544	2686.79991	1
25410	C	66.60500	59.53580	77.92290	-820.78401	-16.32267	-410.49309	1

25411	O	67.97300	59.58680	77.66090	-657.14196	-390.63375	201.56302	1
25412	H	68.15200	60.22280	76.96390	1756.12133	-2575.75318	-405.88925	1
25413	C	64.61200	58.27280	78.57190	-389.04374	437.27601	694.91365	1
25414	H	64.11800	57.43480	79.04090	2257.40182	-996.58226	1941.85223	1
25415	C	66.01500	58.33080	78.34490	-480.10183	-367.84540	677.96337	1
25416	H	66.62900	57.44280	78.37690	955.45519	-2912.16914	-711.08916	1
25417	C	60.22600	58.36380	77.44290	37.05971	834.47293	-370.28863	1
25418	O	59.63100	57.65280	78.25890	-325.84923	525.89385	-497.64653	1
25419	N	59.50100	59.13780	76.59090	184.80035	-563.00154	-604.34886	1
25420	H	59.91300	59.78880	75.95890	-2207.73499	1692.09611	1472.51889	1
25421	C	58.09000	58.99580	76.38390	-905.51445	-95.86793	93.04053	1
25422	H	57.66200	59.15280	77.36290	1909.48368	-2197.36945	1183.75963	1
25423	C	57.49900	60.00280	75.39790	-8.27331	-815.80633	402.82954	1
25424	H	57.89000	60.99280	75.71490	-1937.22446	-1895.93125	-1605.40177	1
25425	H	57.90100	59.81880	74.37790	726.15011	-3019.77396	486.06933	1
25426	S	55.72300	60.08580	75.22290	-13.04035	-298.18373	468.12165	1
25427	H	55.62900	59.09380	74.34990	-2342.28634	1913.77637	875.60362	1
25428	C	57.68600	57.57480	75.97290	-729.71906	212.29388	-514.16553	1
25429	O	56.79800	56.98380	76.56690	-679.06989	-371.53951	-176.30881	1
25430	N	58.36000	56.95880	75.04090	8.09640	-814.43915	-224.38680	1
25431	H	58.91300	57.53180	74.44090	-732.18158	2446.19823	1836.04905	1
25432	C	58.10400	55.59180	74.61790	-594.94755	131.40572	676.57127	1
25433	H	57.05600	55.50580	74.37190	1975.86784	-2440.28998	-144.62029	1
25434	C	58.88400	55.19280	73.32890	621.96808	-582.46387	-319.45686	1
25435	H	59.96700	55.39580	73.47690	-2097.39931	1787.72556	-1531.28666	1
25436	C	58.75700	53.70380	73.07890	-709.09967	109.95400	561.75738	1
25437	H	59.12800	53.48880	72.05390	2477.75423	1406.57395	-1334.67679	1
25438	H	59.29400	53.04680	73.79590	2779.83153	-1394.44616	-455.20003	1
25439	H	57.68400	53.41180	73.07590	2815.54171	1396.73836	15.96069	1
25440	C	58.35700	55.95380	72.10590	620.58163	-62.81054	-665.90660	1
25441	H	57.42400	55.51380	71.69390	1378.61682	2826.82428	-66.91023	1
25442	H	58.03500	56.99480	72.32590	2387.24290	2044.85179	36.63227	1
25443	C	59.39500	56.11680	70.97890	692.04483	-525.24606	-264.77266	1
25444	H	59.93700	55.16780	70.78090	1904.86729	-1421.95594	2048.55396	1
25445	H	59.03200	56.60880	70.05190	1915.49614	180.77640	2479.99205	1
25446	H	60.04100	56.97780	71.25290	2521.12411	1582.07890	1004.92652	1
25447	C	58.48800	54.59080	75.69290	-676.48537	35.99850	-620.26861	1
25448	O	57.74000	53.60180	75.90990	-481.87803	-400.26944	-490.12836	1
25449	N	59.64700	54.78980	76.37390	-598.07996	-518.47477	-306.02065	1
25450	H	59.99800	55.71780	76.27190	-2804.99307	-1160.15125	832.74280	1
25451	C	60.34200	53.84080	77.29690	-468.98440	-631.94864	-470.32158	1
25452	H	60.57700	52.90980	76.80290	2101.58109	-1398.49546	-1881.20471	1
25453	C	61.81500	54.30380	77.78890	560.75104	-478.72040	526.35275	1
25454	H	61.72400	55.38780	78.01790	-183.68794	2661.78188	-1673.95999	1
25455	C	62.20200	53.43880	79.01190	-738.27168	495.20263	203.78036	1
25456	H	62.13300	52.35980	78.75490	1742.20933	1919.14072	1772.74128	1
25457	H	63.25500	53.63080	79.30990	-2457.50379	-1863.42726	-640.01204	1
25458	H	61.54700	53.49980	79.90690	-3076.46603	509.65076	-439.93271	1
25459	C	62.82100	54.15980	76.66190	-538.83804	393.54338	-631.96227	1
25460	H	62.32800	54.42880	75.70290	2531.60287	-1815.59591	-421.05835	1
25461	H	63.23200	53.13380	76.55490	634.79353	-2995.48303	-724.70037	1
25462	C	64.08400	54.91880	76.90390	-184.13807	853.32626	260.59174	1
25463	H	63.83200	55.97580	77.13390	-2166.32618	-237.19619	-2279.15350	1
25464	H	64.72100	54.56480	77.74290	-684.98562	-2936.49469	-906.20132	1
25465	H	64.80100	54.81880	76.06190	-106.40325	-379.24058	-3128.92930	1
25466	C	59.39500	53.38480	78.45890	362.73728	-772.25232	313.20819	1
25467	O	59.23700	52.19880	78.85690	-133.38834	-582.76836	-524.39172	1
25468	N	58.74100	54.39080	79.02790	-582.71053	-498.63172	352.20370	1
25469	H	58.82900	55.33080	78.70690	-2468.04052	1949.32524	131.01141	1
25470	C	57.95400	54.24980	80.20890	550.60524	-540.01590	479.40228	1
25471	H	58.55600	53.66780	80.89190	-1938.31132	1680.24537	1815.99635	1
25472	C	57.67700	55.58980	80.88790	-547.28339	522.86882	-514.62002	1

25473	H	57.07200	55.33580	81.78590	2314.41723	-1889.26436	-990.52187	1
25474	C	58.98100	56.16480	81.44990	632.50835	579.78525	295.24144	1
25475	H	58.79600	57.04280	82.10490	2072.59196	-1605.40223	1733.43787	1
25476	H	59.55900	55.40180	82.01390	-3029.52462	728.38312	-452.09881	1
25477	H	59.56000	56.60080	80.60790	489.73541	-3015.18638	751.05713	1
25478	C	56.89100	56.57580	80.03690	-738.17933	-69.24703	-539.44626	1
25479	H	57.59600	57.08480	79.34490	-2014.10563	2110.85900	1175.55937	1
25480	H	56.23000	55.99780	79.35490	-1758.04412	1809.40399	1876.36966	1
25481	C	56.10400	57.58680	80.84990	612.09942	72.72418	665.19675	1
25482	H	55.43400	57.04080	81.54790	2508.33937	1884.31890	185.24347	1
25483	H	55.39900	58.12580	80.18290	-15.38957	59.75542	-3149.29738	1
25484	H	56.80600	58.30380	81.32690	2076.32778	-1737.11946	1597.65195	1
25485	C	56.78400	53.35880	80.02290	-745.79591	510.06983	-136.26126	1
25486	O	56.23600	52.76380	80.96890	586.46816	523.06369	37.22129	1
25487	N	56.27700	53.27880	78.79190	10.70433	587.60088	599.13778	1
25488	H	56.73500	53.86180	78.12490	943.23205	-1979.60866	2249.71654	1
25489	C	55.13000	52.49880	78.47790	-298.45793	790.62413	-348.10402	1
25490	H	54.47900	52.42980	79.33690	841.10892	1699.95694	2502.69370	1
25491	C	54.26500	53.22480	77.40490	751.08208	510.32211	-46.41126	1
25492	H	53.70300	54.02080	77.93790	-1912.50921	-2486.88140	263.83563	1
25493	H	53.51500	52.55080	76.93890	-2514.75430	-1579.36864	1041.97877	1
25494	O	55.06400	53.77880	76.36790	-403.81631	635.29029	-248.82320	1
25495	H	55.77900	53.17280	76.16290	123.48385	3123.82324	345.40259	1
25496	C	55.34500	51.08080	78.13790	727.16410	-447.36364	309.39236	1
25497	O	54.38400	50.33480	77.74290	440.45538	-652.77722	-55.99166	1
25498	N	56.56600	50.60580	78.30390	-110.12572	-766.71739	331.33620	1
25499	H	57.18900	51.23380	78.76590	-206.09660	1793.80309	-2582.87050	1
25500	C	56.93000	49.22180	78.07690	647.42298	-640.49008	-4.87502	1
25501	H	56.17700	48.60980	78.54990	-1685.57563	-2009.33410	1733.18203	1
25502	C	56.90500	48.80080	76.58590	547.78093	503.05454	517.03139	1
25503	H	55.84500	48.89880	76.26890	-1916.10626	2467.70100	375.89510	1
25504	H	57.16400	47.73180	76.43290	1243.65199	2688.00758	1050.04261	1
25505	C	57.61500	49.74880	75.55590	-527.85145	657.26409	345.25500	1
25506	H	58.66700	49.92380	75.86590	50.75156	-3096.96792	-557.03030	1
25507	H	57.07500	50.71580	75.64090	810.84637	1730.29012	-2505.59484	1
25508	C	57.50000	49.15880	74.14190	-223.35265	495.37736	726.09066	1
25509	H	58.09000	49.79580	73.44890	-2574.82200	-1810.75131	51.97719	1
25510	H	58.01800	48.17680	74.12790	2255.03114	444.43995	-2153.50318	1
25511	C	56.08000	49.16180	73.63190	566.76327	-673.03576	220.94543	1
25512	H	55.39300	48.50380	74.20690	1469.41986	-1730.98496	-2182.57190	1
25513	H	55.70700	50.20880	73.64390	2310.54238	135.47811	-2134.07279	1
25514	N	56.00100	48.71280	72.26790	-368.51878	-341.35732	-687.30492	1
25515	H	56.26500	49.45680	71.59090	161.08552	-2616.85465	1728.81374	1
25516	H	55.01000	48.47780	72.05990	1481.87613	2106.56126	1798.00185	1
25517	H	56.61600	47.89280	72.09290	2552.09690	-659.51715	-1719.47830	1
25518	C	58.25800	48.62980	78.70690	528.68676	544.68588	494.17694	1
25519	O	58.67000	47.50480	78.41790	-485.64995	-551.48467	284.81516	1
25520	N	58.87400	49.39780	79.67090	-11.15353	-841.05502	75.23653	1
25521	H	58.55300	50.33080	79.81490	2295.09230	2050.43469	-650.28071	1
25522	C	60.05300	49.01480	80.43090	-739.76577	51.35025	524.23380	1
25523	H	60.85900	48.83280	79.73490	-211.97496	1445.24612	2777.44621	1
25524	C	60.48400	50.11080	81.40890	-592.92340	417.79370	-561.22024	1
25525	H	60.55300	51.07380	80.85790	-1983.46346	-902.11708	2263.60544	1
25526	H	59.62900	50.22680	82.10890	-1608.99885	-1669.53969	-2136.84080	1
25527	C	61.81200	49.86180	82.09690	-17.39217	53.57775	901.39075	1
25528	H	61.77700	48.88480	82.62590	486.97202	2619.74135	1660.67321	1
25529	C	62.94700	50.01980	81.06690	703.63325	-577.47312	-52.21045	1
25530	H	62.97300	51.01480	80.57190	-2307.21941	1828.12275	1104.24845	1
25531	H	62.94200	49.14980	80.37590	-379.88308	-367.68946	-3110.90518	1
25532	H	63.86500	49.83680	81.66490	2804.40415	1331.11270	-510.19502	1
25533	C	61.98100	50.95380	83.20990	-530.35700	-529.07068	-531.23309	1
25534	H	61.11500	50.89480	83.90290	-2600.96689	-13.23639	1763.31772	1

25535	H	62.95000	50.78680	83.72690	-2858.15912	-1165.87505	-625.01334	1
25536	H	62.00600	51.98380	82.79390	-1979.55886	-1095.81766	2180.26988	1
25537	C	59.83400	47.69080	81.19690	28.16078	588.78346	-703.32129	1
25538	O	60.73700	46.80980	81.21890	-396.42664	-156.47903	656.28573	1
25539	N	58.64700	47.46780	81.86090	189.50305	-795.22824	-225.45440	1
25540	H	57.93700	48.16280	81.93990	-2343.97394	-2095.72374	151.12772	1
25541	C	58.32400	46.20480	82.43990	-698.23026	578.72050	-95.57311	1
25542	H	59.16000	45.72380	82.92390	-136.09305	-1222.11680	2887.34584	1
25543	C	57.25300	46.40580	83.55490	438.60519	-369.65632	701.24722	1
25544	H	56.46500	47.09480	83.18390	-2984.15346	-796.47279	-613.66978	1
25545	H	56.84700	45.42880	83.89290	-1528.64299	2388.34080	-1366.96455	1
25546	O	57.79400	47.05480	84.72390	-58.51501	-274.67543	-747.85507	1
25547	H	58.33600	46.39680	85.16390	-3067.73636	-108.12397	680.97552	1
25548	C	57.74300	45.15880	81.47690	-761.43432	366.34712	-351.86501	1
25549	O	57.44700	44.02980	81.86390	658.42406	-57.23348	-441.32801	1
25550	N	57.64000	45.44880	80.18090	-28.83271	-201.47557	-828.86920	1
25551	H	57.87600	46.33480	79.79090	-2407.00087	1967.31608	477.22477	1
25552	C	57.07300	44.51080	79.22090	222.25047	528.66122	-717.09076	1
25553	H	56.64100	43.64980	79.70890	-2195.30224	2068.21296	885.19037	1
25554	C	55.93600	45.12680	78.34290	-520.52782	-146.23133	726.73201	1
25555	H	56.29600	45.99180	77.74590	2182.80936	100.04034	2253.02174	1
25556	H	55.54800	44.49680	77.51490	1246.64597	-603.21103	-2833.27020	1
25557	N	53.71900	46.31980	78.70290	-452.32544	534.44687	-479.57797	1
25558	H	53.67500	46.71180	77.78490	2143.22087	691.28098	-2202.42025	1
25559	C	54.76900	45.59380	79.19390	746.12048	318.95916	403.86066	1
25560	C	52.84700	46.50780	79.73890	-655.23277	360.15652	514.97758	1
25561	H	51.89400	47.02380	79.61890	820.15980	-3006.18718	-451.25623	1
25562	N	53.29900	45.96080	80.86590	-522.22342	-366.13709	547.70996	1
25563	C	54.52600	45.35480	80.48390	149.93693	171.97960	873.78990	1
25564	H	55.14700	44.83680	81.20490	-1934.56761	1912.99514	1569.65665	1
25565	C	58.04800	44.00880	78.19490	735.63683	259.59731	459.54437	1
25566	O	57.88200	42.94680	77.55890	259.17027	-502.59429	540.59931	1
25567	N	59.14200	44.76280	78.02990	-230.88063	-767.62611	-277.16269	1
25568	H	59.21600	45.65280	78.47390	2721.07718	-1531.93880	-383.15218	1
25569	C	60.37000	44.45780	77.32690	473.70491	-634.32786	440.10410	1
25570	H	60.06600	43.86780	76.47490	1924.74792	-1447.26938	-2032.90251	1
25571	C	61.19700	45.73880	76.87590	-755.21103	-28.76892	503.24446	1
25572	H	62.10800	45.47580	76.29590	-205.32545	-2886.01693	1224.11527	1
25573	H	61.43300	46.19080	77.86290	-2219.75341	860.90680	-2068.62879	1
25574	O	60.39300	46.65880	76.10090	297.03439	658.41511	308.52724	1
25575	H	59.93500	47.30180	76.64590	-933.61401	1922.18738	2301.14223	1
25576	C	61.25600	43.57680	78.15690	-180.20461	-160.99100	868.69469	1
25577	O	61.74400	44.02380	79.23190	667.69655	408.95211	81.23428	1
25578	O	61.55900	42.43480	77.70390	606.02463	-496.79187	-99.16065	1
25579	N	68.09800	39.69880	83.86190	572.14840	348.49268	499.13078	1
25580	H	68.31400	38.85080	84.42290	910.88142	2167.50233	2074.67999	1
25581	H	68.24600	39.59180	82.83790	1776.28789	-2242.63956	1296.88740	1
25582	H	67.12500	40.02180	84.03590	1021.91205	1010.50969	-2812.12598	1
25583	C	68.95200	40.75780	84.30590	778.07659	145.19269	439.13499	1
25584	H	68.94300	40.82480	85.38390	1946.89076	224.15770	2447.69469	1
25585	C	70.47100	40.56280	83.91090	-111.17474	612.18102	650.97023	1
25586	H	70.98000	41.53880	84.06090	2031.63668	2398.07471	-140.54322	1
25587	H	70.47900	40.45980	82.80490	230.87820	-2500.71031	-1910.58185	1
25588	C	71.15500	39.33080	84.51890	-125.96207	-756.64873	479.63392	1
25589	H	72.17500	39.10180	84.14190	2817.89958	-1317.06781	463.57001	1
25590	H	70.62200	38.43880	84.12690	2587.53815	176.90232	-1797.22989	1
25591	C	71.32300	39.38980	86.03290	464.33305	679.77286	-405.47193	1
25592	H	70.30800	39.45380	86.48090	141.44274	-558.29009	-3108.29175	1
25593	H	71.82700	40.34380	86.29990	-1193.87842	1305.33389	2585.34378	1
25594	C	71.99000	38.13380	86.56490	194.03726	-858.91623	229.05791	1
25595	H	71.54000	37.18180	86.20890	2224.79382	-2113.60034	688.02257	1
25596	H	73.02200	38.05280	86.16090	-2221.81265	-1829.88731	1254.02116	1

25597	N	72.01700	38.08680	88.06190	-229.59529	310.00148	733.44118	1
25598	H	72.40100	38.94980	88.49690	-1217.21774	2185.16780	-1919.72237	1
25599	H	71.06600	37.95380	88.46190	-1433.98301	-2002.52624	-1974.52569	1
25600	H	72.60700	37.30680	88.41590	2887.40422	1133.45820	-547.80871	1
25601	C	68.42100	42.10180	83.76190	-828.68968	-100.29749	353.52751	1
25602	O	67.82500	42.17680	82.71690	-522.46483	-578.24881	-145.69599	1
25603	N	68.61900	43.27580	84.43490	-646.73735	539.43822	-50.62206	1
25604	H	69.20800	43.27780	85.23890	2269.61228	2046.31764	731.39343	1
25605	C	67.99400	44.54780	83.99690	242.22327	239.65341	-857.65584	1
25606	H	68.34000	44.71780	82.98890	859.28505	-1424.96824	-2682.87345	1
25607	H	66.91700	44.46680	83.96490	-771.71817	-607.43786	-3001.32564	1
25608	C	68.37200	45.68480	84.92590	184.71477	-323.15887	821.12600	1
25609	O	68.20000	46.83880	84.64490	-683.00458	-369.89724	136.18410	1
25610	N	68.83800	45.43480	86.17690	-151.39229	591.14501	-593.20456	1
25611	H	69.14100	44.52880	86.46290	2037.86272	2008.17543	1293.47752	1
25612	C	69.04600	46.53980	87.06590	-543.11290	-347.51654	-657.51677	1
25613	H	68.12300	47.09580	87.14390	66.79450	-2805.07552	1417.01724	1
25614	C	69.42500	45.95680	88.48290	-271.04632	-712.62990	-516.04010	1
25615	H	69.61000	46.79780	89.18490	-408.86347	2761.07606	-1457.13173	1
25616	H	70.26400	45.23680	88.37490	2380.76341	925.05122	1824.20722	1
25617	N	68.12900	45.25980	90.58990	462.36708	307.07757	-647.40092	1
25618	H	68.44200	46.05880	91.10290	-328.47456	2959.17630	992.16865	1
25619	C	68.28000	45.18480	89.23290	520.81394	325.89567	-685.24677	1
25620	C	67.11100	44.45380	90.92790	646.22292	-342.19029	537.41111	1
25621	H	66.88800	44.18780	91.96090	1811.91205	2561.03972	-212.46332	1
25622	N	66.50500	43.97780	89.88790	-539.24208	462.16351	-462.61130	1
25623	C	67.24500	44.40280	88.80090	235.07908	628.65201	602.06080	1
25624	H	67.06100	44.12980	87.76890	2201.34033	768.29515	-2124.52362	1
25625	C	70.13100	47.50080	86.71590	173.75021	437.41516	-791.55036	1
25626	O	69.95600	48.68880	86.84090	222.56843	-629.44933	414.01667	1
25627	N	71.22300	46.97380	86.14590	204.81638	808.13477	108.88488	1
25628	H	71.30800	45.98380	86.05590	1395.89859	-1037.40305	2609.96915	1
25629	C	72.34500	47.79380	85.73390	660.79876	626.73078	-9.96498	1
25630	H	72.45100	48.61880	86.42290	-1545.46175	574.38727	-2691.05549	1
25631	C	73.65200	47.05680	85.70090	-425.71347	46.73580	792.00379	1
25632	H	73.55600	46.00080	85.36790	3039.37973	629.25178	-526.64808	1
25633	H	74.35000	47.50180	84.95990	-1972.90628	1037.14966	-2232.97782	1
25634	C	74.30700	47.04680	87.09390	480.98230	149.99186	746.86726	1
25635	H	74.48500	48.04780	87.54190	2371.12486	2027.46513	-411.96702	1
25636	H	75.34400	46.64680	87.06490	1467.72174	-1261.11581	2468.31487	1
25637	C	73.53900	46.29480	88.22990	59.57164	863.48185	266.66990	1
25638	O	73.14300	46.94180	89.21590	701.60397	-339.67769	-151.87416	1
25639	N	73.26100	44.98580	88.05190	-504.81886	156.89550	-670.43680	1
25640	H	73.59700	44.45680	87.27190	3145.80569	6.48472	-99.37089	1
25641	H	72.71800	44.56680	88.77890	2894.65267	211.77240	-1230.25333	1
25642	C	72.00600	48.49580	84.37690	-652.52051	175.99455	-624.18738	1
25643	O	72.38900	49.64980	84.14890	350.31640	169.84020	-698.03500	1
25644	N	71.16500	47.88080	83.49290	-303.15304	-767.22376	-195.94143	1
25645	H	70.90700	46.92780	83.63290	363.98006	-1765.40643	2566.99020	1
25646	C	70.59400	48.62080	82.36290	-863.52263	-289.81833	-73.54308	1
25647	H	71.41900	49.01280	81.78590	1034.78521	2208.28216	-1998.36773	1
25648	C	69.70100	47.63480	81.51590	-165.67591	-344.49176	-839.80251	1
25649	H	69.09700	47.05380	82.24590	657.60912	-2146.65452	2192.75733	1
25650	H	69.01800	48.11480	80.78390	2983.72361	-664.97893	727.25700	1
25651	C	70.56200	46.67680	80.62690	282.31392	211.65759	828.22551	1
25652	H	71.33500	46.24680	81.29890	-1917.83989	822.52708	-2367.84591	1
25653	H	71.11300	47.16180	79.79190	-946.23148	-445.65707	2955.44761	1
25654	C	69.74500	45.52780	80.02090	523.04167	-391.51330	622.48364	1
25655	H	69.31500	44.92580	80.84990	-1230.52272	1844.36171	2220.02125	1
25656	H	70.38800	44.89380	79.37490	1014.29078	-779.65970	-2886.48899	1
25657	C	68.59400	45.99380	79.11190	-665.02027	-12.29125	-637.30567	1
25658	H	67.85700	46.48980	79.77890	2251.65045	-497.05708	-2150.38313	1

25659	H	68.97400	46.63180	78.28490	914.76839	-2519.43065	1633.33235	1
25660	N	68.02900	44.78280	78.47990	-648.23767	412.23324	341.40103	1
25661	H	67.98800	44.08980	79.25490	455.28824	-1690.80126	2600.92417	1
25662	H	67.10500	44.86980	78.00990	1931.05353	1360.88336	2064.70363	1
25663	H	68.67200	44.54580	77.69790	415.92101	2949.46587	1002.53661	1
25664	C	69.71700	49.79980	82.79390	-618.73070	-325.49733	576.16595	1
25665	O	69.79800	50.86580	82.22390	538.81227	474.22327	-336.61224	1
25666	N	68.85600	49.66080	83.84290	593.72544	431.35354	-425.40192	1
25667	H	68.79800	48.77280	84.29290	-979.05634	2661.76826	-1370.23644	1
25668	C	68.00000	50.77580	84.28590	714.36436	-557.77114	93.40731	1
25669	H	67.57400	51.25780	83.41790	2427.90400	1118.77448	1646.74543	1
25670	C	66.81200	50.11480	85.12790	-332.60095	-306.88801	782.72538	1
25671	H	67.22400	49.50880	85.96190	-139.47885	1648.92335	-2684.57783	1
25672	H	66.27300	50.96480	85.59790	-1695.27368	917.34281	2476.55495	1
25673	C	65.87200	49.30880	84.17590	394.90314	649.91124	-510.18056	1
25674	H	66.45800	48.61780	83.53290	-1810.62980	374.50712	2535.42826	1
25675	H	65.40700	50.13980	83.60490	-2339.09592	-443.18660	-2067.66409	1
25676	C	64.58100	48.69080	84.76490	226.09863	672.50352	560.17978	1
25677	H	63.91200	48.26980	83.98490	-2067.14675	-2147.84361	-1021.12150	1
25678	H	64.00700	49.44380	85.34690	2912.33529	1182.06847	97.33367	1
25679	N	64.98200	47.51680	85.61290	-664.91701	242.15192	-469.41606	1
25680	H	64.97100	46.61780	85.17490	-2237.00020	366.26508	2170.62053	1
25681	C	64.91300	47.44980	86.91190	516.27658	617.48760	-434.97523	1
25682	N	65.22000	46.31280	87.50190	290.93333	-638.29790	-485.27461	1
25683	H	65.23700	45.48880	86.93590	-2930.42837	-15.47315	1132.05777	1
25684	H	64.79200	46.14780	88.39090	-218.77295	1128.27858	2916.41874	1
25685	N	64.55700	48.39180	87.74590	367.16060	729.35435	193.37928	1
25686	H	64.32200	49.30080	87.40390	1717.77950	-1468.61692	2181.59809	1
25687	H	64.48300	48.15980	88.71590	897.63727	603.06479	2943.91369	1
25688	C	68.76300	51.77380	85.17190	-286.17697	629.33475	-602.70637	1
25689	O	68.31700	52.89480	85.38790	454.31736	-471.09918	-452.45749	1
25690	N	69.99200	51.44480	85.66490	2.71915	-340.40751	763.10549	1
25691	H	70.22400	50.48180	85.78290	-2461.59986	944.13598	-1726.90626	1
25692	C	71.03900	52.33780	86.14090	-581.93133	505.91242	475.10551	1
25693	H	70.60600	52.99280	86.88290	-1990.94727	-1244.51668	-2105.66098	1
25694	C	72.06500	51.49980	86.96290	573.76024	-556.61345	430.33180	1
25695	H	72.56500	50.79680	86.26290	-1933.07539	2227.85206	-1102.62695	1
25696	H	71.46100	50.99980	87.75090	560.48785	3081.56903	-280.89386	1
25697	C	73.17300	52.34480	87.63990	59.98324	699.62155	-589.78389	1
25698	H	73.64300	52.97080	86.85090	1255.30795	-185.30317	2868.22625	1
25699	H	74.04000	51.75980	88.01390	320.04030	2012.40000	2384.03258	1
25700	C	72.66500	53.24480	88.79790	-478.04769	560.97048	523.67235	1
25701	H	72.29600	54.16380	88.29490	-1899.74746	-2178.60620	1237.00935	1
25702	H	71.81600	52.78380	89.34490	-611.61823	2477.06376	-1846.76659	1
25703	C	73.72900	53.65480	89.76990	779.73216	-157.16668	437.01378	1
25704	H	74.54200	54.24280	89.29390	-2182.34275	-1073.31267	1986.81002	1
25705	H	74.15700	52.71680	90.18490	-257.98359	181.43153	3119.20826	1
25706	N	73.08500	54.51480	90.80690	-312.13178	-450.87323	634.09692	1
25707	H	72.42900	53.95380	91.38690	1691.60202	-1867.58021	-1898.08776	1
25708	H	72.53100	55.23180	90.29690	245.41774	3096.51651	469.38741	1
25709	H	73.73600	55.06480	91.40390	2155.77025	-2112.73157	887.20414	1
25710	C	71.68500	53.15880	85.00390	622.85733	-426.77001	-521.33755	1
25711	O	71.94000	54.39380	85.13790	209.30480	-65.43527	748.84559	1
25712	N	72.06400	52.55680	83.85790	-513.81699	-561.98131	357.08517	1
25713	H	72.02800	51.56080	83.83890	-1341.10324	-2231.97483	-1778.41156	1
25714	C	72.45900	53.18580	82.59290	270.89472	717.25955	481.93228	1
25715	H	73.31700	53.82280	82.75190	-2567.95505	740.50116	-1672.49836	1
25716	C	72.73700	52.17980	81.49090	-527.05995	-457.92153	577.27441	1
25717	H	73.16400	52.69180	80.60190	-871.78771	-2304.71920	-1967.09080	1
25718	H	73.43100	51.39180	81.85490	1351.55292	498.07726	-2807.48892	1
25719	H	71.81100	51.66480	81.15690	-243.12557	2448.19247	-1971.94397	1
25720	C	71.42300	54.10280	82.09390	-691.77939	-586.23721	100.32104	1

25721	O	71.72400	55.20980	81.62890	-554.90869	-246.77717	497.83383	1
25722	N	70.15100	53.68580	82.18190	-344.01806	458.23455	-629.94891	1
25723	H	69.93300	52.74080	82.41190	-2054.59677	-911.74532	2193.24440	1
25724	C	69.05200	54.61880	81.81290	-663.78664	376.71292	492.33719	1
25725	H	69.27300	54.93580	80.80490	2241.01921	930.53964	-2008.67081	1
25726	C	67.72000	53.76380	81.88590	637.38847	-552.42789	335.48284	1
25727	H	67.86000	52.87180	81.23890	-2065.60674	-2289.26734	623.79050	1
25728	H	67.52600	53.54180	82.95690	-1561.18409	-2707.03761	370.42269	1
25729	C	66.42000	54.44080	81.37090	428.16621	-47.04363	-810.77053	1
25730	H	66.26400	55.30580	82.05090	-683.94594	-584.35067	3007.66367	1
25731	C	66.51600	54.88780	79.91790	-175.62812	-435.09582	774.49107	1
25732	H	67.34800	55.61980	79.84090	-806.33307	-2374.20799	-1909.34041	1
25733	H	66.83700	54.05780	79.25390	1896.34991	2069.85276	-1425.70100	1
25734	H	65.61300	55.35880	79.47290	-1670.07846	-79.20129	2659.20964	1
25735	C	65.08700	53.64980	81.60090	-733.23207	300.29283	-461.75133	1
25736	H	64.19400	54.26480	81.35690	-2513.57008	1571.23124	1049.99450	1
25737	H	65.13500	52.68680	81.04990	-597.64101	-3074.51200	-317.04187	1
25738	H	65.04700	53.31080	82.65790	-2824.26134	-1354.05935	309.17022	1
25739	C	68.94000	55.86580	82.65390	-72.35284	-829.56281	365.53057	1
25740	O	68.94800	56.97480	82.06590	-448.98894	136.69942	628.64884	1
25741	N	68.95500	55.70480	84.03490	278.08921	-556.32186	563.10603	1
25742	H	68.90000	54.78480	84.41390	1044.81786	-533.73438	2910.35253	1
25743	C	69.01700	56.76980	84.97390	-535.92622	-435.82794	589.76596	1
25744	H	68.18000	57.41880	84.76190	-1647.45543	-1801.11554	-1995.28869	1
25745	C	68.98700	56.10080	86.37390	385.01593	767.72484	-307.57984	1
25746	H	67.97000	55.65380	86.34790	1888.20486	1407.57866	2075.57676	1
25747	H	69.84200	55.41280	86.55090	-1619.99118	813.48318	2562.50341	1
25748	C	69.01600	57.12980	87.55390	-624.32867	582.34300	308.88132	1
25749	H	68.64300	58.10980	87.18590	2089.26267	-1167.40158	-2050.00407	1
25750	H	70.04000	57.51080	87.75690	2154.55868	1392.64978	-1826.21459	1
25751	C	68.28500	56.64680	88.80690	-56.98660	-653.10276	-644.95100	1
25752	H	67.27800	56.32580	88.46590	-516.84085	-2480.39706	-1877.23848	1
25753	H	68.78000	55.77180	89.27990	-2708.38037	-133.86664	1587.47164	1
25754	C	68.18300	57.76180	89.88990	-301.55837	-724.17842	463.32912	1
25755	H	67.70500	58.60680	89.34890	-1411.51799	-1850.10519	2113.79583	1
25756	H	69.18300	58.07080	90.26390	2505.21264	-25.05664	1895.41186	1
25757	N	67.28600	57.24180	90.94090	-427.35756	-729.30933	-71.60393	1
25758	H	67.23400	57.85680	91.77790	-2217.05297	399.78465	-2202.06030	1
25759	H	66.34800	56.94180	90.60490	2025.02079	1888.25288	-1495.97933	1
25760	H	67.76700	56.37380	91.25190	2451.71403	-668.69683	1849.01909	1
25761	C	70.26400	57.65280	84.87290	241.76368	-476.27354	-747.45930	1
25762	O	70.14300	58.87780	84.98790	-352.00909	641.15756	-303.68038	1
25763	N	71.49100	57.15780	84.71690	523.89146	-578.23634	313.71041	1
25764	H	71.63100	56.17080	84.69590	191.59395	-1748.19240	-2618.33745	1
25765	C	72.71900	57.94580	84.52690	-331.87025	620.69531	570.99214	1
25766	H	72.79500	58.56780	85.40690	-1954.42550	2421.14515	-472.54501	1
25767	C	74.01800	57.10780	84.51390	-90.52778	855.99416	289.60251	1
25768	H	74.13900	56.57280	83.54790	1095.82774	-2285.40230	-1872.96926	1
25769	O	74.08600	56.29880	85.65490	-368.43632	-695.57568	72.57526	1
25770	H	73.52300	55.52680	85.55590	2454.60387	-869.58241	-1774.32266	1
25771	C	75.19200	58.07780	84.76890	18.69959	-910.31488	-71.63354	1
25772	H	75.21200	58.81580	83.93790	3117.04446	66.42821	-416.04279	1
25773	H	76.17100	57.55180	84.75690	2080.31979	-2327.89268	-394.75131	1
25774	H	75.14700	58.74180	85.65790	1241.68768	321.38165	-2880.91332	1
25775	C	72.59200	58.81480	83.22690	-332.57037	260.84769	-816.76451	1
25776	O	73.01500	59.98280	83.18890	-342.83715	-21.05914	-719.99236	1
25777	N	72.00200	58.27580	82.17390	265.99787	-474.49940	-652.99269	1
25778	H	71.78800	57.30480	82.23390	1712.41435	745.21129	-2538.81690	1
25779	C	71.67800	58.96180	80.92490	195.03254	-849.65981	-272.68048	1
25780	H	72.62500	59.27280	80.50790	161.54240	871.21970	3010.79805	1
25781	C	71.09500	58.12480	79.80190	-410.79276	-506.97801	-646.39630	1
25782	H	70.05700	57.80880	80.03990	-2608.66229	1041.90119	1414.45996	1

25783	O	71.89200	56.91180	79.71290	478.08734	457.88590	419.47237	1
25784	H	71.56000	56.30780	80.38190	-2280.70442	2128.77265	-430.74338	1
25785	C	71.17200	58.81080	78.46790	505.92222	21.70086	748.31272	1
25786	H	72.19700	59.09080	78.14290	1928.56641	922.08949	2298.03620	1
25787	H	70.51100	59.70180	78.53390	-411.33798	3062.13109	593.45666	1
25788	H	70.87600	58.20880	77.58290	633.75977	-1571.55403	-2657.07423	1
25789	C	70.83300	60.20580	81.08790	-912.72187	-35.80337	-55.34504	1
25790	O	71.24500	61.35880	80.80990	295.10042	-476.02553	548.15284	1
25791	N	69.70300	59.95480	81.76090	-228.78229	-416.05940	692.20455	1
25792	H	69.43500	59.01180	81.94290	-1317.97085	1569.50928	2380.82814	1
25793	C	68.79200	60.93480	82.26090	-458.66653	36.73231	-795.03063	1
25794	H	68.27700	61.41580	81.44290	-289.04454	1163.99415	2902.68645	1
25795	C	67.64800	60.18880	82.90290	567.99923	-683.92811	-206.01598	1
25796	H	68.05500	59.43180	83.60690	-1278.27981	2173.20884	1875.05957	1
25797	C	66.77000	61.10180	83.78390	324.32109	658.50292	-543.38922	1
25798	H	65.86900	60.56480	84.14890	2407.00446	640.88392	1913.04682	1
25799	H	66.36600	61.97780	83.23390	-1847.25847	2365.13960	-951.09275	1
25800	H	67.30500	61.44380	84.69590	-2709.72009	1600.20873	-20.07739	1
25801	C	66.87700	59.43380	81.79990	-554.76589	-580.77607	-442.42867	1
25802	H	65.98800	58.91880	82.22390	1819.57357	-2565.46117	44.51815	1
25803	H	67.56900	58.76680	81.24290	2703.55368	-1098.30029	-1177.09817	1
25804	H	66.48400	60.21480	81.11490	1607.94260	-16.54917	-2708.42040	1
25805	C	69.33700	61.96280	83.14390	169.41188	748.50247	-496.10866	1
25806	O	69.12900	63.14880	82.91090	-220.16816	-647.16608	392.85936	1
25807	N	70.16800	61.60980	84.15190	637.50710	-180.99071	514.27285	1
25808	H	70.42600	60.68180	84.41090	572.44504	-1722.00824	2563.66015	1
25809	C	70.81100	62.52780	85.05990	763.55127	-90.30022	480.94846	1
25810	H	70.02500	63.10980	85.51790	-1692.24116	-1787.33670	-1968.80163	1
25811	C	71.57800	61.78180	86.15290	-648.39234	65.61318	632.56494	1
25812	H	72.12500	60.95180	85.65690	-2584.37879	1100.14803	-1426.47151	1
25813	C	72.63700	62.69880	86.91090	508.23624	452.91061	-610.45347	1
25814	H	73.14200	62.11380	87.70790	-1398.76934	-1335.44963	2476.50596	1
25815	H	72.14800	63.58180	87.37590	-37.26404	3115.76084	-424.61865	1
25816	H	73.44600	62.89480	86.17490	-1422.22576	-1984.85421	-1993.63522	1
25817	C	70.63500	61.17080	87.20590	552.00393	531.65998	483.26520	1
25818	H	69.64800	60.89180	86.77890	-1579.47180	137.91482	2711.59627	1
25819	H	70.45800	61.96580	87.96190	2867.07509	893.72701	925.00068	1
25820	C	71.26700	59.95680	87.91890	84.39957	-813.60657	-415.19974	1
25821	H	70.48700	59.54080	88.59190	-1871.27492	-1679.13835	-1901.92928	1
25822	H	71.59500	59.21580	87.15890	-1925.74738	-1981.88814	1500.56651	1
25823	H	72.13800	60.22880	88.55390	-2474.32391	-79.39147	1935.29185	1
25824	C	71.66200	63.52580	84.35490	435.65974	632.55091	-493.90992	1
25825	O	71.52800	64.71780	84.59990	-445.84338	-350.72100	546.62306	1
25826	N	72.44000	63.06280	83.35390	-627.02548	556.39101	-118.19203	1
25827	H	72.41000	62.08380	83.16990	383.84384	-135.92728	3112.55464	1
25828	C	73.23300	63.90780	82.52590	362.39557	-426.64716	712.07262	1
25829	H	73.88400	64.42880	83.21190	548.12828	1391.91520	2760.61253	1
25830	C	74.22100	63.07780	81.65290	-149.12935	809.11784	-401.64750	1
25831	H	73.76600	62.28180	81.02690	-2508.59263	-11.29969	1895.72048	1
25832	H	74.79000	62.50380	82.41590	2270.24357	-1218.23418	1794.73879	1
25833	C	75.19500	63.90380	80.72890	-546.25556	264.79055	676.51373	1
25834	H	74.55500	64.48980	80.03390	-770.91263	2581.68519	1621.07082	1
25835	C	76.09000	64.93880	81.32490	10.79118	-877.59966	-251.80790	1
25836	H	76.90300	64.44380	81.89790	1436.57286	-2322.37376	1551.61064	1
25837	H	75.62900	65.65480	82.03890	-742.40897	2217.42357	2099.85397	1
25838	H	76.67100	65.48180	80.54890	-1952.37794	-2389.68158	614.38726	1
25839	C	76.03300	62.90280	79.89590	-462.52171	-254.04080	737.93655	1
25840	H	76.48300	62.22980	80.65690	2597.06825	1526.36507	-907.61133	1
25841	H	76.84200	63.38880	79.30890	1493.32365	-1395.89410	2380.86759	1
25842	H	75.43400	62.30680	79.17490	2297.91662	-2142.76094	-70.83047	1
25843	C	72.43700	64.90980	81.66490	-225.51182	778.97903	412.83319	1
25844	O	72.81300	66.08780	81.57690	-437.05328	-600.29137	-279.71521	1

25845	N	71.36300	64.44380	80.99590	-327.84715	573.58488	522.09923	1
25846	H	71.19000	63.46780	81.10790	1195.00195	1442.99251	2519.91848	1
25847	C	70.42600	65.14580	80.24290	-627.49429	556.92213	358.84352	1
25848	H	71.03900	65.71780	79.56190	-2617.06162	-1464.67174	-965.84898	1
25849	C	69.50000	64.18580	79.47790	244.58674	-7.86921	872.05543	1
25850	H	69.27400	63.33580	80.15590	14.06284	1064.78090	-2966.00371	1
25851	C	68.14600	64.84580	79.02290	715.97755	-206.36765	-524.54766	1
25852	H	67.51200	65.16380	79.87790	856.94058	-3026.00509	18.07280	1
25853	H	67.58600	64.15180	78.35890	-526.86321	2585.20359	-1720.79642	1
25854	H	68.45800	65.75480	78.46590	-664.59282	-2855.71992	1137.20684	1
25855	C	70.28000	63.43880	78.39190	-475.11112	-679.25380	377.45444	1
25856	H	70.44600	64.25280	77.65390	-152.93739	2024.89369	-2409.85080	1
25857	H	71.27200	63.03780	78.69290	-1943.41974	2068.33878	-1370.82799	1
25858	C	69.41000	62.39680	77.58790	23.78904	618.73215	664.34063	1
25859	H	68.96100	61.73580	78.35990	-2870.98804	555.68997	-1176.29594	1
25860	H	68.57700	62.83380	76.99690	973.22887	-2602.95414	1464.43998	1
25861	H	70.16900	61.86880	76.97190	-1507.36810	-2076.57864	-1828.51547	1
25862	C	69.70600	66.19980	80.98090	611.90070	-32.57079	-876.46951	1
25863	O	69.55800	67.36380	80.51690	440.78933	316.90339	566.40349	1
25864	N	69.14000	65.92480	82.22190	-563.64659	575.32766	254.17591	1
25865	H	69.22700	64.99080	82.55990	-2546.75969	-1685.43835	-772.91701	1
25866	C	68.75000	66.92180	83.19690	-552.41564	-558.56522	463.94420	1
25867	H	67.89500	67.41080	82.75390	-1206.00901	2107.82656	1997.53689	1
25868	C	68.34200	66.10180	84.47590	403.66664	-490.82064	649.22373	1
25869	H	68.06800	66.67780	85.38590	740.91520	-752.85466	-2967.32508	1
25870	H	69.24300	65.50480	84.73090	-2012.57951	-2075.32950	-1252.78755	1
25871	C	67.11800	65.15880	84.29590	-83.67110	-74.89202	-909.53009	1
25872	H	67.27600	64.54180	83.38490	-1073.54999	-2565.17986	-1480.50021	1
25873	C	67.17400	64.17980	85.52090	460.95808	-515.50962	-599.13926	1
25874	H	66.20600	63.64480	85.41390	2397.08861	1927.49171	-651.09076	1
25875	H	67.27400	64.75380	86.46590	-2869.85286	1242.90802	-354.59379	1
25876	H	68.06800	63.52580	85.43190	1294.38050	-788.15091	-2761.80874	1
25877	C	65.84000	65.91780	84.21390	867.88328	266.86433	-38.57492	1
25878	H	65.86700	66.56680	83.31290	2134.99966	-2070.77577	-1025.59095	1
25879	H	64.97100	65.22780	84.18490	2228.47620	-826.73611	-2062.74858	1
25880	H	65.68500	66.60280	85.07490	-1730.18241	-1805.67315	-1916.74896	1
25881	C	69.78900	67.93480	83.58990	-669.78685	590.00057	-198.08022	1
25882	O	69.52000	69.15080	83.59590	-330.49488	-501.32361	512.77342	1
25883	N	71.02500	67.45980	83.92190	-671.44398	451.09628	-252.33206	1
25884	H	71.29900	66.50280	83.86090	1263.83761	2404.96265	1577.80273	1
25885	C	72.04000	68.25880	84.44690	12.43074	420.97127	803.71447	1
25886	H	71.72900	68.65180	85.40390	-1705.16054	687.37629	2550.35971	1
25887	C	73.35000	67.44380	84.73490	-747.41729	-368.33650	371.96345	1
25888	H	74.10400	68.14980	85.14490	2986.10525	-698.14654	-696.97013	1
25889	H	73.20500	66.70780	85.55390	-706.38084	-2782.19233	1286.98793	1
25890	H	73.77200	66.98480	83.81490	2025.39785	-2217.41883	927.30008	1
25891	C	72.37500	69.33780	83.44090	-765.84709	-336.03465	-375.15385	1
25892	O	72.35400	70.52480	83.71590	531.60806	466.83134	340.76811	1
25893	N	72.52600	68.93380	82.15690	564.12353	-253.84989	566.61362	1
25894	H	72.48400	67.96680	81.91890	-314.81308	2477.98286	-1917.84791	1
25895	C	72.88600	69.73780	81.06290	277.65989	529.10933	-691.35934	1
25896	H	73.82700	70.20980	81.30690	-2880.40862	100.79266	-1274.94318	1
25897	C	73.15900	68.74380	79.88290	34.36333	904.61594	-118.40888	1
25898	H	72.24600	68.13780	79.70290	1999.54534	-785.60437	-2298.99484	1
25899	H	74.00200	68.08380	80.18090	-1461.50521	2589.81628	-1039.85540	1
25900	C	73.42400	69.35880	78.57890	802.95351	-420.50731	-39.22834	1
25901	C	74.73300	69.62180	78.20490	-892.04944	-170.97013	116.06176	1
25902	H	75.61300	69.41980	78.79790	509.71363	-2656.48449	1597.86512	1
25903	C	74.94800	70.16980	76.88990	501.57512	-145.89548	738.95212	1
25904	H	75.94500	70.40780	76.54990	-2062.67637	-760.48947	-2259.37280	1
25905	C	73.86900	70.43680	76.05490	-120.65328	-901.44540	-42.28973	1
25906	H	74.11800	70.79380	75.06590	-815.94961	2963.08163	-695.42788	1

25907	C	72.34100	69.62080	77.69590	-642.39369	-1.05379	-656.00186	1
25908	H	71.31700	69.47980	78.01090	-918.60612	1687.30015	2490.34961	1
25909	C	72.56000	70.16080	76.43590	-553.31052	-658.73107	-311.56045	1
25910	H	71.70500	70.39580	75.81990	-2803.80628	425.91313	1370.77547	1
25911	C	71.85900	70.76280	80.73490	357.59302	-606.12368	-580.26266	1
25912	O	72.02600	71.98080	80.52490	246.59321	292.18909	686.51055	1
25913	N	70.56600	70.38080	80.67190	-579.23755	539.79530	-304.60005	1
25914	H	70.32800	69.41380	80.71090	1725.41270	2048.84289	-1649.50001	1
25915	C	69.44000	71.27380	80.50690	-835.54156	347.39919	-144.21704	1
25916	H	69.51600	71.89380	79.62590	-667.86940	-2418.62952	-1901.53640	1
25917	C	68.15900	70.43480	80.33790	502.82823	-180.23693	733.49378	1
25918	H	67.91400	69.83780	81.24290	-1466.56316	1425.53450	2390.19653	1
25919	H	68.37400	69.74180	79.49790	1818.13835	2229.53619	-1270.33072	1
25920	C	66.92100	71.17580	80.05790	-388.14025	-228.08235	-797.11912	1
25921	C	66.57200	71.44880	78.74590	-800.44749	442.75501	-55.39110	1
25922	H	67.31800	71.24980	77.98990	977.15023	1485.62864	2591.91995	1
25923	C	65.36200	72.05980	78.40290	-429.74261	560.31165	-582.13009	1
25924	H	65.06300	72.19480	77.37390	2876.06108	178.39252	1249.47696	1
25925	C	64.52500	72.43380	79.47390	282.18653	-522.64791	689.21628	1
25926	H	63.62600	73.01480	79.32790	-1617.44121	2071.06712	1733.95866	1
25927	C	66.02700	71.52980	81.08290	-421.25756	-448.33810	674.61359	1
25928	H	66.30100	71.35380	82.11290	-3039.23074	-818.82495	-131.76491	1
25929	C	64.89600	72.27080	80.79890	302.28465	560.77481	-650.65446	1
25930	H	64.14400	72.56780	81.51590	2262.96875	-344.06780	-2154.66870	1
25931	C	69.33500	72.26180	81.71990	783.29873	-102.68020	-450.21499	1
25932	O	69.08000	73.41680	81.52690	-377.02007	694.18054	47.02147	1
25933	N	69.63000	71.85980	82.96790	429.16608	-326.31243	645.11695	1
25934	H	69.70200	70.91080	83.26390	-1654.39128	-2673.14766	-184.08662	1
25935	C	69.74000	72.75980	84.02890	-879.24586	-118.37682	-228.23466	1
25936	H	68.80600	73.27580	84.19490	2214.35427	-1065.83465	1959.36725	1
25937	C	69.97200	71.99480	85.34890	-259.03649	519.95733	700.32299	1
25938	H	69.16700	71.24180	85.48590	1963.98958	1789.07772	-1682.11755	1
25939	H	70.95100	71.47480	85.41890	-261.32279	-3134.05308	-142.84297	1
25940	H	69.93600	72.73580	86.17590	-1653.36562	1786.38234	1991.95455	1
25941	C	70.81600	73.85580	83.78590	296.03433	613.59929	601.13933	1
25942	O	70.62400	75.02280	84.15090	-639.07849	-333.17333	-333.17520	1
25943	N	71.92800	73.46580	83.15890	215.77116	687.67294	-438.92147	1
25944	H	71.88900	72.59580	82.67490	-2322.62746	-1320.60787	-1669.93115	1
25945	C	73.00100	74.43080	82.80690	-60.52574	505.51068	-758.84717	1
25946	H	73.28100	74.87180	83.75190	556.31376	-260.79097	3082.67980	1
25947	C	74.19600	73.61780	82.23390	-182.61564	-426.62038	-788.85015	1
25948	H	74.96200	74.36980	81.94790	-94.89338	2301.20883	-2146.54057	1
25949	H	73.88900	73.19180	81.25490	-2501.11075	282.04569	-1896.63157	1
25950	S	74.87400	72.35080	83.38990	-394.92036	303.77970	-260.00484	1
25951	H	73.67600	71.91480	83.75190	2081.38285	-1804.24523	1512.43397	1
25952	C	72.62400	75.52980	81.86190	-620.71856	158.62633	651.43853	1
25953	O	72.81800	76.70480	82.13490	777.95765	-104.45792	11.68727	1
25954	N	71.91800	75.07780	80.72890	-228.00471	-529.15225	-620.32588	1
25955	H	71.92300	74.09580	80.55290	-2083.51628	-2344.09634	-286.47068	1
25956	C	71.54200	75.91280	79.63390	155.42880	285.55874	-852.49322	1
25957	H	72.31800	76.64380	79.46390	682.43095	2638.28760	1569.92876	1
25958	C	71.62200	74.98880	78.37290	-20.37741	-543.34072	-733.02230	1
25959	H	71.04500	75.42080	77.52690	541.20451	793.88229	2993.74599	1
25960	H	71.17500	73.99780	78.60090	1742.37550	-1666.60932	-2017.66499	1
25961	C	73.02200	74.78780	77.81290	61.70109	602.11210	680.60857	1
25962	C	73.70700	73.56580	77.87990	102.69375	663.89250	-620.15308	1
25963	H	73.23900	72.61380	78.08190	2247.23856	600.46480	2110.13018	1
25964	N	74.94100	73.72080	77.23790	658.75799	-433.39922	-288.91116	1
25965	H	75.57100	73.04880	76.91690	-2964.47081	-152.45527	-1061.65727	1
25966	C	75.03800	74.99780	76.86390	312.39758	-446.40941	724.64360	1
25967	C	73.88500	75.72880	77.20590	95.39523	-664.22236	-616.48672	1
25968	C	73.84600	77.15180	77.05090	595.93544	-457.06153	506.73611	1

25969	H	72.96800	77.73480	77.28890	-108.41052	3140.34280	190.57743	1
25970	C	74.99200	77.74080	76.45190	-391.25899	-654.92157	-502.97887	1
25971	H	74.97600	78.77380	76.13690	2071.13153	2364.85940	-10.34101	1
25972	C	76.13500	75.64780	76.26290	267.79791	367.50781	-792.10054	1
25973	H	77.00800	75.08280	75.96990	-1850.58696	-2078.20722	-1474.87729	1
25974	C	76.07400	77.02980	76.04390	259.28936	717.23029	497.99242	1
25975	H	76.95300	77.55880	75.70590	-2234.26855	1243.81347	-1844.85262	1
25976	C	70.21200	76.64580	79.76090	-796.44164	346.90135	291.78737	1
25977	O	70.11700	77.79280	79.22390	-403.37842	-249.72626	634.38027	1
25978	N	69.22300	76.15280	80.47990	-743.90175	392.56767	112.15853	1
25979	H	69.32500	75.27080	80.93290	-2387.91572	1962.98996	603.40948	1
25980	C	67.91700	76.79680	80.50690	-234.14640	-612.77389	635.35631	1
25981	H	67.50100	76.72480	79.51290	-2657.90546	586.61038	1587.05541	1
25982	C	67.04200	75.89380	81.32190	248.29829	-868.98166	-115.39297	1
25983	H	67.50300	75.63980	82.29990	1789.97501	-2444.72445	-840.44232	1
25984	H	67.00500	74.91080	80.80590	2387.77954	1489.98580	1396.74492	1
25985	C	65.64000	76.49380	81.61290	-716.85641	-496.90060	280.51405	1
25986	H	65.63400	77.50380	82.07590	-2859.88869	-394.04495	1262.76110	1
25987	C	64.73900	76.55180	80.32490	-190.84838	-392.66461	802.70889	1
25988	H	64.91700	75.65380	79.69490	2026.34317	-632.23737	2317.97766	1
25989	H	63.67100	76.57880	80.62790	-3055.99920	-761.67452	-105.19469	1
25990	H	64.89500	77.50380	79.77390	1262.99409	2145.17464	1921.00230	1
25991	C	64.90600	75.60280	82.61490	213.47330	480.21257	-742.69183	1
25992	H	65.60700	75.23780	83.39590	-1781.11252	1896.39801	1771.56094	1
25993	H	64.05500	76.15680	83.06690	1737.97054	-1255.56394	-2299.26822	1
25994	H	64.60100	74.61180	82.21590	1324.65009	-1924.22409	2105.71085	1
25995	C	67.88300	78.25880	80.97990	-727.01793	-420.78343	-365.14205	1
25996	O	67.19700	79.02380	80.29190	486.37647	472.84692	398.38258	1
25997	N	68.52100	78.78280	82.02490	-55.67475	833.14887	-121.32656	1
25998	C	69.31500	77.97980	82.97190	-779.60307	287.22913	384.57240	1
25999	H	68.96900	76.92580	83.03290	-435.01923	2322.24841	-2077.63935	1
26000	H	70.36000	78.03480	82.59890	-128.46864	-1711.82206	2636.96651	1
26001	C	68.47200	80.19080	82.39590	118.55891	-847.70446	-313.45492	1
26002	H	67.44000	80.42380	82.61490	-723.12595	-2318.46173	-2001.57386	1
26003	C	69.25900	80.17180	83.75390	-404.90442	588.93397	-567.46988	1
26004	H	68.88300	80.87580	84.52690	2871.51761	1211.51990	394.31535	1
26005	H	70.32300	80.40280	83.53390	1013.38486	2830.74964	-917.27071	1
26006	C	69.11600	78.74880	84.28590	821.75306	199.20080	330.00506	1
26007	H	69.94800	78.54280	84.99390	2716.04460	1573.88846	-127.87139	1
26008	H	68.10900	78.61380	84.73490	1971.27042	-1682.05559	1781.62244	1
26009	C	69.05500	81.12380	81.23090	621.74854	121.46666	651.78921	1
26010	O	68.57200	82.24780	81.04590	352.46462	669.19174	218.92168	1
26011	N	70.09900	80.67380	80.54090	-763.64812	-237.66844	286.47718	1
26012	H	70.39500	79.77580	80.85690	1825.96903	-1978.29223	-1621.43128	1
26013	C	70.60700	81.42980	79.40390	-221.20548	877.27987	129.78830	1
26014	H	70.77000	82.44380	79.73990	-1952.75811	-2361.74275	728.38846	1
26015	C	71.94100	80.76680	78.92290	433.01949	-738.04554	-303.76659	1
26016	H	71.86800	79.65880	78.87490	1427.15967	866.49008	-2663.70379	1
26017	H	72.71000	80.96280	79.70090	2491.99726	-1127.55227	1544.77654	1
26018	C	72.44600	81.21980	77.54890	544.92681	365.19204	-628.15294	1
26019	C	73.03200	82.49780	77.40790	119.30009	888.67053	-168.93695	1
26020	H	73.19700	83.12680	78.26990	2991.19652	-928.54855	-215.41398	1
26021	C	73.38000	82.91680	76.12890	-275.75226	689.20129	536.83544	1
26022	H	73.80300	83.90780	76.04790	279.57033	3047.19941	738.93218	1
26023	C	73.21100	82.08580	74.99290	-491.76033	-746.67195	188.57366	1
26024	O	73.66500	82.54480	73.75290	650.82087	-311.22770	-301.27528	1
26025	H	74.19700	83.33680	73.85990	-749.00924	2285.61093	2035.27253	1
26026	C	72.14500	80.45680	76.39290	-387.13295	-826.71248	-9.33084	1
26027	H	71.53000	79.57280	76.46990	-244.03537	-3110.59560	-393.23317	1
26028	C	72.59800	80.86680	75.14790	353.69255	-780.62741	-296.43406	1
26029	H	72.46700	80.20280	74.30690	2562.29264	-1629.33359	-794.83973	1
26030	C	69.60500	81.53480	78.26890	-284.92785	-734.00912	463.65683	1

26031	O	69.34000	82.63880	77.79490	691.35372	-335.39963	154.19752	1
26032	N	68.89900	80.39980	77.87590	711.51531	442.73410	47.88856	1
26033	H	69.15900	79.51980	78.26490	-1648.75348	-2013.70731	-1771.79205	1
26034	C	67.79400	80.35980	76.99690	787.79125	-97.55859	-435.35576	1
26035	H	68.02800	80.90180	76.09190	-816.63774	-1678.82778	-2532.08108	1
26036	C	67.37900	78.88380	76.66290	777.84194	153.26924	-438.64669	1
26037	H	67.35800	78.20080	77.53890	2467.11337	1468.69270	1276.08677	1
26038	H	66.31400	78.74980	76.37590	1799.39135	-973.64395	-2383.53095	1
26039	C	68.31100	78.32080	75.65290	-705.25669	501.89880	-304.93057	1
26040	C	68.11000	78.68280	74.28590	533.59764	542.89476	-496.15951	1
26041	H	67.23800	79.29980	74.12290	1009.12056	2084.39778	2129.37894	1
26042	C	68.99100	78.15880	73.25190	204.71512	-687.42304	557.14316	1
26043	H	68.92600	78.57780	72.25790	-1779.18635	-169.82652	2594.55253	1
26044	C	69.92600	77.15880	73.58790	-495.17626	114.12480	761.64787	1
26045	O	70.77300	76.70680	72.57590	617.60050	259.32096	-410.18511	1
26046	H	70.57700	77.24380	71.80390	-2377.30488	-1730.95893	1128.23690	1
26047	C	69.24800	77.30080	75.92290	393.48833	-445.23166	686.59809	1
26048	H	69.32500	76.81380	76.88390	2432.54882	1986.14299	-108.92899	1
26049	C	70.03300	76.73280	74.90990	268.21968	483.99985	-724.37097	1
26050	H	70.81500	76.02580	75.14390	1691.71228	2139.10077	1563.53039	1
26051	C	66.60900	81.16880	77.39390	-510.15849	535.88567	541.94057	1
26052	O	66.03000	81.91280	76.59390	-562.59245	-29.98994	-557.81211	1
26053	N	66.26200	81.14380	78.69490	-430.12318	461.06752	-564.22658	1
26054	H	66.72900	80.59280	79.38290	225.60819	-420.10098	-3107.63141	1
26055	C	65.22400	82.07880	79.20490	666.80812	-614.12506	-34.68515	1
26056	H	64.38800	81.88480	78.54990	-2069.77189	-1517.12054	-1824.32272	1
26057	C	64.68300	81.72780	80.60790	-837.93004	-44.52736	-367.49663	1
26058	H	65.60700	81.77480	81.22190	-1930.74285	1277.79209	2137.28689	1
26059	C	63.60600	82.80080	81.01090	499.55969	-398.35731	649.99818	1
26060	H	62.70300	82.86080	80.36690	-2013.04249	1127.11753	2147.89753	1
26061	H	63.25600	82.57980	82.04190	-2211.99161	-828.61076	2087.93316	1
26062	H	64.00900	83.83280	81.09290	-2816.39215	-736.52817	-1203.92838	1
26063	C	64.11400	80.29080	80.63890	606.98847	-594.27891	324.62081	1
26064	H	63.25500	80.13980	79.95190	2843.84020	596.01762	-1190.07659	1
26065	H	64.84000	79.61680	80.13490	-1855.40709	-2543.66909	-90.17938	1
26066	C	63.65900	79.83980	81.99690	527.16891	447.82244	-586.28745	1
26067	H	64.50200	79.89380	82.71890	2471.91691	-658.17484	-1823.32103	1
26068	H	63.43900	78.75180	81.95090	2378.40743	-184.80357	2047.32749	1
26069	H	62.80200	80.44580	82.35890	-739.15916	2925.35186	893.08802	1
26070	C	65.58000	83.61280	79.03390	-668.87574	-189.82880	600.29945	1
26071	O	64.77400	84.26080	78.37690	-455.26397	-99.76538	645.83111	1
26072	N	66.82900	84.06580	79.36490	-671.55587	222.80235	-466.74625	1
26073	H	67.45400	83.43180	79.81190	-2956.74293	-175.31124	1080.48037	1
26074	C	67.40078	85.35412	79.02015	-223.21081	-1124.75289	-390.38535	1
26075	H	66.71715	86.02345	79.54725	-3333.46391	-1100.87742	-224.88989	1
26076	H	68.38222	85.39700	79.47008	1333.06766	1208.35926	-1917.99431	1
26077	C	67.40887	85.83971	77.46113	391.75730	-14.17881	-124.34231	1
26078	O	67.08620	86.97267	77.20170	-201.29724	-716.59464	-233.88134	1
26079	N	67.89100	84.89680	76.61290	349.47837	-661.98279	384.43249	1
26080	H	68.32900	84.14080	77.09390	881.12469	2663.55032	1424.31624	1
26081	C	67.81474	85.08916	75.15561	316.72632	-381.29878	389.77317	1
26082	H	68.28067	86.10728	75.07271	-227.02200	-2682.08716	2721.63530	1
26083	C	68.53600	83.92580	74.53290	-684.58583	-543.11628	-273.03382	1
26084	H	68.10500	82.98380	74.93690	-1573.95899	1819.73773	-2032.45044	1
26085	C	68.34900	83.93880	73.05490	-867.92048	290.18588	100.01343	1
26086	H	67.38300	83.53880	72.67890	551.31919	-3031.68844	617.08689	1
26087	H	68.68700	84.91880	72.65490	-2387.55708	1917.70533	758.49530	1
26088	H	69.02400	83.17980	72.60690	2565.01676	-620.57813	-1697.45723	1
26089	C	70.05800	83.94780	74.75490	-867.10462	17.60983	306.27352	1
26090	H	70.56200	83.01280	74.42890	-564.66550	2793.94571	1341.61255	1
26091	H	70.17300	83.76380	75.84390	1851.07309	1315.25961	-2170.48739	1
26092	C	71.00638	85.04773	74.12730	233.35418	130.29709	-769.01397	1

26093	H	72.05045	84.73116	74.29290	-2458.93437	-561.74681	2342.08736	1
26094	H	70.79496	85.16983	73.04123	-519.26625	713.06985	2149.31782	1
26095	H	70.89371	86.05715	74.56702	1279.21698	-3681.65513	977.82901	1
26096	C	66.31158	85.12542	74.48889	67.58103	899.69603	-649.11761	1
26097	O	66.12289	85.74582	73.44674	-513.39466	-298.60487	302.06003	1
26098	N	65.47600	84.30180	75.09290	-422.70430	436.82380	-588.91212	1
26099	H	65.70400	83.60980	75.77290	-84.32858	-2430.43684	1997.81685	1
26100	C	64.05600	84.33580	74.67990	-318.30538	224.05262	-824.07556	1
26101	H	64.10600	84.16680	73.61490	-2588.17039	-1212.04062	-1325.50766	1
26102	C	63.18100	83.19080	75.19690	297.31517	-481.66584	714.56729	1
26103	H	62.22600	83.07180	74.64190	2739.85345	655.49407	1390.24786	1
26104	H	63.77500	82.27180	75.00590	516.93564	-1981.01331	-2382.95225	1
26105	O	62.80900	83.14980	76.55590	282.19169	160.03859	721.07292	1
26106	H	63.47300	83.61580	77.06990	2988.76605	32.74383	-956.87008	1
26107	C	63.42816	85.73776	75.19291	-105.73316	-181.78732	-117.51521	1
26108	O	62.87711	86.46287	74.34640	836.22559	-441.63126	-782.55722	1
26109	N	63.78874	85.98793	76.39912	-395.61382	-196.40437	-983.60238	1
26110	H	64.43593	85.39621	76.96558	904.41797	1308.84348	-1083.54811	1
26111	C	63.39055	87.33266	76.87333	532.06221	114.76626	91.32150	1
26112	H	62.28456	87.44093	76.68986	-123.19008	-1610.89055	1749.35081	1
26113	C	63.63847	87.23550	78.43361	641.29091	1535.90231	-295.80469	1
26114	H	63.90078	86.19740	78.78345	2136.87382	-1941.39922	-756.58838	1
26115	C	64.85234	88.19001	78.73966	-393.71876	353.77115	-388.51838	1
26116	H	65.74028	87.73053	78.17072	532.97029	-899.74644	-233.95129	1
26117	H	65.15773	88.34781	79.84242	1450.68392	1039.54496	-2808.59620	1
26118	H	64.72237	89.20738	78.36431	191.00862	90.99088	-2144.69751	1
26119	C	62.47247	87.82545	79.26909	182.36391	517.69630	1366.04128	1
26120	H	62.25632	88.85160	78.98895	1507.73590	-1400.41718	1071.42106	1
26121	H	62.70346	87.88374	80.34061	370.52676	-320.02052	-2436.43442	1
26122	C	61.32281	86.79247	79.05237	-171.46758	318.68023	-911.07251	1
26123	H	61.29295	86.02270	79.87125	634.80908	-2618.67143	-113.65785	1
26124	H	60.30333	87.29116	79.11300	-1581.31047	-1031.83929	-402.20416	1
26125	H	61.45562	86.27380	78.03817	5224.69184	2246.19457	-968.76085	1
26126	C	64.23870	88.45857	76.14970	10.19393	355.46869	-1094.43934	1
26127	O	63.73310	89.59123	76.19722	71.47336	104.57172	610.70114	1
26128	N	65.33681	88.07343	75.46835	920.79001	-98.80601	-547.80207	1
26129	H	65.44669	87.05880	75.51863	951.97749	-326.01710	447.63485	1
26130	C	66.09565	88.89143	74.58444	-9.30075	-165.12219	235.12627	1
26131	H	65.98751	89.85242	75.12866	534.74015	1657.78500	-2194.18131	1
26132	C	67.52405	88.26950	74.37304	322.09598	335.88707	322.41659	1
26133	H	67.41571	87.40049	73.63349	547.17046	1781.54348	-3436.16214	1
26134	H	67.76088	87.82555	75.35699	-2099.95854	-2227.06190	2077.85740	1
26135	C	68.62464	89.37256	74.00782	19.48712	359.28300	507.98756	1
26136	O	68.64196	90.50173	74.54864	-298.51968	161.60005	456.71935	1
26137	O	69.60751	88.90707	73.38148	11.87555	-2.16048	-713.97776	1
26138	C	65.49082	89.03089	73.09102	-365.48193	143.25293	-881.70112	1
26139	O	65.77197	90.05093	72.45394	261.10617	391.54111	5.59041	1
26140	N	64.83319	87.94755	72.68315	-420.79377	-961.46403	550.10938	1
26141	H	64.81067	87.17037	73.33052	-128.83832	-1723.99244	2045.15183	1
26142	C	64.20767	87.84646	71.38109	-475.44721	-211.18273	626.76679	1
26143	H	64.92377	88.40758	70.69154	-814.05147	-3190.70005	-26.87409	1
26144	C	64.07103	86.33089	71.00141	127.34449	-169.43598	-481.58150	1
26145	H	63.27434	85.89678	71.63091	-1635.40270	114.48509	-1610.08087	1
26146	H	63.71775	86.14729	69.95701	-2117.49956	495.33807	1544.36462	1
26147	O	65.34563	85.51732	70.87626	-235.96592	608.34572	-99.48785	1
26148	H	65.66658	85.67260	71.77968	5162.82502	1106.08350	2351.10222	1
26149	C	62.65207	88.29253	71.18469	-467.25828	-512.38651	-240.78846	1
26150	O	62.20209	88.66368	70.10530	-139.98576	395.56198	553.98488	1
26151	N	62.00778	88.08170	72.33541	-203.40245	236.30986	352.05224	1
26152	H	62.50059	87.63126	73.11935	2857.17709	394.05425	2082.97252	1
26153	C	60.91711	88.99669	72.62379	-690.35535	130.25855	416.36185	1
26154	H	60.28366	88.98871	71.68604	1426.35098	-1589.17815	1324.39103	1

26155	C	60.05312	88.55581	73.84947	-78.20829	-571.23885	-750.99863	1
26156	H	59.15358	89.18380	73.74755	-3828.03485	-323.96515	-1078.32477	1
26157	H	60.43264	88.96890	74.78647	1020.12798	-2730.15073	-3085.04561	1
26158	C	59.77537	87.05741	74.02214	-178.03286	37.94772	462.75133	1
26159	C	59.64820	86.23565	72.88012	61.09823	-16.79619	159.60260	1
26160	H	59.96012	86.57703	71.89404	-1393.57873	813.67080	143.42091	1
26161	C	59.30100	84.85880	73.12290	17.11612	-616.94622	674.88892	1
26162	H	59.12100	84.20580	72.28090	1145.91002	2426.49186	1644.30462	1
26163	C	59.18800	84.30980	74.35190	543.01516	-532.62079	498.38033	1
26164	H	59.20900	83.23180	74.40590	-128.36272	-1413.16777	-2803.06246	1
26165	C	59.67756	86.54308	75.35385	-275.16160	-449.78105	972.95639	1
26166	H	60.00908	87.21656	76.16629	-3886.05984	2006.99295	986.44231	1
26167	C	59.45112	85.18228	75.48423	1077.25571	435.46793	260.30406	1
26168	H	59.40800	84.60080	76.43090	492.51908	3074.37158	450.59690	1
26169	C	61.49539	90.49520	72.98846	42.08448	-902.45893	197.39385	1
26170	O	60.68081	91.43321	73.16383	355.09419	-112.31698	-319.45728	1
26171	N	62.82640	90.59654	73.04309	-287.01054	-864.53581	-207.02111	1
26172	H	63.19923	89.70841	72.67558	-557.75726	3126.35636	-1220.17128	1
26173	C	63.35846	91.91100	72.63797	-1108.64419	532.64008	85.62423	1
26174	H	62.39285	92.41942	72.88480	118.58799	-1982.62746	-2303.27108	1
26175	C	64.58956	92.37258	73.46028	95.64733	548.66644	-335.24311	1
26176	H	65.43662	91.97661	72.89517	1127.82182	1183.01578	1299.84149	1
26177	C	64.75361	93.88583	73.33656	813.42281	67.23960	-24.55626	1
26178	H	64.50479	94.31332	72.32314	-1406.44567	-28.01055	-1113.96697	1
26179	H	64.13704	94.43104	74.13355	160.05085	2004.78765	1226.04342	1
26180	H	65.85972	94.12950	73.52249	1055.65587	2830.50998	2183.31626	1
26181	C	64.69365	91.92535	74.87986	-697.79056	40.07369	-279.65570	1
26182	H	64.42258	90.81556	74.82926	3229.14121	310.13727	-599.90452	1
26183	H	63.95923	92.36511	75.57237	1038.79755	796.03670	-1864.26444	1
26184	C	66.14230	92.31338	75.44380	147.22975	-233.18720	-690.38729	1
26185	H	66.99227	91.86485	74.87587	1556.60762	165.12485	1570.51732	1
26186	H	66.30281	91.94110	76.47782	-3447.68218	-1174.20725	-1966.75609	1
26187	H	66.42826	93.38346	75.33294	1782.86589	1513.01928	-54.23125	1
26188	C	63.85875	92.19805	71.13555	405.72371	-460.89309	76.08410	1
26189	O	63.75885	93.29205	70.66100	-308.27525	291.74971	160.23549	1
26190	N	64.37419	91.11973	70.47018	344.87435	-128.48304	14.53679	1
26191	H	64.62629	90.28571	71.08333	2536.78851	-424.76992	-4621.89963	1
26192	C	64.82153	91.26264	69.12854	-521.65274	278.45660	-180.63044	1
26193	H	65.32175	92.22861	69.03170	885.18517	18.30683	1260.26745	1
26194	C	65.81081	89.97499	68.91543	313.90853	858.97269	-561.54879	1
26195	H	65.21119	89.06860	68.75432	4866.97346	-2806.20745	2401.32630	1
26196	H	66.51135	89.74391	69.68647	2836.17440	-2441.13143	-2299.39087	1
26197	C	66.48131	90.25789	67.58719	-44.58527	-242.17585	-398.07563	1
26198	H	65.89883	90.98391	67.02813	1217.14777	-1132.53849	-2732.43430	1
26199	C	67.87539	90.83819	67.71353	-613.77310	-265.72067	-22.57068	1
26200	H	68.60602	89.96956	67.63942	-2726.39390	-1482.93927	2027.51905	1
26201	H	68.06975	91.38494	68.66784	1016.43832	2026.68898	-1126.67986	1
26202	H	68.14819	91.46537	66.83089	-2124.76667	-1546.70339	306.32220	1
26203	C	66.64332	89.00122	66.71874	-89.21730	12.22692	-756.43836	1
26204	H	65.62421	88.50218	66.57331	478.01470	1101.56978	-327.49544	1
26205	H	66.98728	89.32315	65.71417	-409.25356	-2725.70336	-2073.52904	1
26206	H	67.35807	88.25599	67.19714	944.37158	-1068.07855	716.17408	1
26207	C	63.69156	91.21638	67.95717	-331.42678	443.17305	731.34985	1
26208	O	64.00980	91.83376	66.91957	-16.25377	684.60676	-30.83130	1
26209	N	62.59076	90.59016	68.19312	772.56699	-61.98850	12.62729	1
26210	H	62.35509	90.10833	69.06691	-3221.30305	1975.76295	-87.31216	1
26211	C	61.43866	90.88581	67.44126	926.97153	72.84187	-487.77884	1
26212	H	61.89625	91.30390	66.59343	1248.58450	-2608.41487	-3148.89987	1
26213	C	60.49931	89.58444	67.20379	-439.85480	1080.97219	-304.43148	1
26214	H	61.18696	88.70190	66.98503	-2762.30384	-3173.44284	-1011.79568	1
26215	H	59.76695	89.66839	66.31200	2579.33064	-1196.07620	950.28386	1
26216	C	59.69670	89.30012	68.44911	770.57327	-177.28842	-142.94917	1

26217	H	60.39453	89.50454	69.27502	492.34306	1975.26424	220.30444	1
26218	C	58.49165	90.24958	68.44575	-422.38179	-724.60506	-496.07674	1
26219	H	58.80873	91.33605	68.80420	943.66489	-607.43791	-1081.20946	1
26220	H	57.75416	89.95454	69.19702	820.47747	914.01848	545.36953	1
26221	H	58.03829	90.35046	67.42243	2253.59685	70.39434	1534.01246	1
26222	C	59.26945	87.89155	68.59259	-612.46483	371.52813	-55.86090	1
26223	H	58.78004	87.49767	67.61825	298.46608	774.61087	-3215.83891	1
26224	H	60.04788	87.17796	68.81685	446.36193	-1576.12880	-821.36977	1
26225	H	58.52397	87.79055	69.36320	-968.75234	-609.76074	179.33083	1
26226	C	60.63927	92.19905	68.15277	76.12491	-382.59939	-75.64455	1
26227	O	59.83907	92.71986	67.41279	337.76504	301.54228	8.04589	1
26228	N	60.85322	92.53387	69.43854	-241.61369	316.97022	63.33964	1
26229	H	61.66256	92.01011	69.80848	1107.92842	366.90259	1214.05593	1
26230	C	60.51819	93.72357	70.09217	412.37519	1059.98754	343.41702	1
26231	H	61.17247	93.68332	70.98020	2280.43148	450.80588	153.66606	1
26232	C	60.80151	94.92176	69.02214	118.21557	-399.85322	587.14757	1
26233	H	60.17996	94.79849	68.09779	17.70027	-474.88715	459.83469	1
26234	H	60.50287	95.92646	69.42623	-88.24799	592.81746	-2289.86187	1
26235	C	62.35237	94.96268	68.84902	351.29532	-349.33033	549.78522	1
26236	H	62.62317	93.92805	68.59010	-1283.54499	-231.02188	-1241.65005	1
26237	H	62.87920	95.17889	69.77620	2585.90830	-2156.13094	211.20691	1
26238	C	62.96955	95.82126	67.69450	232.92796	-595.96978	1012.43179	1
26239	O	62.58275	95.76523	66.36278	190.94955	693.95188	-273.34807	1
26240	O	63.80246	96.57681	68.15430	-246.20492	-701.83179	-787.44610	1
26241	C	58.97013	93.64816	70.59635	-158.09314	431.22841	151.08584	1
26242	O	58.09412	94.25863	70.02128	145.19636	-67.15502	750.98462	1
26243	N	58.84099	92.86967	71.71728	1445.81910	-210.32780	-47.90628	1
26244	H	59.65331	92.42564	72.08913	938.25176	-1954.49512	847.67636	1
26245	C	57.95491	93.39307	72.74013	711.61274	223.80041	-27.68920	1
26246	H	57.16152	93.99283	72.21484	3681.78346	1800.10010	645.46875	1
26247	C	57.11403	92.24342	73.46418	-66.69165	-84.24614	-1379.53620	1
26248	H	56.21869	92.69405	73.88674	618.22164	3481.23809	-1940.66333	1
26249	C	56.58746	91.12869	72.47512	-653.34390	-154.45025	232.07451	1
26250	H	55.54775	90.80959	72.71783	-1627.43194	-907.95894	1082.12101	1
26251	H	56.64641	91.39427	71.40211	-1310.25793	-2782.57811	-1985.23538	1
26252	H	57.20912	90.16980	72.52029	553.22697	-608.64253	-172.07013	1
26253	C	57.80815	91.42997	74.62387	1247.41801	-299.35575	-181.56560	1
26254	H	58.46878	92.01644	75.30018	-2751.30086	-538.82928	1224.89936	1
26255	H	58.56506	90.86928	73.97777	-903.64895	285.24068	3427.28822	1
26256	C	56.96365	90.38820	75.41389	-42.66666	-375.81969	-161.66796	1
26257	H	57.53179	89.49820	75.80348	-1773.08063	9.78157	1756.45723	1
26258	H	56.67722	90.74969	76.46148	248.61059	1971.30371	-750.96058	1
26259	H	56.02053	89.99623	74.94255	339.97995	-2533.76794	1490.55134	1
26260	C	58.66241	94.33366	73.80061	366.65987	-272.76666	215.04033	1
26261	O	58.13131	95.35215	74.13483	15.39616	-277.64841	57.73420	1
26262	N	59.84209	93.86540	74.36582	146.43493	-167.40049	-81.07058	1
26263	H	60.25588	92.99137	73.93417	4609.95821	1521.70184	1569.89444	1
26264	C	60.83843	94.72891	74.96272	-765.46809	-1376.40536	47.59431	1
26265	H	60.46095	95.54895	75.54778	-1621.49338	-679.50519	1392.57319	1
26266	C	61.84069	93.78398	75.66688	-706.23630	574.72999	985.99458	1
26267	H	62.12594	92.97045	74.99654	-901.81883	-995.11457	-3686.14399	1
26268	C	62.90292	94.73924	76.32045	-271.04482	433.29534	379.08255	1
26269	H	63.60114	94.18328	76.99980	-1269.19692	-1026.43743	-3445.05014	1
26270	H	63.48816	95.23427	75.46587	-2449.33665	-1047.15680	1150.15126	1
26271	H	62.40588	95.50608	76.97491	-1396.26967	1520.71536	1623.61158	1
26272	C	61.30975	93.10284	77.03341	-1082.36532	118.40598	-71.20131	1
26273	H	60.24540	93.20155	77.24089	-149.49693	1892.41962	3366.43991	1
26274	H	61.81736	93.63396	77.89730	-2065.03253	-1753.91820	995.78033	1
26275	C	61.80602	91.61297	77.23291	-848.10367	799.10460	-193.58066	1
26276	H	61.29815	91.25452	78.19165	731.57766	-625.28888	-2030.60341	1
26277	H	62.87781	91.47325	77.27839	901.93823	2046.32506	2203.81021	1
26278	H	61.38955	91.00059	76.42649	259.00679	101.95593	399.94034	1

26279	C	61.68636	95.32471	73.66313	94.44158	-396.50568	142.57230	1
26280	O	61.85629	94.63363	72.63734	-579.68634	324.50464	-389.36649	1
26281	N	62.21132	96.46487	73.93212	-17.61694	-99.51575	-234.76525	1
26282	H	61.83719	96.81919	74.81684	2078.94788	862.31458	-3007.22006	1
26283	C	62.75886	97.31115	72.87472	-66.92117	-111.65298	-136.78264	1
26284	H	62.92883	96.56965	72.02086	-1002.67972	-3735.80057	-2115.06735	1
26285	C	61.77706	98.51027	72.62094	759.89808	-240.22811	-84.25543	1
26286	H	62.34059	99.52245	72.35778	4223.39334	-2165.41534	5404.53568	1
26287	H	61.13968	98.72917	73.52046	2294.77519	3566.41871	730.26953	1
26288	C	60.74860	98.08598	71.50109	-418.24205	-386.73667	146.42344	1
26289	H	60.20421	98.98914	71.04935	-2031.64626	-734.07853	504.21615	1
26290	H	61.39200	97.72736	70.63088	-2827.50516	1924.42467	3136.42575	1
26291	C	59.68819	97.04691	71.81127	-501.99252	-46.93214	516.77315	1
26292	H	59.33229	97.12683	72.85493	1385.22885	191.09645	775.17548	1
26293	H	60.13775	95.99468	71.72016	1047.98745	-2277.98014	632.24598	1
26294	C	58.51612	97.35582	70.81296	-427.34193	458.15224	-871.21172	1
26295	H	58.17889	98.38253	70.78254	-2841.98405	1313.97842	567.32959	1
26296	H	57.67493	96.66259	70.98488	672.44890	977.06196	-3558.61982	1
26297	N	58.80683	96.95497	69.48036	-814.72387	143.05937	313.25428	1
26298	H	63.29466	96.36679	65.93515	203.58522	819.21314	492.72393	1
26299	H	58.35555	96.11406	69.11259	-1815.94645	204.37080	-1864.27085	1
26300	H	58.60859	97.69916	68.78619	528.09392	2086.76085	-1691.43011	1
26301	C	64.02990	98.06786	73.50597	-6.40522	120.61723	1256.38043	1
26302	O	63.92476	98.98754	74.34412	290.36649	-254.83969	-31.14916	1
26303	N	65.14327	97.62891	72.93314	-1026.77140	-152.86479	-160.84149	1
26304	H	65.04020	96.76330	72.38166	1195.58513	-3501.33616	1185.84329	1
26305	C	66.47547	98.12535	73.21706	-389.01507	-438.01373	866.19752	1
26306	H	66.57249	99.29252	73.23279	2234.23851	-1480.82772	1157.08637	1
26307	C	66.91320	97.36558	74.57653	-259.74286	-514.70272	435.33043	1
26308	H	68.00207	97.21832	74.71365	2490.15086	137.16427	978.30684	1
26309	H	66.48915	96.30122	74.60411	1006.35662	-738.58260	1462.31408	1
26310	C	66.40008	98.26660	75.71775	-89.50834	167.68473	-503.61723	1
26311	H	65.34343	98.35391	75.69539	-1374.63230	-523.91457	-3071.50512	1
26312	H	66.65252	97.87640	76.72695	-1657.05165	4464.11739	-1418.26066	1
26313	C	66.90369	99.77927	75.57627	-333.72805	-385.43136	186.94898	1
26314	O	68.01696	100.12734	75.84849	48.14766	-1467.50099	310.68375	1
26315	N	65.91583	100.49239	74.99807	87.16794	115.04773	362.67302	1
26316	H	64.92239	100.18777	74.83526	-757.01260	761.89600	-387.25761	1
26317	H	66.15596	101.45438	74.53924	240.40426	-3439.32142	-2439.63484	1
26318	C	67.30322	97.52900	71.97233	15.90680	290.22721	-154.69366	1
26319	O	66.91289	96.53514	71.36947	-1113.64897	968.31676	59.15763	1
26320	N	68.41197	98.23926	71.79011	-8.66012	-192.61452	98.37745	1
26321	H	68.66329	99.10173	72.29002	838.14000	1596.66855	686.63678	1
26322	C	69.30258	97.79744	70.78729	419.18850	582.00923	149.09732	1
26323	H	69.70925	98.68787	70.26806	2863.06063	-2329.78747	4052.19334	1
26324	H	68.57654	97.24568	70.12583	-2694.03737	3210.27395	-1038.23235	1
26325	C	70.40429	96.93164	71.66468	712.43247	418.51559	-42.98648	1
26326	O	70.75192	97.32285	72.80301	136.40860	314.32996	-105.66289	1
26327	N	71.03082	96.04140	70.98280	297.34679	-418.80361	367.85631	1
26328	H	70.72537	95.68382	70.04331	2110.88390	526.31410	-2804.64880	1
26329	C	71.65959	94.99082	71.74448	40.59260	33.88720	-331.52779	1
26330	H	70.87292	94.76932	72.48349	-933.71374	1898.67129	-1321.68361	1
26331	C	72.19422	93.78898	70.83224	1235.25189	211.41764	789.83916	1
26332	H	72.66116	92.99109	71.48359	427.59256	-256.42563	-2226.95908	1
26333	H	73.06066	94.17848	70.27261	2567.90208	-400.02588	473.74100	1
26334	S	70.88832	92.94050	69.74794	-729.74287	417.29143	275.66357	1
26335	C	73.02070	95.54162	72.39733	359.10691	1395.54192	-143.57333	1
26336	O	73.57856	94.91561	73.30554	-214.26938	999.13785	187.68795	1
26337	N	73.50826	96.59140	71.69316	371.94996	22.24917	-61.60296	1
26338	H	72.76802	97.04370	71.07488	-2342.88018	1053.17085	-3614.47281	1
26339	C	74.67467	97.39390	72.09786	-514.64597	401.26303	815.98461	1
26340	H	75.38898	96.63609	72.36618	4252.57410	-93.75927	856.25526	1

26341	C	75.15254	98.04456	70.73303	102.66913	-846.05079	-1012.50748	1
26342	H	74.40512	98.74049	70.36623	426.21844	-855.73619	864.11463	1
26343	H	75.15725	97.25843	69.95897	2142.60435	1776.42701	1526.10021	1
26344	C	76.51184	98.77497	70.62373	267.37893	-243.10178	-244.24267	1
26345	H	76.65333	99.63153	71.31136	1652.44031	430.08243	1662.67596	1
26346	H	77.31856	98.06769	70.97037	-876.13340	37.75548	3459.70699	1
26347	C	76.70553	99.10998	68.99749	312.24545	-329.85787	400.14049	1
26348	O	77.56519	99.93859	68.69872	-1.81457	189.66540	201.05276	1
26349	O	76.17433	98.26581	68.23181	-629.61490	308.86489	165.89593	1
26350	C	74.41724	98.47569	73.21490	-737.98151	238.04123	-126.44796	1
26351	O	75.29426	99.24068	73.56614	118.55719	-118.28700	-171.26768	1
26352	N	73.11141	98.46284	73.57409	1095.76313	-703.57893	211.60404	1
26353	H	72.34991	97.77393	73.17853	-3920.53488	2339.40134	606.88979	1
26354	C	72.94339	98.95364	74.91594	-953.58433	-168.55633	-241.10395	1
26355	H	73.62685	99.84940	74.91423	-289.45397	-1230.29456	2431.24216	1
26356	C	71.36615	99.43940	74.99053	1098.07791	53.09732	-176.41403	1
26357	H	70.92023	99.25563	73.98476	-2878.95013	-696.09876	-60.06897	1
26358	H	70.85318	98.78404	75.64782	-2717.44243	-3542.74374	1681.91341	1
26359	C	71.26379	100.92313	75.34562	-443.27852	685.88543	-331.60867	1
26360	C	71.73681	101.04974	76.66189	312.16234	-84.43572	699.96817	1
26361	H	72.18244	100.17444	77.13498	-1404.66159	1430.18286	306.90305	1
26362	C	71.46201	102.28406	77.30295	594.53958	-44.67000	-268.28612	1
26363	H	71.67953	102.34801	78.34764	250.56678	489.20245	-133.01696	1
26364	C	70.94506	103.39266	76.61886	335.29178	-650.42116	30.98994	1
26365	H	70.73584	104.39077	77.14208	-518.70862	1788.94679	1771.59508	1
26366	C	70.76749	102.04511	74.58775	-83.39458	196.46581	-94.93877	1
26367	H	70.41223	101.88351	73.52766	1493.48370	-894.52116	-575.97182	1
26368	C	70.67607	103.31347	75.22672	223.81114	-219.40751	-606.13881	1
26369	H	70.53092	104.22509	74.67042	1413.61237	-2425.97005	-1665.39234	1
26370	C	73.27432	97.98189	76.11877	493.47412	80.94648	-494.58327	1
26371	O	73.12815	98.31243	77.30571	427.16915	397.12304	-52.88220	1
26372	N	73.60973	96.77562	75.63406	-1278.30153	-85.63360	-900.33297	1
26373	H	73.66490	96.62237	74.62287	-186.24890	1753.05654	2504.17364	1
26374	C	72.79602	95.75399	76.26993	390.21731	-587.54869	-296.70785	1
26375	H	72.56748	96.22695	77.23916	-424.62673	2976.19843	-2778.82021	1
26376	C	71.48875	95.63441	75.31573	837.66077	268.51319	-312.45318	1
26377	H	71.42477	96.47244	74.52908	3883.79841	-2967.28623	-1744.28345	1
26378	H	71.79537	94.69964	74.66753	2267.57648	206.86511	-1030.75481	1
26379	C	70.18145	95.38167	76.07778	730.26418	596.96958	1580.06913	1
26380	H	69.77747	96.27921	76.64138	-272.99692	-898.04194	-863.25979	1
26381	H	70.27893	94.72560	76.96536	-2712.32239	687.45228	987.60355	1
26382	C	69.11170	94.83781	75.00403	-77.02870	-128.92451	1112.02307	1
26383	O	67.95366	94.80378	75.45125	639.39309	225.33357	33.41516	1
26384	O	69.50285	94.50835	73.88056	166.04799	-175.38064	-127.31985	1
26385	C	73.54575	94.35878	76.32979	452.76718	382.74074	410.89867	1
26386	O	72.91555	93.35238	76.54052	-136.95494	178.99382	453.41926	1
26387	N	74.91473	94.47188	76.43134	283.08903	-0.64068	1106.60702	1
26388	H	75.22291	95.39969	76.20255	287.48961	-644.44174	1364.56035	1
26389	C	75.55146	93.93871	77.63178	-160.32175	788.92707	-65.26268	1
26390	H	75.20433	92.84738	77.63105	-984.46211	2750.07433	-118.87620	1
26391	C	77.08823	94.27967	77.42880	-213.86053	-1198.31943	-97.43106	1
26392	H	77.54418	95.04443	78.09162	-778.14937	280.56157	340.97320	1
26393	H	77.36695	94.62700	76.35331	-1047.22632	-763.46164	1883.97352	1
26394	C	77.77580	92.88082	77.65346	402.59357	-296.57730	-193.97073	1
26395	O	77.71002	92.20779	78.66854	618.83721	371.69275	-35.39601	1
26396	N	78.17731	92.36407	76.41986	675.62341	-401.54438	-418.08252	1
26397	H	78.28738	92.80477	75.55371	3288.62889	1253.15188	2783.37418	1
26398	H	78.94854	91.71025	76.52297	2032.44890	-2030.03956	2113.69471	1
26399	C	75.07004	94.79286	78.89371	-223.11959	899.40939	1217.20500	1
26400	O	75.77846	95.68180	79.44403	-459.51842	132.80903	30.72611	1
26401	N	73.91637	94.31902	79.22510	723.47068	-416.86554	-731.28419	1
26402	H	73.59837	93.45276	78.79372	502.46778	-1040.67320	-1561.02951	1

26403	C	73.09078	94.99581	80.17157	259.76785	447.90840	-23.65653	1
26404	H	73.70095	95.01615	81.06097	-1119.68495	321.23779	1898.68352	1
26405	C	72.70234	96.44703	79.80505	-752.44848	707.06434	514.49026	1
26406	H	72.26608	96.57911	78.73561	-316.29988	-107.10392	398.06675	1
26407	O	74.04369	97.64558	79.69790	-61.14743	-1036.07269	-194.13388	1
26408	H	73.61366	97.93224	78.76069	-3057.50194	1340.46102	2578.62154	1
26409	C	71.77201	96.76217	80.99178	-59.50778	399.37397	639.02946	1
26410	H	71.06403	95.97803	81.37900	3814.55725	1284.87167	1175.48754	1
26411	H	71.23150	97.72074	80.92736	2747.62284	2610.91809	-1995.04514	1
26412	H	72.47046	96.91292	81.80692	-2136.95123	2787.49259	1289.64156	1
26413	C	71.73692	93.93333	80.32849	-425.26632	-140.20707	-783.45939	1
26414	O	71.38423	93.72748	81.46668	168.26075	767.79693	-766.17591	1
26415	N	71.15351	93.56607	79.19083	-430.90646	1011.63536	26.84908	1
26416	H	71.68308	94.03682	78.46186	1911.70247	-976.13785	-1200.60299	1
26417	C	70.36126	92.33572	79.27631	-460.78098	845.60360	-214.50704	1
26418	H	69.83881	92.51663	80.20590	-699.09116	265.77888	809.03185	1
26419	C	69.55388	92.32631	77.91107	494.67628	-410.31451	-735.00239	1
26420	H	70.29360	92.54010	77.11581	331.23044	-4985.72237	4.49030	1
26421	C	68.84589	90.96291	77.61614	-102.23219	-441.88230	-70.93595	1
26422	H	68.26037	90.60628	78.46560	-2216.59160	-109.68567	159.96461	1
26423	H	68.15022	90.96024	76.75391	-304.92166	134.54442	-1260.10195	1
26424	H	69.59591	90.09490	77.43541	-3240.75252	1189.88325	-410.65386	1
26425	C	68.41122	93.36243	78.09859	369.85634	759.00737	-196.67505	1
26426	H	67.70599	93.46045	77.21234	-2867.42606	-1287.19561	-2396.25648	1
26427	H	67.78583	93.18935	79.05656	1798.45553	1078.46388	-3022.08548	1
26428	H	68.91056	94.36999	78.16511	-1624.65601	2006.83445	-599.31804	1
26429	C	71.42493	91.15011	79.21620	-198.95242	-221.86083	373.47623	1
26430	O	71.40443	90.30422	80.09398	81.03610	-21.81761	-417.91380	1
26431	N	72.23854	91.23251	78.16158	-20.58613	63.73459	454.15133	1
26432	H	72.21231	92.01727	77.50777	1060.53471	507.10811	2850.44066	1
26433	C	73.11616	90.15733	77.85584	-350.00611	322.76177	-214.84140	1
26434	H	72.40477	89.30939	78.11087	-86.48972	-992.99614	-934.44964	1
26435	C	73.42844	90.24383	76.26887	-728.26990	-465.07383	615.40052	1
26436	H	74.20372	91.02815	76.17238	-2979.34907	-316.86726	-2875.55593	1
26437	H	72.55322	90.59466	75.74608	-614.30159	2855.29697	-355.73661	1
26438	N	73.22125	88.01417	75.02132	110.67342	-81.46461	599.43379	1
26439	C	73.90994	88.81521	75.85599	98.35831	1011.69437	-195.19762	1
26440	C	73.95682	86.97575	74.75900	-339.49284	-428.97941	1004.57435	1
26441	H	73.63000	86.10828	74.08395	-1410.37698	-28.98829	-790.28660	1
26442	N	75.17190	87.09319	75.42435	-405.57113	26.28936	-310.20670	1
26443	H	75.88148	86.39877	75.38402	1528.34604	1549.14898	2613.70858	1
26444	C	75.18794	88.18097	76.12324	98.90136	504.67260	-323.48047	1
26445	H	75.98573	88.44367	76.81727	739.98150	2740.51425	-2938.16620	1
26446	C	74.38070	90.19200	78.77559	-39.24365	338.94694	484.13031	1
26447	O	75.22928	89.33635	78.57050	-985.41832	-128.67702	-316.55324	1
26448	N	74.49408	91.22270	79.63873	-695.33054	-167.35818	594.68196	1
26449	H	73.71657	91.80270	79.85489	1091.94793	-1035.50628	3799.09017	1
26450	C	75.38652	91.00062	80.75202	-241.30880	57.46769	-422.16192	1
26451	H	76.27142	90.70070	80.11063	-1520.68688	-855.24435	-3012.81247	1
26452	C	75.55104	92.40586	81.42649	838.97830	659.67720	-348.62373	1
26453	H	75.76321	93.16104	80.72305	1301.26080	-3473.22327	-1518.46133	1
26454	H	76.50540	92.42172	82.05783	-984.83117	-2413.27950	-1056.97510	1
26455	C	74.42420	92.78124	82.43090	-467.44354	-155.37381	-596.64001	1
26456	H	73.42282	93.06207	81.91068	-1439.30214	1801.79267	-1019.94306	1
26457	H	73.93201	91.98677	83.11592	-1816.93807	-983.60049	-2408.20514	1
26458	C	74.98650	94.05347	83.23656	-11.91106	199.70072	520.63316	1
26459	H	75.24872	94.88811	82.54751	-2706.42692	295.25255	-1097.34583	1
26460	H	75.93017	93.79874	83.75735	-923.04998	-590.70746	-1247.34922	1
26461	C	73.95346	94.52049	84.35388	-568.53662	637.20829	-67.13207	1
26462	H	73.04969	95.01329	83.96359	1760.81918	-2307.69627	341.91227	1
26463	H	73.57160	93.66704	85.03559	-326.32920	-1901.43256	-906.94451	1
26464	N	74.70406	95.32386	85.29703	27.16745	247.90688	-138.86168	1

26465	H	74.81232	96.90233	79.58416	-690.40863	828.83434	-1567.92245	1
26466	H	74.02763	95.75833	85.96860	3141.41497	2101.82021	-444.97046	1
26467	H	75.11839	96.09906	84.80930	761.39311	-2819.69798	-1206.87044	1
26468	C	74.90833	89.76673	81.73888	212.19500	-627.64802	210.43756	1
26469	O	75.74076	89.02242	82.29820	-60.00488	413.59701	2.71099	1
26470	N	73.62149	89.73776	81.85724	621.53572	-458.66224	652.50142	1
26471	H	73.10342	90.29482	81.16334	1152.78399	1734.69249	339.59457	1
26472	C	72.88390	88.97030	82.78158	-297.78556	-189.02406	-84.15087	1
26473	H	73.51397	89.09134	83.71845	-788.72446	37.65256	-236.85020	1
26474	C	71.35588	89.54391	82.96473	-794.64654	124.38731	-600.14035	1
26475	H	70.67268	88.63810	83.04198	578.13713	90.66432	1345.02136	1
26476	H	70.95505	90.06325	82.02965	1147.11673	462.56177	2497.33530	1
26477	C	71.25524	90.47745	84.15519	-101.80990	-351.74049	-74.53668	1
26478	C	71.40662	91.87298	84.19084	-531.44570	463.73348	-119.95143	1
26479	H	71.53190	92.55424	83.35244	3979.69522	2350.67742	1191.17184	1
26480	N	71.47686	92.32169	85.44258	-332.22879	-221.63165	-374.87691	1
26481	H	71.64206	93.25727	85.78334	-1307.27164	-754.29541	1177.24397	1
26482	C	71.27656	91.24958	86.33788	80.29125	103.82601	-598.69167	1
26483	C	71.14241	90.02343	85.57408	257.56206	438.02716	-552.08036	1
26484	C	71.00955	88.73659	86.17362	-102.91511	-480.31198	549.00656	1
26485	H	71.02275	87.78923	85.67689	-1558.38932	2109.09032	2235.26933	1
26486	C	70.78396	88.81533	87.57428	-439.12104	639.34620	274.98789	1
26487	H	70.59346	87.81439	87.98433	-515.25300	597.43414	-549.05547	1
26488	C	70.98942	91.24005	87.74658	-37.17764	-55.99710	-2.84805	1
26489	H	70.81732	92.17830	88.27348	-2627.97466	-4031.34069	-1006.34290	1
26490	C	70.71204	89.99814	88.35154	-472.41433	-498.83077	663.40817	1
26491	H	70.27709	89.98094	89.40099	1136.85797	879.75084	-2572.01461	1
26492	C	72.77024	87.47761	82.17959	691.25767	-132.21748	-264.63863	1
26493	O	73.08913	86.51448	82.85979	505.43520	-5.65285	-72.85124	1
26494	N	72.52931	87.47533	80.86759	-544.67010	965.18622	-392.05632	1
26495	H	71.99104	88.31842	80.64596	-1328.40896	3818.78886	-178.86468	1
26496	C	72.69701	86.34196	79.89221	-431.25829	-68.75649	477.49999	1
26497	H	71.90699	85.63540	80.20491	981.54481	-1194.81100	1512.77445	1
26498	C	72.35605	86.92167	78.54319	461.40917	1110.03705	-14.65166	1
26499	H	73.06665	87.72587	78.19757	-2695.31221	-5495.65476	-2486.56738	1
26500	C	72.58189	85.80410	77.52087	369.64646	-753.99313	-892.31429	1
26501	H	73.43677	85.00790	77.86771	-3629.60661	-2860.02760	2040.00345	1
26502	H	72.86769	86.11845	76.49434	-49.96206	2769.77061	830.14173	1
26503	H	71.54986	85.31150	77.34431	1673.88184	-234.17643	2807.18701	1
26504	C	70.95533	87.39575	78.38233	634.16701	-172.58628	-647.18638	1
26505	H	70.91878	88.34638	78.98745	-879.53625	-435.80187	3248.69875	1
26506	H	70.15740	86.81713	78.93033	-3768.51653	1361.14338	-190.64108	1
26507	C	70.50806	87.80535	76.92337	70.63798	804.71539	-85.80495	1
26508	H	70.62236	86.96469	76.24920	-189.08086	-2442.32605	2435.84595	1
26509	H	69.46674	88.18851	76.81782	335.72644	-827.06515	2082.27210	1
26510	H	71.25204	88.49476	76.39379	747.17610	-1392.46101	3316.37896	1
26511	C	74.21572	85.74486	79.92106	-544.01421	159.80109	914.12804	1
26512	O	74.43095	84.58790	79.52982	-57.34474	773.53321	261.44631	1
26513	N	75.04264	86.77093	80.02243	77.99243	139.76101	699.89106	1
26514	H	74.53685	87.61660	80.19378	2857.08941	-2323.54242	-393.70615	1
26515	C	76.44833	86.60871	80.11829	128.52567	-249.30262	-583.55013	1
26516	H	76.61717	85.84779	79.36498	318.92379	1257.42499	1178.62142	1
26517	C	77.28561	87.94743	79.84117	691.98208	631.58278	-652.96099	1
26518	H	76.79274	88.12232	78.84842	-3476.67039	-1565.64703	1671.07063	1
26519	H	76.98342	88.78273	80.54624	2804.34738	-1501.13447	571.74003	1
26520	O	78.74734	87.98496	79.92611	315.09460	-178.51603	-433.22117	1
26521	H	78.91346	88.82840	80.35787	786.41514	1874.65979	522.06428	1
26522	C	76.99194	85.74615	81.44299	-263.27983	123.03977	-357.44140	1
26523	O	77.93022	84.97492	81.37459	317.33843	-785.70622	372.97394	1
26524	N	76.37786	86.30607	82.46720	594.46379	-603.28187	250.99029	1
26525	H	75.70520	87.04050	82.37055	1457.42055	1610.12770	1936.29559	1
26526	C	76.42538	85.65838	83.83355	445.16203	-448.12120	-594.68822	1

26527	H	77.50666	85.69075	84.06313	939.50287	-1349.65208	486.65194	1
26528	C	75.62352	86.43323	84.88591	327.58185	754.00069	-1049.30762	1
26529	H	74.58706	86.36153	84.51337	450.27349	1507.24888	-1701.07540	1
26530	C	75.78604	85.80468	86.20944	90.64619	934.54643	1261.62468	1
26531	H	75.08724	86.22366	86.98764	3836.65808	960.75086	3219.37313	1
26532	H	75.51400	84.69780	86.20590	-1210.19279	-2378.29733	1672.75445	1
26533	H	76.83669	85.85169	86.57747	-1117.73716	-1426.48507	913.61413	1
26534	C	76.17036	87.81689	85.11971	343.85216	-664.62603	6.42475	1
26535	H	77.23306	87.77132	85.47567	2981.97791	965.69405	-1031.90872	1
26536	H	76.17126	88.26046	84.05564	-2821.88021	-963.12667	-219.03799	1
26537	C	75.45268	88.79831	86.14853	352.84020	423.62593	-232.71522	1
26538	H	74.43302	89.17636	85.74751	101.93215	-574.17761	-997.22038	1
26539	H	76.15900	89.66156	86.46187	-2080.80966	1610.23657	-1148.60037	1
26540	H	75.15045	88.17383	87.02702	560.57650	2881.88908	245.78909	1
26541	C	75.78700	84.21280	83.67290	780.31815	-42.05103	-460.38069	1
26542	O	76.22800	83.19180	84.17690	-765.27036	-48.04301	208.39534	1
26543	N	74.61500	84.11980	83.04490	563.20368	-188.35068	-594.00104	1
26544	H	74.13500	84.95480	82.78790	-344.74458	2869.01526	-1243.85815	1
26545	C	73.91400	82.81280	82.88690	-719.42455	390.17044	411.74553	1
26546	H	74.00400	82.22380	83.78790	622.53462	2152.83758	-2205.75129	1
26547	C	72.40500	82.98880	82.63790	723.38832	-305.89760	-453.87018	1
26548	H	71.80800	82.06780	82.46190	-1944.91760	-1720.08361	1783.86333	1
26549	O	72.05500	83.93480	81.60190	-717.74869	-76.49643	334.57649	1
26550	H	72.41500	84.72780	82.00590	2023.09370	-1577.95939	-1812.74049	1
26551	C	71.88900	83.50080	83.95390	605.19602	-360.84239	575.43011	1
26552	H	72.21200	84.53380	84.20790	2191.98616	-1939.79265	-1143.63599	1
26553	H	72.03100	82.81280	84.81390	1804.13016	83.53454	-2571.57819	1
26554	H	70.78500	83.62080	83.92590	-1627.98852	-2139.21008	-1639.27001	1
26555	C	74.57400	81.90580	81.81590	615.11118	-665.98768	50.39140	1
26556	O	74.51000	80.70880	81.83790	-646.40062	129.20151	442.37445	1
26557	N	75.20800	82.54480	80.80190	473.22167	678.21242	155.44275	1
26558	H	75.17800	83.52780	80.63590	-843.16064	-1004.02016	2862.01060	1
26559	C	76.14000	81.91880	79.89590	157.54242	868.30725	229.26375	1
26560	H	75.54400	81.19980	79.35290	2575.64173	1357.49996	-1180.98157	1
26561	C	76.52300	82.92480	78.72290	274.80268	730.76521	-469.81833	1
26562	H	75.62500	83.11680	78.09690	2064.45991	-1558.99425	-1780.98404	1
26563	H	76.66500	83.94280	79.14390	2168.63932	-2264.39534	-181.36611	1
26564	C	77.84600	82.66780	77.99590	-617.88482	139.01027	662.10949	1
26565	H	77.88700	81.63180	77.59590	-1871.15522	2012.70360	-1543.45540	1
26566	H	78.72200	82.60580	78.67690	3002.02647	-856.50807	331.90877	1
26567	C	78.18500	83.71880	76.95690	-107.09657	-886.05157	178.43420	1
26568	O	77.71100	83.55580	75.80090	688.66903	4.89886	373.05333	1
26569	O	78.82900	84.76080	77.27790	519.75083	296.00622	509.88549	1
26570	C	77.35300	81.31380	80.52590	117.92664	726.35021	537.73369	1
26571	O	77.70100	80.15980	80.26390	-53.26553	738.27135	-280.80070	1
26572	N	77.95800	82.09480	81.38790	495.48075	644.69541	-217.44805	1
26573	H	77.75900	83.05180	81.58290	-1885.02414	-2215.29954	-1206.82803	1
26574	C	79.11300	81.64780	82.15290	-457.98023	500.28608	-615.16454	1
26575	H	79.84000	81.34180	81.41590	780.66261	-2555.38934	-1658.29313	1
26576	C	79.73600	82.80780	82.92590	549.17241	-702.71038	171.11183	1
26577	H	79.00500	83.27380	83.62090	1999.56534	-30.14525	2423.97242	1
26578	H	80.07200	83.58180	82.20390	1767.14693	-1970.10006	1693.77958	1
26579	H	80.64900	82.46280	83.45690	-2.29933	2332.10223	-2113.46025	1
26580	C	78.82700	80.48580	83.13890	-369.72256	-599.40209	-583.64553	1
26581	O	79.55900	79.51980	83.22390	151.02221	287.45757	716.81727	1
26582	N	77.64800	80.51980	83.78290	444.56591	348.57190	622.58497	1
26583	H	77.05800	81.29980	83.58990	1779.18934	2071.99204	-1556.86411	1
26584	C	77.12500	79.38880	84.44290	-299.54306	-726.86723	464.00053	1
26585	H	77.86300	79.04080	85.15090	-2731.74188	-1206.94478	-1003.67782	1
26586	C	75.91800	79.80180	85.39390	-762.21498	-221.68741	-457.36341	1
26587	H	75.08100	80.21480	84.79090	1544.49869	-1156.93705	2481.76326	1
26588	H	75.49200	78.90680	85.89490	1941.08079	1924.31596	-1552.78144	1

26589	C	76.28200	80.82580	86.48490	-433.68999	80.49815	799.35650	1
26590	H	76.98000	81.55880	86.02790	3038.75223	526.66718	-600.28091	1
26591	C	74.98200	81.56780	86.85190	-743.94729	-314.23761	-431.80640	1
26592	H	75.18900	82.57080	87.28190	-2664.27821	-1224.78041	-1151.31104	1
26593	H	74.37200	80.96780	87.56090	443.52838	-2206.43547	2199.49783	1
26594	H	74.21300	81.76580	86.07590	-2698.85106	-1172.60111	-1125.07857	1
26595	C	77.11200	80.14080	87.64290	466.13626	-363.27208	-694.04991	1
26596	H	78.19900	80.15580	87.41590	-736.13953	-2435.33703	-1855.73748	1
26597	H	76.72400	79.10680	87.76490	761.84484	-723.60456	-2966.56632	1
26598	H	77.02300	80.76480	88.55790	-1927.48794	-2481.23504	223.08475	1
26599	C	76.81200	78.16480	83.60190	-26.82592	583.22529	698.49627	1
26600	O	76.88800	77.02780	84.09590	681.22562	-368.80145	-136.66817	1
26601	N	76.40900	78.34580	82.33290	114.66656	-327.71632	-770.39121	1
26602	H	76.25200	79.28280	82.02990	-483.74399	1308.05306	-2822.50135	1
26603	C	76.00000	77.24280	81.44990	221.43886	-710.22362	522.39625	1
26604	H	75.30300	76.60780	81.97590	-1977.38274	1232.28114	2116.61964	1
26605	C	75.34000	77.71080	80.16190	-751.87236	357.12298	-385.50321	1
26606	H	74.36600	78.17280	80.43090	-565.96182	2524.84230	-1793.63221	1
26607	H	76.02600	78.35680	79.57290	2899.03508	-1129.43192	425.94841	1
26608	H	75.07000	76.89780	79.45490	-1757.36868	-2496.71814	765.97636	1
26609	C	77.21500	76.45580	81.18090	249.35453	646.81953	588.44193	1
26610	O	77.05800	75.22780	81.01690	80.95629	473.47460	623.69477	1
26611	N	78.42600	76.99280	81.18490	353.50510	-72.86015	757.92946	1
26612	H	78.51000	77.98480	81.24190	2126.23700	-950.17224	2107.29385	1
26613	C	79.72500	76.37280	80.94990	785.96613	-212.30841	396.94714	1
26614	H	79.67100	75.84580	80.00890	-2584.28796	-1693.07951	-615.66348	1
26615	C	80.84500	77.40480	80.87490	-632.04512	614.08060	-254.32493	1
26616	H	81.81300	76.89780	80.67290	1825.76699	-2196.20209	-1313.64380	1
26617	H	80.83100	77.90280	81.86790	-795.73915	1508.53313	2642.69033	1
26618	C	80.72800	78.48680	79.85590	474.14589	136.81949	-766.44319	1
26619	C	79.79900	78.45180	78.78390	-189.58507	-154.53623	-881.91141	1
26620	H	79.19800	77.57480	78.59390	1920.23573	2017.96696	1454.83543	1
26621	C	79.71500	79.51180	77.92990	-495.83879	-673.05800	366.00043	1
26622	H	78.93100	79.51880	77.18690	-2296.60452	317.46210	2132.05000	1
26623	C	80.60300	80.61280	78.00890	-887.28632	133.26319	193.55837	1
26624	H	80.63700	81.41480	77.28690	-1407.85576	-531.31333	-2767.49837	1
26625	C	81.56500	79.61080	80.03390	-35.74170	721.58742	556.30169	1
26626	H	82.29100	79.66680	80.83190	-3120.79393	374.95255	228.33405	1
26627	C	81.49000	80.62980	79.09190	-437.80542	-323.57572	-736.36429	1
26628	H	82.21500	81.42980	79.14390	983.73118	1267.48202	-2707.20231	1
26629	C	80.06500	75.30780	81.89290	27.30115	-618.60110	-672.21477	1
26630	O	80.91900	74.45080	81.59690	669.55248	394.83134	114.57914	1
26631	N	79.44000	75.24380	83.07190	600.03055	-486.27441	-336.42566	1
26632	H	78.65900	75.82680	83.28190	101.08731	2691.73377	1622.30433	1
26633	C	79.63100	74.13880	83.98890	-70.88053	63.60258	902.95116	1
26634	H	80.68900	74.07380	84.19190	2813.27829	-1089.67613	875.60325	1
26635	C	78.87000	74.41180	85.37190	-414.99990	-611.29493	-541.67634	1
26636	H	78.83600	73.47280	85.96590	-1802.79406	-1149.07688	-2315.39983	1
26637	H	77.82200	74.75780	85.24390	735.28626	2930.02592	870.10279	1
26638	C	79.70500	75.33080	86.30090	12.88302	410.03656	810.08980	1
26639	C	79.44800	76.73280	86.29990	325.07925	-574.76938	-630.91415	1
26640	H	78.60500	77.12880	85.75290	2069.89167	1838.29736	1485.77699	1
26641	C	80.18400	77.60480	87.17890	-242.64569	832.26937	-285.37039	1
26642	H	79.91800	78.64980	87.23690	-72.92502	880.94857	-3021.71432	1
26643	C	81.22300	77.03480	87.99790	-590.06330	16.44092	-701.17183	1
26644	H	81.76900	77.73080	88.61790	19.09342	-2099.49312	2340.94424	1
26645	C	80.73400	74.83380	87.05290	-302.81803	444.90462	-740.99522	1
26646	H	80.89600	73.77180	87.15890	-2130.08363	-1155.89099	-2014.64186	1
26647	C	81.50200	75.61880	87.92690	-216.42402	884.75216	26.57408	1
26648	H	82.33500	75.21480	88.48390	-444.31235	1999.57651	-2391.91189	1
26649	C	79.16300	72.79280	83.47990	-516.03174	551.59781	-519.39448	1
26650	O	79.55200	71.72080	84.04290	543.43098	-435.00758	-372.79849	1

26651	N	78.30700	72.68380	82.44790	-842.74127	81.23730	48.92391	1
26652	H	77.94400	73.50180	82.00890	1034.72283	-614.70237	2901.18759	1
26653	C	78.01100	71.39980	81.79690	-313.67359	392.23880	-767.87771	1
26654	H	77.51000	70.87580	82.59890	1351.13833	1384.29953	-2484.13175	1
26655	C	77.14300	71.47680	80.57290	-600.58337	-476.18448	493.83867	1
26656	H	76.78100	70.46380	80.29490	-989.85260	-235.68810	-2983.26254	1
26657	H	76.21100	71.97380	80.91690	-391.91194	-1088.12666	2922.06180	1
26658	N	77.72300	73.44280	79.04490	336.80945	-769.90044	-25.40563	1
26659	H	77.43600	74.19280	79.63990	-1943.86398	-1987.71228	-1480.99796	1
26660	C	77.73900	72.10080	79.28290	339.14265	658.71439	525.86555	1
26661	C	78.21500	73.63280	77.79190	-506.62262	-648.66746	-399.85372	1
26662	H	78.09200	74.62580	77.35890	2922.70215	-606.54080	971.99507	1
26663	N	78.44100	72.46680	77.21390	484.93487	-381.97566	-574.05936	1
26664	C	78.16100	71.51680	78.14890	-693.65672	-586.15218	101.86778	1
26665	H	78.36500	70.47680	77.92590	1211.23453	1925.83611	-2177.43227	1
26666	C	79.20000	70.61280	81.39290	730.93323	476.73181	249.08226	1
26667	O	79.29400	69.44680	81.75690	-87.31612	42.16951	-790.08111	1
26668	N	80.23700	71.24080	80.70990	568.52704	431.88150	-451.64135	1
26669	H	80.12400	72.15080	80.31990	-1149.65240	-2405.00055	-1677.19991	1
26670	C	81.53600	70.68980	80.37790	258.21674	-780.87818	-393.50393	1
26671	H	81.30400	69.88380	79.69790	314.79765	-2655.03250	-1660.70039	1
26672	C	82.43700	71.71380	79.66390	590.88523	255.48703	-648.09388	1
26673	H	82.58700	72.59480	80.32390	632.99086	938.19797	2929.51452	1
26674	H	83.49300	71.39880	79.52090	1354.74289	-2170.45508	-1830.98012	1
26675	S	81.70000	72.38080	78.16590	94.19767	-446.02503	311.04487	1
26676	H	80.97600	71.33580	77.79290	1219.71884	-1563.72376	2432.53615	1
26677	C	82.28600	70.13480	81.59390	-540.84005	550.98076	484.57662	1
26678	O	82.97200	69.12480	81.49390	-436.28164	392.33045	525.78051	1
26679	N	82.03700	70.65580	82.81090	6.28899	-151.64923	824.09626	1
26680	H	81.50900	71.49380	82.92690	-1336.11792	1919.09811	2102.10231	1
26681	C	82.76200	70.16280	84.01490	-512.17584	510.78451	-565.19630	1
26682	H	83.68700	69.72280	83.67190	2439.51831	1691.80363	-1041.58248	1
26683	C	82.99500	71.37380	84.95390	744.21846	-516.55823	69.92031	1
26684	H	83.61300	70.98680	85.79290	-2664.13642	1489.10131	767.28321	1
26685	H	82.07200	71.89880	85.27890	-563.61484	-2073.30590	-2304.88871	1
26686	S	83.97900	72.63280	84.11290	-397.01144	170.82368	351.11502	1
26687	H	85.18200	72.12980	84.34390	-938.37215	707.11658	-2926.23502	1
26688	C	81.93800	69.10780	84.71990	-666.21271	500.18023	369.45573	1
26689	O	82.51800	68.29280	85.42290	-492.56503	-377.88381	-498.13078	1
26690	N	80.65300	69.10580	84.45990	617.44633	-132.70146	550.37538	1
26691	H	80.19800	69.73580	83.83490	-2558.68239	-1828.00004	-168.48568	1
26692	C	79.68700	68.14480	85.04490	-414.70060	252.94468	-779.56284	1
26693	H	80.05800	67.92580	86.03490	-1439.03520	-2776.68828	-365.24589	1
26694	C	78.28300	68.75380	85.06290	-348.58929	763.02345	353.13191	1
26695	H	77.45500	68.03180	85.23190	2179.34118	2180.30691	610.28256	1
26696	H	78.09100	69.16680	84.04990	1965.51469	-958.23108	-2264.97901	1
26697	C	78.00400	69.82480	86.20890	18.93232	197.72398	884.25036	1
26698	H	78.90500	70.47180	86.14290	-1127.50894	652.24411	-2870.13829	1
26699	C	76.81100	70.73680	85.85990	-445.46179	602.41885	516.27520	1
26700	H	76.67900	71.41480	86.72990	-1427.37923	2301.11806	-1606.68973	1
26701	H	77.14500	71.31780	84.97290	-1678.51077	734.77856	-2564.06769	1
26702	H	75.93600	70.06580	85.72890	2454.70188	1187.43975	1559.14909	1
26703	C	77.83700	69.07980	87.51390	256.78752	559.00886	665.26225	1
26704	H	76.86500	68.54180	87.53190	2628.44439	883.92489	1475.49212	1
26705	H	77.89600	69.81380	88.34590	1039.96745	-1663.74612	-2465.11651	1
26706	H	78.56200	68.26680	87.73190	97.91267	2292.23283	2144.86671	1
26707	C	79.65200	66.80780	84.29190	-499.89939	-497.87065	573.19609	1
26708	O	79.37600	65.74280	84.89590	480.47712	-540.34317	-321.51431	1
26709	N	79.98800	66.80280	82.99990	627.33225	-66.11519	550.29628	1
26710	H	80.13000	67.65680	82.50490	1399.56376	-2146.65873	-1828.56647	1
26711	C	80.27200	65.57980	82.21990	345.04682	-447.31261	-721.31110	1
26712	H	79.38000	64.97580	82.30090	1650.38530	1519.17424	-2211.71191	1

26713	C	80.25600	65.98080	80.69390	-334.08369	572.27963	622.10040	1
26714	H	80.91000	66.86380	80.53090	2645.86741	-535.00409	1601.81543	1
26715	H	79.24200	66.28180	80.35290	24.17996	-799.50259	-3049.45710	1
26716	C	80.67100	64.84780	79.76590	91.34875	864.86093	270.29622	1
26717	O	80.29900	63.70080	79.96890	491.28809	510.54753	337.64568	1
26718	N	81.33000	65.20580	78.66090	434.66559	-587.78336	-422.71164	1
26719	H	81.30100	66.17680	78.42390	-92.79501	2773.24980	-1495.12667	1
26720	H	81.92300	64.53680	78.21290	-1624.95742	-662.28272	2604.85185	1
26721	C	81.38000	64.62380	82.85090	824.62520	-11.99987	374.33151	1
26722	O	81.10700	63.45380	83.05790	-131.30189	779.54121	-26.00616	1
26723	N	82.53700	65.11480	83.31390	-339.31920	-721.36209	271.21287	1
26724	C	83.22100	66.26080	82.69590	541.99876	-110.44546	714.18945	1
26725	H	82.94100	67.16080	83.28390	1545.85470	-2007.91833	1853.47843	1
26726	H	82.92800	66.49280	81.64990	905.93180	-1202.84435	-2768.61406	1
26727	C	83.43800	64.25680	84.07790	-240.66065	-339.22390	-820.98939	1
26728	H	83.55400	63.29780	83.59490	2124.14329	-1229.66546	1955.69865	1
26729	C	84.69700	65.12580	84.13990	-796.93056	-125.24448	420.87301	1
26730	H	85.61200	64.50480	84.24490	2279.45514	694.58323	2042.14911	1
26731	H	84.61000	65.77680	85.03590	-1601.06150	-1253.62059	2393.51044	1
26732	C	84.69800	65.91280	82.85790	-749.02680	-523.18608	-22.76480	1
26733	H	85.34200	66.81680	82.82290	1912.45638	-1909.98823	-1613.38983	1
26734	H	85.02000	65.31480	81.97890	2193.15415	-1269.24227	1850.88229	1
26735	C	82.95000	63.89680	85.48290	697.69511	-16.75617	-593.25326	1
26736	O	83.29800	62.85680	86.07890	428.57217	-589.35192	-311.73354	1
26737	N	82.18500	64.85480	86.18890	645.82068	-462.76646	272.96605	1
26738	H	82.04200	65.79680	85.89690	-1849.64782	-2155.75735	-1364.44491	1
26739	C	81.67900	64.58180	87.53990	885.92957	203.76482	31.83323	1
26740	H	82.46700	64.31080	88.22590	1309.38994	1452.35775	-2471.81257	1
26741	C	80.99100	65.83580	88.13590	-476.64914	755.68161	-188.64709	1
26742	H	80.39700	66.35780	87.35590	2519.49885	1875.91449	122.99791	1
26743	C	80.07500	65.51980	89.33090	-485.51541	740.08288	207.84173	1
26744	H	79.23600	64.80180	89.20790	-1421.71086	-681.01690	2716.24615	1
26745	H	79.60200	66.50280	89.53890	-349.83941	1608.09408	-2687.41356	1
26746	H	80.59200	65.06380	90.20190	-2653.86935	1244.66657	1134.91797	1
26747	C	82.10400	66.82480	88.54790	341.08039	750.76400	377.33682	1
26748	H	82.94700	66.77280	87.82690	1058.26083	252.17697	2943.41535	1
26749	H	82.54800	66.39380	89.46990	209.75222	-1466.86417	2768.20379	1
26750	C	81.75600	68.27980	88.67090	766.68587	473.15800	-131.44538	1
26751	H	81.18400	68.37880	89.61690	-1084.69897	-2625.11562	1351.13845	1
26752	H	82.69900	68.86180	88.75190	-1629.90670	-1947.70046	1853.02194	1
26753	H	81.16100	68.59880	87.78890	-1720.56889	-507.26516	2579.63256	1
26754	C	80.71800	63.40580	87.53890	683.54933	525.37521	282.69148	1
26755	O	80.75900	62.52280	88.33690	-298.59033	284.26585	-682.36881	1
26756	N	79.82600	63.35580	86.53090	-566.62785	397.63625	-492.91382	1
26757	H	79.63700	64.12880	85.92890	1418.38124	-2166.98211	-1793.44966	1
26758	C	78.94800	62.20480	86.22690	1.72425	434.54089	-809.68156	1
26759	H	78.49300	61.75780	87.09790	1786.71034	-1480.63809	2115.61906	1
26760	C	77.77100	62.67180	85.34990	-249.35766	-653.93048	-594.24492	1
26761	H	78.14500	63.09380	84.39290	-1171.49152	2061.37804	2060.99536	1
26762	H	77.13300	61.79380	85.11490	2694.88822	114.66173	1607.88303	1
26763	C	76.80000	63.71180	86.07290	-91.33357	-903.89690	84.73427	1
26764	H	77.33300	64.63980	86.37290	239.21745	257.58420	-3133.38059	1
26765	C	75.74100	64.25280	85.11390	506.58859	-687.78010	-324.21865	1
26766	H	76.09600	64.59780	84.11990	1287.60724	-2287.00147	-1740.47961	1
26767	H	74.99800	63.47780	84.82990	-1472.58561	176.09258	-2782.81107	1
26768	H	75.09800	65.00780	85.61490	2431.81597	-1732.59108	981.31642	1
26769	C	76.08600	63.16980	87.28090	-700.51006	-474.68831	-352.69832	1
26770	H	75.75700	62.14180	87.01690	-445.91568	-2546.92932	1787.32991	1
26771	H	76.70900	63.27280	88.19590	1110.91061	2058.54317	2093.75705	1
26772	H	75.17000	63.75080	87.51990	-1082.79162	-1746.74136	2377.32573	1
26773	C	79.71000	61.03980	85.48290	405.84824	566.87794	-595.13298	1
26774	O	79.10700	60.24680	84.78490	-161.99185	548.21819	535.70323	1

26775	N	81.05000	60.89580	85.67690	533.44919	-565.23425	-337.12746	1
26776	H	81.56300	61.63580	86.10390	1083.00552	-1558.87255	2499.16215	1
26777	C	81.67900	59.58380	85.48290	566.41868	-236.18358	662.89105	1
26778	H	80.94000	58.86180	85.16790	-1779.55896	935.28051	2410.77127	1
26779	C	82.84300	59.77880	84.44790	537.99138	-555.58610	470.10495	1
26780	H	83.72900	59.14880	84.67490	1891.56470	1319.59888	2127.45893	1
26781	H	83.19000	60.83380	84.42090	1058.83435	2830.06142	864.61293	1
26782	C	82.46800	59.21580	83.06090	636.62532	-67.41624	-657.69896	1
26783	C	82.09700	57.87180	82.98090	-616.46879	665.01433	-123.55983	1
26784	H	82.06500	57.29180	83.89090	-1041.04369	258.09811	-2969.56608	1
26785	C	81.76000	57.32380	81.74990	-202.38448	-398.99101	783.39511	1
26786	H	81.57400	56.26280	81.67190	1130.34981	2820.92157	-826.66260	1
26787	C	81.73300	58.12080	80.62590	792.16737	-444.58203	-34.48110	1
26788	O	81.35100	57.56780	79.39290	471.29654	615.46945	-160.40697	1
26789	H	80.98200	56.68280	79.44890	-2195.96720	-317.63284	-2244.19934	1
26790	C	82.57200	59.98580	81.93490	659.83917	-599.41313	-188.97373	1
26791	H	82.88300	61.01080	82.07090	2142.39099	-1741.45441	-1513.40529	1
26792	C	82.18800	59.43480	80.71690	-588.71559	-484.68450	-512.22335	1
26793	H	82.27300	60.00980	79.80690	-2935.15819	-991.50955	550.76615	1
26794	C	82.20300	59.06980	86.83590	540.15733	111.71175	714.48925	1
26795	O	82.67700	57.91880	86.94890	331.10550	30.83105	704.60580	1
26796	N	82.03300	59.88880	87.89690	-706.34432	-271.89267	-386.88693	1
26797	H	81.63800	60.79980	87.80690	-2287.23878	229.78604	2139.29466	1
26798	C	82.49000	59.51680	89.18790	-429.20347	-660.19071	-473.10306	1
26799	H	83.47100	59.07480	89.09290	-657.11568	-2946.19267	880.94793	1
26800	C	82.64400	60.75380	90.06890	594.23746	560.14118	-412.36388	1
26801	H	83.36700	60.50080	90.87390	1955.46588	-1228.50243	2127.20429	1
26802	H	81.69200	61.08180	90.53790	2704.79006	-865.49660	1344.79205	1
26803	H	83.13700	61.58380	89.51890	-2831.82718	-1373.82942	-30.85665	1
26804	C	81.62000	58.45680	89.91790	690.34928	501.76332	306.72671	1
26805	O	80.36400	58.52880	89.88090	473.03440	532.29965	-347.94812	1
26806	N	82.22900	57.62180	90.79390	-74.87698	-712.65972	438.65210	1
26807	H	83.21700	57.48780	90.80390	-2531.19794	1333.42174	1295.09487	1
26808	C	81.49200	56.95580	91.86190	-484.62087	580.97427	494.19771	1
26809	H	82.21900	56.51580	92.52890	416.64956	-2022.48046	-2387.80927	1
26810	C	80.59000	57.87080	92.75390	-490.73562	-662.08290	384.23252	1
26811	H	79.86600	58.38380	92.08590	1816.37410	1149.34821	2285.88985	1
26812	H	80.09300	57.24080	93.52290	2202.62792	-1704.50842	-1479.46018	1
26813	C	81.46100	58.86380	93.52190	-583.08386	603.40092	-360.55788	1
26814	C	82.52500	58.47380	94.32090	-96.83068	-762.18108	485.40403	1
26815	H	82.86400	57.44780	94.30990	2841.33140	-962.60301	943.09466	1
26816	C	83.30600	59.40880	95.01490	403.18420	461.44573	662.51970	1
26817	H	84.13400	59.10480	95.63690	2264.94488	-1691.66042	-1398.49004	1
26818	C	82.96400	60.78380	94.84590	563.44879	507.20968	493.64990	1
26819	H	83.47000	61.57380	95.38290	2291.46047	1100.77322	1842.29204	1
26820	C	81.16500	60.24680	93.35090	630.69665	592.55679	271.39685	1
26821	H	80.29800	60.48480	92.75290	-1223.81537	2157.31707	-1941.40482	1
26822	C	81.88600	61.18680	94.02290	-515.77355	731.46685	147.62958	1
26823	H	81.69100	62.24580	93.93990	-140.87734	-1689.51412	2643.20526	1
26824	C	80.76400	55.70980	91.43490	-500.17464	188.56098	-749.21014	1
26825	O	79.70800	55.31080	91.95290	-20.07980	606.17021	490.74313	1
26826	N	81.30300	54.90280	90.49790	-613.18897	137.01729	-574.84867	1
26827	H	82.18100	55.22180	90.14890	-1239.52519	2115.28659	1957.30459	1
26828	C	80.71900	53.68480	89.94390	612.36223	595.14129	-328.81222	1
26829	H	79.65100	53.83680	89.97990	2834.10760	-1176.69575	-710.99315	1
26830	C	81.27100	53.31280	88.53290	-560.34836	452.98662	-570.11317	1
26831	H	80.83700	52.33080	88.24890	1578.65255	-2693.59292	385.49362	1
26832	H	82.36400	53.11580	88.57390	1257.75788	-2242.97224	-1827.20116	1
26833	C	80.98500	54.38180	87.51690	-842.38085	348.28366	7.74413	1
26834	H	81.51500	55.32680	87.76390	2395.00217	-730.48098	-1916.62867	1
26835	C	81.53700	54.10480	86.08490	671.22173	-472.59731	384.01449	1
26836	H	81.59600	55.10380	85.60390	-966.79973	2725.76877	1226.50630	1

26837	H	82.55700	53.69280	86.23790	-2211.60947	-2225.26126	-257.81645	1
26838	H	81.03200	53.33780	85.45890	-1645.61523	-2509.74390	933.98114	1
26839	C	79.54200	54.65580	87.23390	-438.91318	551.49441	-589.28025	1
26840	H	79.04100	54.79480	88.21590	-1489.54258	-1962.09022	-1970.19780	1
26841	H	79.34300	55.38180	86.41690	-2621.10783	1268.91685	1180.27756	1
26842	H	79.14800	53.69780	86.83090	-876.22058	-2193.97233	2067.27869	1
26843	C	80.97300	52.63780	90.95190	-294.66308	223.74628	819.74815	1
26844	O	82.06500	52.10580	91.11790	-626.47854	130.80062	447.55994	1
26845	N	79.89800	52.16980	91.66690	700.99672	-393.49591	252.15640	1
26846	H	78.97800	52.45280	91.40590	-681.63258	2386.12313	-1942.29263	1
26847	C	80.08900	51.23780	92.72590	-237.47494	599.79763	627.86329	1
26848	H	79.15000	50.75680	92.95390	2215.78107	-2233.10999	-167.79085	1
26849	H	80.83200	50.52280	92.40490	-1665.28805	2601.75139	-592.67696	1
26850	C	80.71500	51.67880	93.95290	776.65550	-248.54192	-426.41797	1
26851	O	81.35700	50.96780	94.71090	243.12424	-651.31031	368.95954	1
26852	N	80.54900	52.96080	94.25390	211.98757	-726.81273	369.09334	1
26853	H	80.17900	53.60180	93.58590	2803.25639	227.75806	1399.95341	1
26854	C	81.11800	53.58680	95.39990	-685.69174	594.61897	4.05934	1
26855	H	82.06300	53.10980	95.61590	-2112.39479	-2276.13884	502.42633	1
26856	C	81.44900	55.05980	95.20090	16.05675	-477.49194	767.20087	1
26857	H	82.12800	55.25980	94.34390	-3142.33105	64.73887	92.46630	1
26858	H	80.47800	55.52680	94.93090	1236.55968	-2887.79133	226.48613	1
26859	H	81.73900	55.58780	96.13490	-2907.70078	-1189.64873	-179.67213	1
26860	C	80.21700	53.42580	96.59890	725.72974	-559.59322	-14.76808	1
26861	O	79.01700	53.23880	96.46890	633.46152	-312.66261	349.01780	1
26862	N	80.81200	53.47280	97.79790	-253.56058	538.26796	580.84249	1
26863	H	81.79700	53.59180	97.89590	-553.73820	1892.11503	2434.83529	1
26864	C	80.10400	53.53380	99.00590	-83.91579	658.51692	606.60021	1
26865	H	79.05200	53.39680	98.80390	-472.42510	2324.38280	-2071.82914	1
26866	C	80.72100	52.50880	100.05290	233.58968	-434.99622	-783.60778	1
26867	H	81.81400	52.47280	99.85790	1872.56749	-1434.83900	-2101.36641	1
26868	H	80.40300	52.62580	101.11090	2233.18072	-1205.53046	1855.24459	1
26869	C	80.28200	51.06780	99.72490	740.64847	379.18767	360.40302	1
26870	H	80.89900	50.69980	98.87790	-907.38103	-2108.23571	-2169.25623	1
26871	H	80.52600	50.40280	100.58090	1209.73044	-2451.22492	1556.65493	1
26872	C	78.78400	50.94080	99.35690	-217.71049	-415.53200	-796.90687	1
26873	H	78.65100	51.25080	98.29890	595.16338	637.83785	-3034.80129	1
26874	H	78.23800	51.66280	100.00090	-862.47632	1992.59939	2257.72148	1
26875	C	78.18400	49.58980	99.52590	659.39928	471.49349	-429.22298	1
26876	H	78.30600	49.19080	100.55490	2214.81220	2199.79166	-390.32189	1
26877	H	78.65300	48.87980	98.81090	2552.35577	-729.39431	1682.68986	1
26878	N	76.74200	49.65680	99.25790	419.64495	488.64067	530.02827	1
26879	H	76.66100	49.91580	98.25390	-1358.22428	737.50074	2724.66510	1
26880	H	76.41300	50.36980	99.93990	2247.84457	-1622.33881	1487.61010	1
26881	H	76.27200	48.73580	99.36890	-541.39753	465.54450	3049.52035	1
26882	C	80.22600	54.95980	99.62690	-375.40057	-102.13516	-835.74657	1
26883	O	81.26600	55.62880	99.55690	-512.39704	-305.30105	-529.87790	1
26884	N	79.06500	55.53180	100.15290	73.66002	-573.14662	-632.57827	1
26885	H	78.24600	54.96680	100.20890	2167.21604	2068.83019	941.74550	1
26886	C	78.96600	56.92180	100.51590	-586.63207	-559.92563	-431.97535	1
26887	H	79.79100	57.47180	100.08790	-1673.28905	-839.22354	-2539.50586	1
26888	C	77.72400	57.53680	99.83390	625.78443	193.50274	-644.88255	1
26889	H	76.80700	57.08980	100.27490	1414.55464	-2630.82724	-1018.83450	1
26890	H	77.67100	58.59880	100.15690	-2146.38526	707.25787	-2193.92999	1
26891	C	77.84300	57.42380	98.31090	-240.48154	-882.54119	50.38544	1
26892	C	78.61700	58.35580	97.58790	107.15079	-792.97961	437.15073	1
26893	H	79.29400	59.02580	98.09690	-523.54230	2286.42711	-2100.25588	1
26894	C	78.64100	58.25080	96.16690	852.53770	-143.13388	-306.48573	1
26895	H	79.20400	58.96380	95.58290	-2919.23626	1086.50141	413.47539	1
26896	C	77.93600	57.23580	95.50590	-628.64119	-498.04666	426.86338	1
26897	H	78.04600	57.12480	94.43790	1999.98856	246.97922	-2426.77750	1
26898	C	77.15700	56.45480	97.64590	579.92030	-624.38988	328.11635	1

26899	H	76.68800	55.65580	98.20190	-265.05029	-1298.00640	2845.58841	1
26900	C	77.20800	56.31680	96.28190	563.01934	441.87114	-573.10795	1
26901	H	76.74300	55.47580	95.78890	-1999.53975	2382.98360	427.23241	1
26902	C	78.97800	57.25380	102.00090	-765.50594	342.37163	334.02720	1
26903	O	79.06900	58.41480	102.47090	128.43460	441.95748	627.39383	1
26904	N	78.95100	56.16180	102.83090	543.64501	-564.88512	-342.38822	1
26905	H	78.58300	55.30280	102.48390	-2357.29774	1729.77235	-1154.72275	1
26906	C	78.88800	56.33080	104.26790	679.17118	-605.61759	-144.88744	1
26907	H	78.72600	57.37580	104.48790	2701.74597	368.13041	1563.79394	1
26908	C	77.73800	55.52780	104.91990	588.08092	-616.19941	-358.26986	1
26909	H	77.73700	55.67180	106.02190	-2147.71108	2278.52679	178.17059	1
26910	H	78.02200	54.47280	104.71790	858.28534	-2379.80617	-1893.68340	1
26911	C	76.39500	56.07880	104.37490	-383.79535	-464.25291	-698.00178	1
26912	H	76.33400	56.03080	103.26590	2425.37538	-1985.51195	-359.09172	1
26913	H	76.43600	57.17880	104.52490	2446.90820	832.89736	1785.24220	1
26914	C	75.12500	55.41780	105.00790	101.32343	-461.54444	-795.46715	1
26915	H	74.21200	55.89580	104.59090	-825.78325	-2244.34704	-2061.66732	1
26916	H	75.24900	55.59280	106.09790	-2541.87240	-795.10878	-1682.31856	1
26917	C	75.05000	53.89580	104.84890	-163.65939	-558.79052	-718.04817	1
26918	H	75.91600	53.36880	105.30390	2469.56089	-395.49511	-1927.35616	1
26919	H	74.88900	53.64780	103.77790	-1769.52098	2588.36478	93.79002	1
26920	N	73.87300	53.41980	105.56690	-546.67977	341.26623	-545.45288	1
26921	H	74.07600	53.58480	106.57290	2819.51493	-470.17905	-1338.42872	1
26922	H	73.01100	53.99980	105.60990	-236.68518	2570.82327	-1794.53762	1
26923	H	73.73800	52.42180	105.30890	1436.11924	1826.99246	2105.46168	1
26924	C	80.16700	55.94380	104.98190	-562.18634	-642.96543	316.52428	1
26925	O	80.39300	56.21780	106.18890	-470.53643	-359.15762	-535.59274	1
26926	N	81.09000	55.32780	104.18990	-619.69063	43.27505	554.96531	1
26927	H	80.83000	54.95680	103.30190	-1474.99399	1661.73147	2207.71545	1
26928	C	82.53200	55.16980	104.40690	226.13765	819.78284	300.81604	1
26929	H	82.59600	54.28380	105.02190	-3140.20118	-79.86815	57.79492	1
26930	C	83.29300	54.91580	103.09090	66.83758	737.53381	-535.45073	1
26931	H	82.81500	54.08480	102.53090	-1220.46249	-2210.60774	1869.37159	1
26932	O	84.67700	54.54080	103.24590	-721.25168	-116.57650	-305.93974	1
26933	H	84.78500	53.96080	104.00290	-300.20061	-2268.60807	-2178.96832	1
26934	C	83.23200	56.06680	102.10790	-553.19055	-380.70547	605.74554	1
26935	H	83.45200	55.63380	101.10790	-1789.32235	-2557.03716	409.14435	1
26936	H	83.82700	56.93980	102.45090	-1817.78697	-634.51282	2475.59782	1
26937	H	82.23100	56.54280	102.03790	1183.58087	2418.86174	-1631.03719	1
26938	C	83.20700	56.25880	105.24790	-481.45484	570.84800	-522.89598	1
26939	O	83.00500	57.44880	105.00190	551.04298	-574.82111	-60.89647	1
26940	N	83.99000	55.88980	106.24490	534.03243	232.42701	-624.23858	1
26941	H	84.16600	54.94980	106.52790	92.68837	-92.15621	3131.08234	1
26942	C	84.73700	56.88680	106.99290	825.62441	-392.31486	-109.99574	1
26943	H	84.96900	57.66880	106.28490	-2000.53873	1608.73753	-1819.11862	1
26944	C	83.91500	57.42980	108.20490	906.36631	113.15543	-72.95035	1
26945	H	84.21500	58.48080	108.40390	63.17842	-2977.20480	1029.07161	1
26946	H	82.85200	57.49980	107.89190	1202.89448	1388.87616	2539.98305	1
26947	O	83.89700	56.69080	109.40790	-26.14491	767.95928	125.34871	1
26948	H	83.44200	57.18580	110.09290	1297.80650	1801.40383	2212.90352	1
26949	C	86.04500	56.31880	107.48390	914.97952	-61.74150	-10.40376	1
26950	O	86.23700	55.11080	107.49890	229.61591	378.33656	-664.21723	1
26951	N	86.96200	57.19680	107.92490	597.14599	-123.50356	-602.85420	1
26952	H	86.55800	58.10780	107.88190	-192.35619	-3025.64718	856.28963	1
26953	C	88.24100	56.92680	108.44490	-39.70392	31.43055	-922.93234	1
26954	H	88.79900	56.31480	107.75190	-2308.74034	-399.30065	2082.40514	1
26955	C	88.99900	58.27680	108.62790	533.06131	267.21247	-703.06754	1
26956	H	88.48300	58.99280	109.30190	1621.58566	2506.23513	967.89022	1
26957	H	90.03800	57.98680	108.89590	2283.11093	-1524.00781	-1565.51550	1
26958	H	89.10200	58.71980	107.61390	-2188.71036	-1996.25869	1052.30564	1
26959	C	88.23700	56.08880	109.70490	642.22866	267.23352	578.02159	1
26960	O	89.01500	55.11480	109.84290	674.29431	-417.58623	81.31770	1

26961	N	87.28400	56.41280	110.61790	548.16637	453.94747	-464.45808	1
26962	H	86.91200	57.33580	110.56290	2027.54104	-1421.14751	1940.78371	1
26963	C	86.97200	55.47480	111.74990	-583.22133	-420.93382	-574.57245	1
26964	H	87.90700	55.26180	112.24790	2301.34493	482.26405	-2108.41189	1
26965	C	85.97400	56.15380	112.70390	-434.42365	325.26577	711.77238	1
26966	H	85.55200	55.42080	113.42490	-2652.15769	-446.62730	1611.85439	1
26967	H	85.16200	56.58080	112.07790	1392.34311	-1341.84480	2478.04443	1
26968	C	86.51500	57.41880	113.51390	-518.76209	579.66808	443.45980	1
26969	H	85.63700	57.75580	114.10590	-397.27039	-2877.35012	-1243.82266	1
26970	H	86.86800	58.20880	112.81690	3085.93597	285.05713	557.56108	1
26971	C	87.65700	56.97980	114.46190	-373.18304	533.00404	-638.86655	1
26972	O	87.51800	56.06080	115.23690	-561.92578	-242.26106	-509.74084	1
26973	N	88.78900	57.67580	114.32290	112.31106	827.20148	-17.50210	1
26974	H	88.76800	58.52780	113.79990	-1540.90061	-1709.45619	2136.17914	1
26975	H	89.56800	57.40480	114.88790	31.83797	-2360.60773	-2104.68758	1
26976	C	86.38100	54.13380	111.32290	186.04227	17.84476	-907.08440	1
26977	O	86.84900	53.05580	111.69790	-198.53370	-517.33565	554.93721	1
26978	N	85.41700	54.13580	110.31590	-571.07270	-506.66814	-377.32812	1
26979	H	85.05700	54.93680	109.84490	1272.48260	-2500.38249	1431.54664	1
26980	C	84.85500	52.81180	109.85490	422.34363	477.98314	-662.29753	1
26981	H	84.53200	52.34680	110.77490	305.41600	-736.83651	-3060.04183	1
26982	C	83.70500	53.01180	108.93090	-9.75433	-684.18590	-625.88094	1
26983	H	84.01300	53.65080	108.07590	1434.14690	-2809.32224	-123.33248	1
26984	H	83.34100	52.09480	108.41990	2245.34169	-1331.23701	-1783.46068	1
26985	N	82.20500	53.38680	110.95190	-129.12814	-123.37351	-838.31457	1
26986	H	82.76300	52.85980	111.59290	2115.43274	325.34364	-2323.35424	1
26987	C	82.52300	53.64980	109.61990	-540.65560	-371.89490	620.93352	1
26988	C	81.11100	54.09780	111.23090	-446.76210	109.55486	770.17287	1
26989	H	80.61100	53.96480	112.18990	521.94149	-1096.21733	-2919.64429	1
26990	N	80.67200	54.79180	110.20390	-666.45331	-506.17666	108.82604	1
26991	C	81.57800	54.50080	109.14890	-409.69791	161.45830	781.53908	1
26992	H	81.39700	54.85780	108.14190	-2404.64671	-1642.49524	1180.83233	1
26993	C	85.90800	51.89980	109.19590	-51.36434	492.02505	745.55590	1
26994	O	85.88900	50.70180	109.38790	753.04817	-263.70656	-37.54943	1
26995	N	86.82900	52.50780	108.42890	440.28802	-705.24858	180.35530	1
26996	H	86.68300	53.45680	108.15990	2068.26808	-2382.14230	-97.00836	1
26997	C	88.02200	51.87180	107.84890	687.84369	530.90858	-289.39722	1
26998	H	87.57200	51.13580	107.19990	-1838.47594	-2546.19589	219.49772	1
26999	C	88.70700	52.92580	106.97790	-738.12864	-526.64736	83.75863	1
27000	H	89.07900	53.71380	107.66690	1487.63967	-2251.13827	-1647.74815	1
27001	H	88.02500	53.45380	106.27890	1603.01873	-2662.02562	530.27210	1
27002	H	89.64100	52.60980	106.46590	-665.85474	1160.27859	2828.39221	1
27003	C	88.99100	51.29980	108.85590	661.82690	-508.57586	-403.50394	1
27004	O	89.45100	50.19180	108.67390	-261.51197	-84.85822	-755.02024	1
27005	N	89.27600	51.98380	109.97890	-424.66527	-558.07716	459.47263	1
27006	H	88.76800	52.80380	110.22890	-905.13376	-2832.92282	1030.39139	1
27007	C	90.10100	51.42580	111.06990	-679.22628	543.23924	222.29926	1
27008	H	91.01100	51.07180	110.60790	-931.55511	2643.68285	-1424.58670	1
27009	C	90.26000	52.46080	112.19890	-143.87362	-562.27375	-724.56451	1
27010	H	90.54900	51.99480	113.16490	-2806.66635	1346.09134	364.68259	1
27011	H	89.29800	53.00080	112.32690	-1961.06028	1876.47468	1556.88599	1
27012	C	91.46800	53.42280	111.91590	554.07711	-543.53918	480.44117	1
27013	H	91.24700	53.92980	110.95190	951.11569	-937.59130	2838.44685	1
27014	C	91.52600	54.66780	112.80790	-317.99455	-553.30851	641.25410	1
27015	H	91.94300	54.47580	113.81990	-1363.63520	-1646.74124	-2325.95455	1
27016	H	92.19500	55.45480	112.39790	-1476.00409	2647.15703	-818.10281	1
27017	H	90.49100	55.02780	112.99190	-1674.09359	1651.52184	-2091.62519	1
27018	C	92.83900	52.70780	111.87190	-394.74455	613.22564	-548.39512	1
27019	H	92.94400	52.02380	111.00290	-145.83781	-2017.17187	2400.52263	1
27020	H	93.60500	53.51180	111.82990	2253.68213	2149.78808	417.84540	1
27021	H	93.04000	52.07480	112.76290	1895.46477	1835.56317	-1727.23128	1
27022	C	89.46100	50.19980	111.71690	-547.96712	168.13184	685.77758	1

27023	O	90.15700	49.23380	112.03990	-661.52465	407.88855	-70.00391	1
27024	N	88.19500	50.21680	112.07190	511.12975	-579.90554	349.03531	1
27025	H	87.72300	51.07580	111.88590	-1719.24051	1948.27710	-1772.04816	1
27026	C	87.47100	49.11180	112.69890	401.63311	392.16534	701.22189	1
27027	H	88.04300	48.79080	113.55590	-2396.87845	-1930.18719	640.69576	1
27028	C	86.10000	49.48680	113.13590	609.09279	-214.22935	-669.10143	1
27029	H	85.43700	48.61080	113.30090	-2432.90355	-207.11611	-1991.56016	1
27030	O	85.50100	50.38680	112.30590	210.34657	647.94102	371.65154	1
27031	H	85.67800	50.08280	111.41290	-2036.83915	380.86807	-2375.07761	1
27032	C	86.15600	50.20880	114.52090	-419.66067	228.70361	-784.28352	1
27033	H	85.14000	50.56980	114.78890	-2906.61975	52.20097	-1198.92605	1
27034	H	86.84200	51.06980	114.37390	-867.58561	-3008.30891	367.90175	1
27035	H	86.58700	49.54880	115.30390	-2513.79285	-1578.55899	-1056.06460	1
27036	C	87.33200	47.86380	111.81290	744.96388	-539.93151	58.07691	1
27037	O	87.28100	47.98280	110.59890	402.96599	-511.80725	446.23403	1
27038	N	87.22900	46.69980	112.39890	-242.12019	603.26164	-540.72166	1
27039	H	87.31500	46.64780	113.38990	1729.81744	-1504.06017	-2184.71464	1
27040	C	87.00800	45.43480	111.73590	793.47529	-469.94647	20.09701	1
27041	H	87.60700	45.49580	110.83890	774.51587	2892.98738	-958.92929	1
27042	C	87.63800	44.22280	112.49690	-380.31524	-664.56034	484.48118	1
27043	H	87.57500	43.32580	111.84390	-1405.00239	-1588.99201	-2343.57422	1
27044	H	88.73700	44.38180	112.50190	-2503.19484	-1323.57475	1348.66127	1
27045	O	87.05400	43.98480	113.80390	461.47569	464.54060	421.09403	1
27046	H	87.22400	44.78680	114.30390	-835.70238	-2922.49211	-858.01661	1
27047	C	85.56100	45.12680	111.38790	-844.04850	-314.10052	-135.47984	1
27048	O	84.61300	45.60580	112.09190	52.51541	695.48013	-368.33181	1
27049	O	85.32200	44.42480	110.35290	-393.53940	238.55721	616.83476	1
27050	H	80.70072	97.72288	71.05723	-28.75021	1354.14069	2313.32998	2
27051	N	80.25309	98.01071	70.15004	360.98639	-362.65453	477.77466	2
27052	H	79.63085	98.74526	70.44620	1370.84166	-4683.21762	-2759.38871	2
27053	C	81.18283	98.64816	69.20254	-504.76223	78.29735	-855.48651	2
27054	H	82.08899	98.00168	69.21014	2483.91312	207.59651	-616.85338	2
27055	C	80.34442	98.48705	67.85642	-496.13976	17.93884	531.59301	2
27056	H	80.22673	97.40890	67.62391	-1071.71275	401.29279	-720.38173	2
27057	H	79.28467	98.86237	67.94548	2732.78852	-2326.65779	23.62752	2
27058	C	80.83949	99.15104	66.57334	260.08705	-266.37593	-540.53333	2
27059	H	81.06594	100.25370	66.81422	1.35464	-1073.68480	1006.70541	2
27060	C	82.09017	98.38608	66.15167	64.65722	-113.46308	280.71794	2
27061	H	81.78491	97.31899	65.86563	1336.99985	2395.70981	-674.63175	2
27062	H	82.56385	98.73833	65.27371	-1959.19126	-1145.00055	-2083.89292	2
27063	H	82.97735	98.25060	66.95839	124.34951	-4140.80952	984.51144	2
27064	C	79.72187	99.02509	65.58252	-208.83081	-772.89618	-724.28084	2
27065	H	79.88684	99.65297	64.63588	942.67767	-69.65364	2683.59115	2
27066	H	79.47806	97.90343	65.25993	2141.46893	1361.99553	1389.73637	2
27067	H	78.76500	99.45812	66.06836	-1231.88962	1380.81974	-1007.73671	2
27068	C	81.52052	100.17235	69.64400	48.92880	-75.89637	-528.98638	2
27069	O	81.42633	101.09678	68.78902	-512.04881	-347.44463	-74.67701	2
27070	N	81.94757	100.22398	70.85722	35.97771	273.20649	0.08554	2
27071	H	82.05459	99.27935	71.30377	4053.81932	825.83713	-599.26871	2
27072	C	81.34035	101.24950	71.70099	-10.84229	270.08836	599.69294	2
27073	H	80.31679	100.76345	71.94554	-532.92365	1244.71796	2811.43163	2
27074	C	82.40567	101.37639	72.88842	514.59915	-843.49857	540.88512	2
27075	H	83.46291	101.26230	72.41166	-784.43090	-1729.14143	-1018.79247	2
27076	O	82.73903	100.19363	73.72821	-188.41785	64.13248	-589.59926	2
27077	H	81.75728	99.87772	73.83543	-726.95990	2331.52832	190.53821	2
27078	C	82.22223	102.84793	73.41833	362.06353	-340.36570	553.01129	2
27079	H	82.98327	103.56890	73.00792	-12.09749	642.93273	734.51267	2
27080	H	81.23480	103.27067	73.18715	2345.32475	-40.50010	747.43973	2
27081	H	82.21168	102.87070	74.52741	2381.10464	1198.40850	-2291.90661	2
27082	C	81.09391	102.65997	70.99113	819.14438	594.88011	-283.15446	2
27083	O	82.09519	103.38029	70.85309	69.96079	-103.82350	90.58532	2
27084	N	79.86447	102.81358	70.56383	230.14922	-481.43646	322.01977	2

27085	C	79.46004	104.05112	69.93795	-968.65900	-216.01707	-101.92498	2
27086	H	80.29721	104.29833	69.19042	1453.75334	-1158.12107	860.72431	2
27087	C	78.02469	103.65530	69.40417	163.98244	-12.42136	83.06769	2
27088	H	77.32316	104.51946	69.17819	1652.18405	1291.46670	2492.28156	2
27089	H	78.13076	103.20105	68.32778	2328.02755	-1404.76033	1028.46884	2
27090	C	77.41006	102.59413	70.36588	-387.04026	681.81602	-583.65057	2
27091	H	76.90299	103.03788	71.21996	2150.25629	-745.10984	-956.29671	2
27092	H	76.54840	101.92809	69.93064	1290.52388	1970.79120	398.00284	2
27093	C	78.74925	101.85446	70.73505	616.42056	326.87515	35.53862	2
27094	H	78.74544	101.41527	71.75547	-947.33490	-3711.95528	726.08716	2
27095	H	78.79510	101.02609	69.96673	1010.93024	1466.47691	-1467.92604	2
27096	C	79.22506	105.18089	71.08956	-227.22892	-515.80612	836.78668	2
27097	O	78.15523	105.76156	71.06658	-653.55050	230.73929	-862.68968	2
27098	N	80.23089	105.31173	71.94965	20.07116	-310.61109	350.92518	2
27099	H	81.05466	104.68564	71.84908	1023.75924	-706.45054	-3080.09039	2
27100	C	80.48262	106.60322	72.49351	226.36416	-489.93454	83.46435	2
27101	H	79.47437	107.16002	72.36903	228.97534	3774.11449	2215.24514	2
27102	C	81.01452	106.30707	74.00354	-667.90851	-906.54075	-124.83595	2
27103	H	81.31103	107.38128	74.21714	512.61221	-1574.96934	2.52164	2
27104	O	82.21016	105.43763	74.24249	-38.55283	664.20327	591.31246	2
27105	H	82.81520	106.11226	74.60988	334.52575	984.22406	1338.98634	2
27106	C	79.73801	105.90790	74.74431	221.26345	37.20300	266.26847	2
27107	H	79.50631	104.81954	74.62950	-3.04439	-651.00758	2110.69912	2
27108	H	79.89006	106.09522	75.84231	-1102.24234	-2033.17735	2820.29737	2
27109	H	78.79541	106.45735	74.43899	3741.64350	-317.71822	1824.13154	2
27110	C	81.70727	107.08528	71.57265	-272.13185	229.43416	90.21554	2
27111	O	81.53716	107.95622	70.70360	-695.51261	-111.64484	-1203.44307	2
27112	N	82.78823	106.37242	71.81168	82.00173	-435.66041	325.80728	2
27113	H	82.80152	105.84248	72.75829	368.55647	-1680.43771	2903.07882	2
27114	C	84.05344	106.84502	71.32684	-475.57109	-956.75740	359.77281	2
27115	H	83.81356	107.95881	71.16997	-1103.18334	4619.81417	-1149.04781	2
27116	C	85.11214	106.42072	72.41527	722.49972	-307.02261	867.27107	2
27117	H	85.16981	105.32086	72.56457	926.83144	-278.11890	-1439.95530	2
27118	H	86.08905	106.80776	71.99199	631.03610	4822.16619	1337.86680	2
27119	O	84.78452	107.06802	73.77877	942.84355	-177.78089	352.63188	2
27120	H	85.22554	106.38663	74.33981	2215.64715	4200.69675	1538.87461	2
27121	C	84.57491	106.15317	69.95461	1130.03065	34.81480	-817.46462	2
27122	O	85.32747	106.69191	69.15609	-201.99061	228.22805	54.70781	2
27123	N	83.95677	105.01604	69.65963	391.00108	-28.32421	-320.29611	2
27124	H	83.13860	104.71402	70.17018	-1650.75143	-583.11808	-2520.26056	2
27125	C	84.10970	104.40414	68.32401	945.60334	-224.24374	-208.33368	2
27126	H	85.12174	104.64983	67.94729	807.29532	2547.70367	-1101.12701	2
27127	C	83.99888	102.80107	68.63324	165.51385	-816.30458	-416.99695	2
27128	H	82.97390	102.38268	68.96164	-1224.77387	243.01590	2231.15141	2
27129	C	84.54631	102.10652	67.33949	702.88601	159.31653	318.18348	2
27130	H	85.08692	101.13518	67.52843	-2653.59665	923.99692	-2434.04962	2
27131	H	83.70762	101.71411	66.71119	-161.98272	752.74553	-1071.58427	2
27132	H	85.27496	102.75705	66.76774	170.49722	137.87745	-602.88810	2
27133	C	84.91306	102.63955	69.87381	-994.09105	-191.88038	389.31686	2
27134	H	85.07422	101.57146	70.15131	2067.60197	-1129.25701	-53.36024	2
27135	H	85.98061	103.02728	69.66201	626.94480	2499.40609	-2638.54559	2
27136	H	84.44734	103.24516	70.68908	-1102.23125	-120.98075	-3088.28412	2
27137	C	82.92983	104.94425	67.42262	937.53311	601.45755	175.38210	2
27138	O	81.73403	105.05155	67.76640	-6.07773	547.81531	60.25378	2
27139	N	83.42042	105.06930	66.17314	-410.63743	-702.40132	191.48497	2
27140	H	84.39321	104.81853	66.04426	-1877.19658	1961.52001	2416.08248	2
27141	C	82.70581	105.77887	65.16266	249.53592	-517.80599	-365.52789	2
27142	H	81.60640	105.86996	65.54425	2636.95057	-3667.40529	195.68022	2
27143	C	83.47374	107.18566	65.09598	-23.34043	736.90690	401.40617	2
27144	H	84.38209	107.03106	64.48461	2743.79978	335.34493	534.04956	2
27145	H	82.69706	107.74414	64.50162	-1999.73130	607.41408	239.35026	2
27146	C	83.94030	108.03077	66.27807	-887.19363	-317.46497	467.34939	2

27147	H	84.62711	107.36938	66.89084	-5189.09204	1608.40716	-1608.98085	2
27148	H	84.63754	108.85750	65.88087	1622.91834	786.98681	-1173.60313	2
27149	C	82.67261	108.60229	67.08727	72.19562	-472.03962	123.48414	2
27150	O	81.83443	109.22076	66.45535	452.36222	106.68792	79.18109	2
27151	N	82.75666	108.30650	68.38605	253.98509	570.73130	-18.78595	2
27152	H	83.53223	107.74326	68.93972	-4570.31399	-2332.45216	-2484.42597	2
27153	H	81.99730	108.39167	69.15386	-19.48640	-2484.14906	41.34676	2
27154	C	82.88509	105.05527	63.69913	-320.88763	-198.49436	521.01958	2
27155	O	83.50551	105.67199	62.82958	62.71213	59.60043	891.55807	2
27156	N	82.38218	103.80466	63.71882	-416.66466	173.91593	926.26397	2
27157	C	81.96407	103.16193	62.49537	-952.55485	573.20652	232.95923	2
27158	H	82.82995	103.32902	61.79658	886.67306	-3336.00857	-1684.50430	2
27159	C	81.48933	101.67820	62.83429	-525.29811	645.87965	-240.86441	2
27160	H	80.38423	101.52297	62.76824	502.92008	-919.59243	-362.52581	2
27161	H	81.92784	100.93271	62.14044	1005.54312	1654.01060	1281.84787	2
27162	C	81.87252	101.53411	64.33711	555.76398	130.13216	-163.68436	2
27163	H	80.93416	101.25494	64.90575	-403.79991	-895.95840	3093.90531	2
27164	H	82.51203	100.70033	64.48434	-1715.42086	415.17553	78.91519	2
27165	C	82.62930	102.86250	64.79063	1057.52223	-366.75064	323.07254	2
27166	H	82.20891	103.21670	65.78886	-3504.01772	-727.36832	1121.38089	2
27167	H	83.75827	102.83506	64.86690	-956.25622	-283.49698	-1777.92764	2
27168	C	80.86952	104.06113	61.62955	-61.11325	-583.30037	680.02075	2
27169	O	80.76433	103.98371	60.42084	132.47571	-315.63984	-76.22998	2
27170	N	80.00048	104.51809	62.51960	-77.73079	629.80830	267.82809	2
27171	H	80.38289	104.37699	63.45582	3129.16004	1331.18029	4128.61955	2
27172	C	79.26082	105.77992	62.26628	314.30949	500.90384	679.73404	2
27173	H	79.70943	106.23590	61.35714	753.93467	-3505.47991	-5172.10618	2
27174	C	77.81871	105.36191	62.03958	-191.62711	293.44951	237.58129	2
27175	H	77.38262	105.08444	63.03704	-1114.90838	2958.55707	-475.93595	2
27176	C	76.99286	106.56765	61.61491	-232.54886	168.49871	416.51443	2
27177	H	77.25083	107.41750	62.30186	-1472.99464	-1574.74892	227.39517	2
27178	H	77.18943	106.90716	60.56696	5077.31293	-2285.40903	1255.19862	2
27179	H	75.81659	106.37092	61.60056	-1695.21235	-1404.35268	1513.12560	2
27180	C	77.57665	104.09417	61.23167	1660.51300	647.68457	453.64498	2
27181	H	77.95120	103.26413	61.80660	65.69729	749.99564	-3697.68522	2
27182	H	76.45209	104.05706	60.98651	-3513.91482	-4609.69178	1368.60254	2
27183	H	78.23509	104.21555	60.30728	-1118.21582	-399.18199	1753.36931	2
27184	C	79.52697	106.66811	63.63172	148.25055	552.00386	560.53938	2
27185	O	79.59130	106.29354	64.82185	-88.84061	158.68919	-304.87079	2
27186	N	79.80651	107.85375	63.18848	301.72485	749.47134	179.11913	2
27187	H	79.67276	107.94177	62.12123	-1013.97595	1432.73274	-716.27723	2
27188	C	79.80176	109.06574	63.98195	172.15695	-198.95290	139.30126	2
27189	H	80.24251	108.85318	64.95734	37.60281	-1785.42374	-2616.62926	2
27190	C	80.48445	110.22863	63.15429	174.63251	484.38678	-482.67134	2
27191	H	79.88578	110.58134	62.26612	615.99999	-1011.12308	-166.31671	2
27192	H	80.47998	110.90437	64.00936	1469.67704	-2499.71533	-1231.98514	2
27193	C	81.95532	109.83293	62.82341	49.54531	566.73334	204.44089	2
27194	H	82.23203	108.93711	63.38482	-178.92641	119.54585	-1317.38683	2
27195	H	82.19638	109.69941	61.71786	1461.20904	-1576.96142	-913.53117	2
27196	C	82.80403	110.99933	63.47244	-957.59101	-1400.74985	-592.04217	2
27197	H	82.35079	111.44199	64.41116	821.07748	2754.41192	-2554.36023	2
27198	H	83.74997	110.63909	63.74058	3173.29254	-504.01636	-840.22361	2
27199	C	83.10659	112.24784	62.53870	-206.26892	401.06198	193.96222	2
27200	H	83.69334	113.10070	63.00258	252.99661	807.00934	-851.79697	2
27201	H	83.71191	111.79430	61.68030	-943.39907	671.53689	3896.28578	2
27202	N	81.95848	112.68883	61.86361	108.56539	199.35058	-98.31947	2
27203	H	81.53355	113.56398	62.03426	-866.02593	874.53063	-906.98038	2
27204	H	76.54034	113.16297	61.56230	-2352.01525	-90.87398	-1320.78321	2
27205	H	81.87893	112.49704	60.82699	-130.07029	247.99392	-332.20978	2
27206	C	78.28610	109.68460	64.05720	-456.81791	-424.87041	360.50883	2
27207	O	77.56972	109.52427	63.08260	-105.88395	248.75307	370.13465	2
27208	N	78.15239	110.73326	64.91522	-663.32108	516.49087	-354.22193	2

27209	H	78.83708	110.57111	65.64296	461.21945	-1620.19000	-842.04772	2
27210	C	76.74440	110.97115	65.38367	-501.30686	677.84830	635.21172	2
27211	H	76.42264	109.89442	65.07946	-1663.84502	-424.49928	-1057.84904	2
27212	C	76.74389	111.40742	66.85730	-47.37151	-5.64595	-100.41544	2
27213	H	77.04138	110.61303	67.63383	1135.40097	-2620.51262	-2003.69202	2
27214	H	77.40823	112.30130	67.08304	1354.84551	-742.28870	-3029.38312	2
27215	C	75.27807	111.94702	67.23313	-1282.13054	945.08159	-1453.24139	2
27216	H	75.16015	112.14443	68.32273	739.84922	1265.28435	1561.37836	2
27217	H	75.31583	112.98267	66.89797	-3556.78700	-1230.75417	494.05768	2
27218	C	74.16746	110.94039	66.76650	345.71343	158.73572	-282.85375	2
27219	H	74.19997	110.91926	65.63089	-397.07820	-164.97582	-1314.77090	2
27220	H	74.42798	109.91480	67.14040	-801.23129	3145.04019	1622.32353	2
27221	C	72.76812	111.43532	67.28085	104.17644	-551.90025	-30.46575	2
27222	H	72.49227	110.99831	68.27413	1928.41828	-1313.00660	74.59029	2
27223	H	72.67112	112.52892	67.28507	1350.27284	3222.60664	-4083.30941	2
27224	N	71.60913	110.86897	66.37917	-114.51997	-62.88541	-383.23871	2
27225	H	71.67708	111.17190	65.32816	315.36821	879.02963	-405.86485	2
27226	H	71.41041	109.82585	66.28244	1131.35423	612.98728	-202.25555	2
27227	H	70.68981	111.19293	66.66749	2715.95336	1317.95196	732.71932	2
27228	C	76.08708	112.19766	64.61926	541.87455	-94.41914	-426.12797	2
27229	O	75.94391	113.36319	64.86706	-31.20100	-517.14259	-515.71617	2
27230	N	75.91043	111.67145	63.35779	-20.66778	-175.10698	406.91899	2
27231	H	76.25649	110.71296	63.23939	-1848.16589	-313.59347	-2411.00000	2
27232	C	74.65594	112.14655	62.69790	977.68676	459.24225	194.01762	2
27233	H	74.59552	113.19278	63.04936	-2264.59134	-10.81969	1005.01083	2
27234	C	74.85871	112.00080	61.21131	190.45219	-112.56114	-158.15616	2
27235	H	75.20321	111.00993	60.82709	-2080.35985	1610.39122	658.81965	2
27236	O	76.18887	113.13576	60.60366	325.50167	133.33409	412.00458	2
27237	H	76.76371	112.37323	60.25221	1618.61717	972.00502	-3590.42268	2
27238	C	73.47909	112.45021	60.65632	53.99568	-72.63180	-408.22027	2
27239	H	73.31227	112.44371	59.51451	-1009.79518	-2045.99359	-2775.22030	2
27240	H	72.57339	112.05458	61.23668	-2252.04137	-3905.98031	-2036.16445	2
27241	H	73.40456	113.56292	60.81981	611.46636	-2279.73633	-2383.79908	2
27242	C	73.52546	111.16309	63.41096	-509.83330	88.89100	-534.78720	2
27243	O	72.57872	111.69264	64.02130	-710.83571	-753.22309	-31.13778	2
27244	N	73.78575	109.91972	63.16308	241.02248	-843.72505	433.88144	2
27245	H	74.66596	109.83614	62.60800	4454.22132	153.88356	-1398.69913	2
27246	C	73.19131	108.73898	63.71681	230.02788	44.61916	-857.47522	2
27247	H	72.62967	109.12089	64.57794	-662.92852	3030.09898	599.95960	2
27248	C	72.42344	108.19360	62.45202	-410.78279	763.15558	230.67138	2
27249	H	72.05136	109.01651	61.77029	-2034.27236	3501.52928	-2268.65805	2
27250	H	73.10915	107.72464	61.74418	-3255.63919	44.56585	-545.18471	2
27251	C	71.45471	107.04242	62.87397	5.77863	-843.05347	-521.93677	2
27252	C	71.70646	105.98961	63.81050	302.11008	101.04057	-131.45881	2
27253	H	72.38859	106.11220	64.70400	723.87970	-195.78880	-2064.53807	2
27254	C	70.50373	106.76188	61.87151	547.02862	-706.29920	370.32408	2
27255	H	70.29827	107.48600	61.14708	1315.06357	2225.91966	2373.74863	2
27256	C	70.87053	104.90919	63.81792	-702.86456	-971.81020	-435.15572	2
27257	H	71.13884	104.26782	64.67019	-724.65286	-1216.21186	1461.17808	2
27258	C	69.70635	105.57041	61.94359	811.80398	-652.43382	299.78567	2
27259	H	69.06635	105.34523	61.07324	-2168.39937	1224.33611	-148.41596	2
27260	C	69.80057	104.55963	62.93906	-21.44231	-325.84247	424.32441	2
27261	O	68.99041	103.38306	63.22096	-325.54213	-315.93557	-488.78698	2
27262	H	69.57389	102.95867	63.92118	-1205.99506	4334.93225	-1281.95080	2
27263	C	74.24030	107.56281	64.13015	-446.11705	25.60516	-570.14706	2
27264	O	74.95605	107.02284	63.33322	-847.51149	3.67111	86.25363	2
27265	N	74.45907	107.49333	65.48522	365.05105	194.35332	-391.98237	2
27266	H	73.83338	108.10178	66.07118	-2851.96396	-872.27866	-1161.65454	2
27267	C	74.82217	106.17315	66.00113	855.88610	445.99586	-992.33811	2
27268	H	73.87617	105.65658	65.94025	4815.31547	-3350.73326	4449.73285	2
27269	C	75.75663	105.41078	65.01359	867.94395	-961.33992	301.99752	2
27270	H	75.17060	104.88874	64.22747	126.67348	782.80221	-78.11920	2

27271	H	76.36698	106.19127	64.54225	-255.34691	103.76659	2029.55993	2	
27272	C	76.66308	104.36416	65.71521	-104.88923	137.21335	328.41458	2	
27273	H	77.27543	104.87487	66.52144	1283.63213	813.75921	-1598.74943	2	
27274	H	75.96439	103.62732	66.22487	-563.54187	1215.86375	-57.77553	2	
27275	C	77.64796	103.60226	64.65470	-1279.60015	1134.06096	669.83822	2	
27276	H	77.21144	102.94706	63.81800	1260.03019	-768.24037	4645.96856	2	
27277	H	78.58435	104.16136	64.26796	1581.36774	1418.52550	-91.87554	2	
27278	N	78.00348	102.69619	65.61681	61.54134	-473.45915	-219.31027	2	
27279	H	77.47927	101.84681	65.63845	-4162.54141	1591.26466	427.47039	2	
27280	C	78.97437	102.84388	66.46261	1086.67877	380.70695	179.25455	2	
27281	N	79.69049	104.06845	66.30687	27.46201	374.11419	-279.10761	2	
27282	H	79.48775	104.86535	65.66734	618.39204	-422.78355	-1281.15099	2	
27283	H	80.51319	104.29669	66.89179	-817.39436	-724.79210	1238.99969	2	
27284	N	79.07014	101.75899	67.27036	67.38315	-284.13118	725.14269	2	
27285	H	78.42414	100.99745	67.38123	979.78749	2523.54919	-295.89263	2	
27286	H	79.82922	101.65914	67.98652	-1999.64371	-2107.43231	626.48061	2	
27287	C	75.40804	106.43981	67.50324	181.37567	448.09956	328.68016	2	
27288	O	75.18509	105.68362	68.46805	-109.86441	-792.42009	-472.65058	2	
27289	N	76.36102	107.32742	67.39396	301.23228	222.77616	-219.65122	2	
27290	H	76.54843	107.79810	66.47181	2840.46534	4091.49967	776.90159	2	
27291	C	77.12856	107.53295	68.59424	-383.83246	-168.56348	113.52110	2	
27292	H	77.38891	106.50844	68.96381	-500.83316	1691.07902	743.18886	2	
27293	C	78.32726	108.42172	68.05609	357.47706	-596.51459	-202.73486	2	
27294	H	78.02693	109.25043	67.36413	2428.95716	939.76298	-395.51823	2	
27295	C	79.03796	109.12951	69.30543	-444.06139	181.18198	57.27239	2	
27296	H	78.31606	109.68061	69.92451	-914.28044	-261.97256	449.75099	2	
27297	H	79.56909	108.38852	69.97309	-2543.37545	3190.65011	945.52461	2	
27298	H	79.85210	109.84823	68.95233	-907.34543	-2046.71310	279.33543	2	
27299	C	79.46030	107.48394	67.59606	255.89646	-186.60740	-434.05043	2	
27300	H	80.28610	108.10416	67.17568	-1607.40923	-593.51045	-1179.49456	2	
27301	H	79.79267	106.92844	68.43102	329.43263	413.28972	-145.97563	2	
27302	H	79.13438	106.80944	66.68833	3647.26968	-470.70318	-3702.50779	2	
27303	C	76.28265	108.31173	69.75116	-504.80690	-736.05669	-186.85475	2	
27304	O	75.72904	109.36051	69.48966	346.12675	851.98860	176.30697	2	
27305	N	76.26287	107.66395	70.96586	499.27987	-483.43183	84.76302	2	
27306	H	76.70336	106.78004	71.01413	-1268.39408	-864.34584	618.97866	2	
27307	C	75.06086	107.93333	71.72532	-63.05321	-11.30148	212.75295	2	
27308	H	74.81740	109.01072	71.61861	449.34344	-787.95242	-1160.36341	2	
27309	C	73.87265	107.07910	71.06104	-176.70843	519.02450	982.30082	2	
27310	H	74.16842	106.60642	70.05229	201.72207	993.21356	90.97991	2	
27311	H	73.77946	106.25640	71.76303	-1797.23387	574.81436	-64.27406	2	
27312	C	72.54880	107.80344	70.94382	-723.58339	-195.46982	-1123.63805	2	
27313	H	71.67011	107.18606	70.68307	1411.11843	-1062.43026	572.14153	2	
27314	C	72.26057	108.34254	72.33362	-349.40568	-1075.98414	223.61543	2	
27315	H	71.21653	108.70124	72.34070	-1689.42356	-3142.59478	-1158.65053	2	
27316	H	72.41664	107.48883	73.08034	466.54713	-657.47916	620.71876	2	
27317	H	72.99581	109.17687	72.65656	1409.00882	86.94478	401.89744	2	
27318	C	72.63325	108.85200	69.87054	646.14090	625.34829	-607.34174	2	
27319	H	71.54677	109.20160	69.79892	1785.41700	-1926.17410	-568.32983	2	
27320	H	73.33173	109.71197	70.02023	-3851.70880	-919.36960	2413.82570	2	
27321	H	72.78068	108.38462	68.82226	-3330.93433	-1944.60454	1484.89263	2	
27322	C	75.34524	107.45679	73.20304	255.14128	43.74177	-488.52876	2	
27323	O	74.51288	106.87049	73.81250	-96.30975	386.76015	-186.32589	2	
27324	O	76.65263	107.65704	73.75665	-358.63377	702.42604	738.89109	2	
27325	H	77.10372	108.07894	73.01183	-822.68361	1343.08897	139.40547	2	
27326		5463							
27327		150.0000	150.0000	150.0000	0.0000	0.0000	0.0000***** 250.0000	1000000	
		0.2500	400.00	0.00	0.00	0.00	-25973.0287	0.2268	400.0000
27328	N	57.27141	97.55846	58.87991	223.83994	-101.90287	372.66777	1	
27329	H	57.37328	98.10578	59.71824	-2142.52195	-1037.52776	145.71361	1	
27330	H	56.80967	98.14250	58.17978	-1590.79522	-2082.55268	192.18837	1	
27331	H	65.45529	101.45577	56.80579	784.43016	2140.69514	1972.07577	1	

27332	C	58.44549	96.93641	58.34561	-3.96221	-856.97858	91.29554	1
27333	H	59.25530	96.92875	59.16285	1496.06083	2074.90424	-3435.44620	1
27334	C	58.05548	95.53718	57.74697	-496.34520	-675.23278	451.50467	1
27335	H	58.76931	95.18203	56.94870	-274.64575	1276.00949	-4171.97117	1
27336	H	57.14719	95.51357	57.18299	-549.47739	-7.93573	-144.35018	1
27337	C	58.07278	94.50658	58.93098	598.10324	171.20862	-72.22022	1
27338	H	57.37847	94.77166	59.82103	859.17111	-1975.42267	1326.78250	1
27339	H	58.88442	94.78751	59.68251	-2898.37212	3322.79497	-2983.15550	1
27340	S	58.05033	92.90700	58.20049	399.30544	636.60173	-473.57315	1
27341	C	58.16626	91.96574	59.80195	-337.87428	154.14824	-357.08131	1
27342	H	58.00723	90.84317	59.63181	-2682.83358	202.87996	193.88211	1
27343	H	59.21888	92.06566	60.26749	-2916.74131	-277.61173	1745.14866	1
27344	H	57.50550	92.34045	60.65112	-522.81693	5019.59325	-170.42904	1
27345	C	58.99618	97.78526	57.08010	177.87656	526.61997	-675.33308	1
27346	O	58.37746	97.98938	56.04116	-462.95898	-74.28650	-372.85397	1
27347	N	60.16293	98.33924	57.48667	1086.22787	-475.82708	427.91659	1
27348	H	60.36103	98.26374	58.48269	-1671.05218	527.14628	-1257.58353	1
27349	C	61.12427	98.35589	56.39938	-158.85132	282.38350	-915.48546	1
27350	H	60.42127	98.30181	55.54044	-2122.32369	3021.50215	309.51748	1
27351	C	62.00579	99.63329	56.55342	788.34156	373.73982	474.63822	1
27352	H	62.47129	99.89742	55.56791	1407.57195	-229.43230	-88.13700	1
27353	H	61.28790	100.52349	56.77039	2128.35497	-2342.21224	-207.33603	1
27354	C	63.03488	99.44501	57.70349	-95.44621	1307.00313	1137.73544	1
27355	H	63.44935	98.45511	57.68587	997.09550	-799.02037	-466.98014	1
27356	H	62.53671	99.70639	58.67345	-1629.93621	-1901.32039	1350.30907	1
27357	C	64.44239	100.20423	57.75271	-576.61342	-329.78069	-463.01011	1
27358	O	65.24214	100.08361	58.67294	-238.96285	209.77551	495.53168	1
27359	O	64.63407	100.93426	56.57114	232.21765	197.70878	419.22716	1
27360	C	61.94899	96.95590	56.32181	339.05332	-307.62035	-103.07817	1
27361	O	62.58192	96.68879	55.30839	-65.11166	242.54330	343.94936	1
27362	N	61.98365	96.25821	57.47532	-385.04173	54.68295	477.76583	1
27363	H	61.27292	96.59870	58.13923	272.27842	771.72105	1377.58006	1
27364	C	62.30478	94.84205	57.29295	-256.36276	150.25203	162.81083	1
27365	H	62.11466	94.57963	56.21530	-1291.04698	415.16344	-1233.71910	1
27366	H	61.61493	94.27141	57.95005	380.90484	-1834.61783	1364.06344	1
27367	C	63.85174	94.64847	57.54530	665.67957	671.50643	-228.24625	1
27368	O	64.20696	93.49086	57.91644	557.38900	-35.98427	415.55234	1
27369	N	64.69034	95.71555	57.38763	-943.50101	-164.26427	536.84470	1
27370	H	64.12446	96.44875	56.90953	888.03099	2257.73858	1995.48658	1
27371	C	65.78903	95.89646	58.33909	838.98336	-236.75818	504.51230	1
27372	H	66.14827	94.82601	58.57252	-1407.71303	649.82461	-2371.37603	1
27373	C	66.91952	96.70886	57.78221	-124.15470	-96.86912	-498.65822	1
27374	H	66.46157	97.69089	57.51162	-563.93077	-2437.25687	-604.22076	1
27375	C	68.01097	97.24908	58.71656	67.61415	137.30774	54.26577	1
27376	H	67.67942	98.17765	59.32974	1137.79354	565.06887	1321.39728	1
27377	H	68.98466	97.41271	58.16588	816.47410	1192.08505	232.55993	1
27378	H	68.26596	96.53791	59.53464	-1996.86414	-716.65410	136.88505	1
27379	C	67.67264	96.01671	56.66362	856.69011	35.33764	-60.97192	1
27380	H	67.80382	94.89918	56.88595	927.68628	-2297.06562	1297.24378	1
27381	H	68.71848	96.37010	56.50394	1958.41266	50.27662	-1840.57427	1
27382	C	66.84519	96.35829	55.34179	413.51732	305.03268	-205.93044	1
27383	H	67.16934	95.68980	54.45469	-752.67458	-2028.42053	829.57944	1
27384	H	67.04320	97.45887	55.13384	-876.13005	-3055.43762	660.85391	1
27385	H	65.70197	96.16617	55.39397	778.95555	-2348.47632	1933.45130	1
27386	C	65.40638	96.52613	59.84019	432.90416	-117.39365	195.48026	1
27387	O	66.23465	96.66902	60.71128	439.06534	162.80042	-165.65715	1
27388	N	64.09046	96.85281	59.82858	973.96130	-854.07216	-548.98415	1
27389	H	63.56412	96.58449	59.00860	45.73217	-790.14428	1251.14235	1
27390	C	63.52261	97.25889	61.11781	-975.81455	107.98848	-149.24664	1
27391	H	64.30663	97.93822	61.50817	695.09684	-1643.30687	382.44087	1
27392	C	62.20131	98.05061	60.85604	512.40910	760.99619	874.80041	1
27393	H	61.89491	98.41784	61.83295	-298.57684	-3015.13255	-1204.04103	1

27394	H	62.40206	98.97093	60.26926	367.64825	1893.75731	511.59865	1
27395	O	60.97327	97.37909	60.16409	-269.88069	-267.64247	609.84134	1
27396	H	60.31939	97.49498	60.85303	-414.02405	-2203.22157	1950.22292	1
27397	C	63.33525	96.04773	62.16936	-107.55504	704.87887	-1248.35683	1
27398	O	63.21031	96.11896	63.39932	173.42926	-140.14576	195.93924	1
27399	N	63.07982	94.96328	61.41718	-386.99728	6.14206	711.85412	1
27400	H	63.66037	95.10062	60.56890	-2513.59844	262.93059	-571.74591	1
27401	C	62.80869	93.63339	61.79551	730.29051	-425.67784	-375.75323	1
27402	H	63.19098	92.90241	60.97935	581.98120	917.63575	-1485.37579	1
27403	C	63.58033	93.34189	63.17015	199.29655	377.44038	113.34335	1
27404	H	63.42889	94.16397	63.89169	676.35224	1432.55759	688.85595	1
27405	C	63.13159	91.97888	63.83415	142.03138	-685.25507	798.22513	1
27406	H	63.55846	91.83413	64.91846	-1852.30099	-491.14193	-731.46553	1
27407	H	62.03722	91.94034	63.93890	2223.81520	989.22035	-1022.13541	1
27408	H	63.36792	91.11021	63.25466	272.31634	-2703.95446	2484.24909	1
27409	C	65.11510	92.93565	62.96667	-838.85351	-536.69233	712.54879	1
27410	H	65.14505	92.29262	62.08373	2785.14254	1582.16731	181.98432	1
27411	H	65.52593	92.42422	63.86412	727.21214	1658.05388	2488.50096	1
27412	C	65.82959	94.20935	62.44835	1762.36466	-391.85899	-1030.94925	1
27413	H	65.40474	94.60197	61.41247	-1281.04059	-2588.49885	1950.91718	1
27414	H	65.57122	94.94447	63.27601	2480.19761	826.07261	1043.37373	1
27415	H	66.96319	94.24281	62.27586	-222.06256	1941.64329	39.77507	1
27416	C	61.20197	93.46798	62.12841	352.63826	444.68963	44.76667	1
27417	O	60.48140	92.82851	61.37652	3.17021	-692.61759	-169.28677	1
27418	N	60.84617	94.02153	63.30736	-158.44428	-310.27800	8.82672	1
27419	H	61.51682	94.65739	63.76297	0.06581	3521.40151	-17.62877	1
27420	C	59.47213	94.24582	63.53146	-134.90599	-532.27502	353.25048	1
27421	H	58.89411	93.36886	63.11649	1314.01374	-2883.07375	138.18612	1
27422	C	59.15659	94.63796	65.06681	-722.55980	-332.86256	1434.85925	1
27423	H	59.11228	95.77718	65.05600	-238.17492	-759.25451	1426.60252	1
27424	H	60.03686	94.21445	65.67039	2451.89923	1578.39567	1299.06414	1
27425	C	57.84287	94.31614	65.76442	-48.94270	-238.58598	421.40903	1
27426	C	57.33096	92.96164	65.88581	920.62983	11.61425	369.99068	1
27427	H	57.94619	92.15364	65.44052	-896.43915	-2394.36749	-589.10971	1
27428	C	55.95009	92.76528	66.18955	-973.74614	150.53031	-900.44944	1
27429	H	55.55349	91.74136	66.10587	-969.01815	-233.17376	350.91611	1
27430	C	55.18102	93.85784	66.63208	1302.73046	-801.68459	-79.60416	1
27431	O	53.84822	93.68527	67.01986	513.74526	810.36864	-479.38343	1
27432	H	53.73845	92.72991	67.14139	2389.20555	-580.45487	-2059.82187	1
27433	C	57.00500	95.40132	66.19430	-1157.90132	-130.96347	-466.50571	1
27434	H	57.47406	96.37937	66.10587	-863.81718	1638.80912	1172.70623	1
27435	C	55.73725	95.17354	66.65823	-601.19008	235.49415	-1134.82887	1
27436	H	55.14206	96.04131	66.99146	-749.77417	1581.78423	-1908.76264	1
27437	C	59.15787	95.63096	62.75896	-338.48172	1036.85071	530.45681	1
27438	O	58.16072	95.74896	62.05686	121.94000	465.36202	936.49152	1
27439	N	60.00201	96.62075	63.04480	725.17539	-955.29523	448.94573	1
27440	H	60.82281	96.27008	63.58040	967.92479	-718.84485	1701.73994	1
27441	C	59.72624	98.03147	63.22581	-556.42046	-602.21134	-537.17850	1
27442	H	60.59033	98.62857	62.85763	851.22731	-6.73694	1020.00079	1
27443	C	58.29354	98.47697	62.90838	182.97329	-660.58202	-22.67783	1
27444	H	57.46436	97.85563	63.36532	-2096.65786	737.97975	1074.05465	1
27445	O	57.88567	98.21359	61.40446	-323.80136	747.97949	318.03008	1
27446	H	58.19839	97.31225	61.29527	1923.96986	2292.04882	-2524.03878	1
27447	C	58.12106	99.97444	63.17638	1026.09326	510.25566	-1101.74271	1
27448	H	58.37274	100.18363	64.29834	2800.01145	32.07560	3029.35397	1
27449	H	58.88264	100.56665	62.62921	662.92992	-2103.04040	2674.30133	1
27450	H	57.05444	100.33753	62.97694	964.24341	-278.05074	3334.01694	1
27451	C	59.82819	98.20092	64.92355	-360.94615	-369.33659	277.60833	1
27452	O	58.74855	98.02904	65.52113	-285.53464	-159.50482	-326.98798	1
27453	N	60.95879	98.69166	65.30960	-395.04506	208.17867	649.44863	1
27454	H	61.64016	98.80913	64.58553	993.63212	2031.55949	72.00047	1
27455	C	61.12637	99.45292	66.52560	1156.11402	-420.46343	826.98264	1

27456	H	60.55617	98.91145	67.23971	-1943.89326	-750.32719	208.68890	1
27457	C	62.69823	99.71819	66.95796	-95.92796	-148.06102	-258.94289	1
27458	H	62.78108	100.07676	68.04910	1083.22949	205.12219	-1763.63080	1
27459	H	63.20130	98.66439	66.85665	3339.08538	1186.79885	-2285.15101	1
27460	O	63.32629	100.91922	66.35275	-125.39473	-539.02174	-250.30686	1
27461	H	63.17854	101.54025	67.07231	675.98476	1696.18494	-2596.35745	1
27462	C	60.54720	100.89199	66.20759	-303.67101	644.20945	10.93313	1
27463	O	60.33098	101.34683	65.10532	-467.79830	93.24809	231.35954	1
27464	N	60.34794	101.46474	67.42058	-538.92228	344.19105	-726.49763	1
27465	H	60.19592	100.77685	68.21864	-4658.96832	-1196.15326	41.74528	1
27466	C	59.54137	102.70384	67.57628	453.44347	580.42898	-1669.14722	1
27467	H	58.61156	102.27703	67.14358	-2275.26415	-3504.36177	-443.83204	1
27468	C	59.44491	102.99145	69.07875	-391.92154	865.27714	-250.26989	1
27469	H	58.79767	103.86594	69.24009	91.75915	202.90248	1268.48113	1
27470	H	60.42053	103.40000	69.47141	-2338.72835	-465.48887	-949.43949	1
27471	C	58.86104	101.73783	69.88902	67.10442	172.57570	-37.83967	1
27472	O	58.17434	101.96849	70.86663	-69.89069	188.38432	261.50696	1
27473	O	59.08854	100.54463	69.46715	-42.03242	553.28577	-398.00371	1
27474	C	60.02548	103.99483	66.65291	95.24854	-913.35529	-520.00746	1
27475	O	59.27603	104.87406	66.31047	-890.10473	75.58527	-147.88990	1
27476	N	61.36334	103.96581	66.60447	501.01913	279.14011	-15.08164	1
27477	H	61.92868	103.19109	67.03619	2645.87577	-3282.07524	943.43993	1
27478	C	62.01001	104.89051	65.76488	139.57832	-18.19336	-273.23789	1
27479	H	61.20239	105.52655	65.30494	1216.97260	723.79783	-528.05763	1
27480	C	63.01924	105.73504	66.68287	790.47951	229.35307	-452.61236	1
27481	H	62.47392	106.43959	67.30339	-1638.63748	40.33434	89.77868	1
27482	H	63.54936	106.30615	65.90177	838.11398	-1622.70994	192.03501	1
27483	C	63.96795	104.84607	67.50350	94.69847	323.66110	-224.89426	1
27484	O	63.73450	103.64002	67.69048	258.79406	493.49716	-53.01587	1
27485	N	65.21103	105.48981	67.64683	686.95071	-238.45382	498.90890	1
27486	H	66.06175	104.99088	67.97616	3498.52040	1772.14804	-433.48655	1
27487	H	65.40824	106.49849	67.65375	913.82090	-1268.60799	-1941.74576	1
27488	C	62.87061	104.17582	64.58239	-1190.54851	-570.44258	-503.11954	1
27489	O	63.75974	104.90296	64.11691	381.19051	29.10440	-458.14414	1
27490	N	62.43362	103.01770	64.19387	251.26802	285.20818	-939.49094	1
27491	H	61.73849	102.46318	64.72860	-2733.27123	-231.53084	53.54857	1
27492	C	63.30348	102.38619	63.24091	-584.32311	-176.71679	-251.36220	1
27493	H	64.30060	102.66509	63.53554	-37.25588	109.60759	1252.67964	1
27494	C	62.98548	100.85529	63.31372	618.07649	20.82617	21.65291	1
27495	H	62.80290	100.54767	64.40505	-1085.77292	1271.20730	2788.01866	1
27496	H	62.08262	100.52217	62.74538	1190.37143	373.79723	5292.72956	1
27497	C	64.22192	100.12631	62.72657	132.98820	-86.02102	156.11491	1
27498	C	65.08799	100.52648	61.64749	-892.70284	187.38838	14.55031	1
27499	H	64.80260	101.27769	60.88643	-3533.58294	2961.81080	1439.97501	1
27500	C	66.40730	99.98161	61.65642	-37.37695	421.47089	-110.51479	1
27501	H	67.04196	100.29402	60.84541	425.63478	-1249.35562	-786.93588	1
27502	C	66.87486	99.00874	62.57008	-636.50803	154.03008	-354.45449	1
27503	O	68.23472	98.55244	62.57669	-703.34731	20.08629	-444.35482	1
27504	H	68.81869	99.35069	62.59707	-3193.98058	-827.14245	1432.18976	1
27505	C	64.67695	98.98018	63.44026	360.34557	-10.78063	440.62829	1
27506	H	63.98305	98.49074	64.17301	1634.51905	-698.36153	1823.20161	1
27507	C	65.92398	98.39216	63.37728	-140.56791	507.71861	33.60724	1
27508	H	66.28020	97.52171	64.01249	1087.86601	-931.37523	-2083.43329	1
27509	C	62.98793	102.98559	61.74260	-450.12780	830.88066	674.00304	1
27510	O	63.85544	103.17805	60.92300	-310.71077	-139.14906	131.48981	1
27511	N	61.68659	103.15770	61.61471	83.40986	-328.48047	863.97421	1
27512	H	61.07738	103.05367	62.43835	1812.04954	-1946.54652	-2683.18687	1
27513	C	61.07029	103.54653	60.39261	-715.62265	-225.53368	290.10262	1
27514	H	61.99266	103.59427	59.83342	-1177.51190	1999.17862	4190.33347	1
27515	C	60.09939	102.41002	59.84414	373.51195	276.45041	889.08190	1
27516	H	59.42876	102.45865	60.74371	3296.90272	321.74699	356.00724	1
27517	O	60.62611	101.13805	59.48124	8.81012	242.36330	-99.51536	1

27518	H	60.32639	100.59307	60.25654	2221.77736	1537.60090	-60.95838	1
27519	C	59.38923	103.15418	58.65809	-189.01865	448.53529	951.02184	1
27520	H	60.09093	103.68146	57.89833	110.84116	1862.17306	-554.59230	1
27521	H	58.67504	103.92069	59.11233	-2338.87366	2290.50079	1558.66994	1
27522	H	58.84994	102.37111	58.05762	1480.25065	5444.98257	1960.16341	1
27523	C	60.38859	104.99348	60.79791	477.35664	-507.14817	388.39016	1
27524	O	59.19705	105.15127	60.78780	352.90294	70.91248	-103.20221	1
27525	N	61.42208	105.83830	60.98393	-780.40559	28.76172	319.76036	1
27526	H	62.33393	105.40240	61.01486	-410.01932	-1931.83804	2909.46328	1
27527	C	61.33505	107.13295	61.58598	-621.09049	-87.74697	567.56631	1
27528	H	60.61132	107.82918	61.09880	-1594.03434	295.09401	-1006.46991	1
27529	C	60.85407	106.89689	63.08004	-40.31486	485.05383	200.88366	1
27530	H	60.94432	105.87095	63.47235	-3860.15489	3600.49066	-627.75077	1
27531	H	61.35165	107.63818	63.73524	3605.86055	-1736.08610	111.53335	1
27532	C	59.34731	107.23636	62.90082	217.15978	341.43735	-765.93324	1
27533	H	58.88791	106.71262	61.99355	-2130.71131	-2243.13424	672.01326	1
27534	H	58.83335	106.74300	63.73416	749.31484	82.13135	-829.90380	1
27535	C	58.90229	108.82747	62.81468	-689.64429	725.77995	378.79114	1
27536	O	57.72648	109.08058	62.90729	121.38360	-425.43291	395.58262	1
27537	O	59.83867	109.56342	62.43930	-159.68404	570.20102	554.10430	1
27538	C	62.78729	107.89315	61.73675	-626.60334	-81.90946	-70.02929	1
27539	O	63.84278	107.37083	61.55272	293.36709	374.82498	-659.78524	1
27540	N	62.49480	109.12676	62.15069	134.83385	485.73266	499.65953	1
27541	H	61.54348	109.46140	61.88923	774.93538	-1031.23249	1462.87748	1
27542	C	63.52176	109.70845	63.02394	-414.30374	143.07157	-797.90657	1
27543	H	64.47941	109.71073	62.48620	2577.19530	-817.92377	1683.69584	1
27544	C	63.04676	111.21351	63.23136	-352.40122	-217.04860	-206.96424	1
27545	H	61.92200	111.13070	63.24400	-3936.71469	-434.67940	-540.42601	1
27546	H	63.25745	111.85491	62.28265	1480.76594	-2397.33392	-893.52785	1
27547	C	63.62421	111.85566	64.50171	584.27051	16.87414	-9.58048	1
27548	H	63.07732	112.70064	65.01548	1873.19125	444.18595	330.28681	1
27549	H	63.61327	111.01529	65.25717	-1266.49352	-314.96222	-2844.17439	1
27550	C	65.21118	112.42110	64.09968	649.83735	258.34675	346.47738	1
27551	O	65.30432	113.66057	63.88836	888.77942	-788.13281	-59.55699	1
27552	O	66.08286	111.57721	63.92659	-354.93047	-256.74499	-568.52097	1
27553	C	63.81718	108.87925	64.37061	503.34361	160.39647	-101.01292	1
27554	O	62.88673	108.31053	64.91747	-152.00592	-312.08504	478.23051	1
27555	N	65.03478	109.20567	64.86718	291.49763	-776.01023	-102.85939	1
27556	H	65.59001	109.81467	64.26869	1469.88412	-1284.81542	-84.31721	1
27557	C	65.78046	108.12335	65.46294	-214.64465	56.09512	140.88516	1
27558	H	65.02788	107.52435	65.94286	-1357.46492	299.63849	1513.23903	1
27559	C	66.38254	107.26399	64.26858	-205.17874	-1141.12594	20.90700	1
27560	H	65.65918	107.21641	63.40578	683.32875	920.95889	4630.76559	1
27561	H	67.27180	107.78093	63.82479	-1448.25347	-426.77856	4495.70038	1
27562	C	66.69950	105.79570	64.61248	-314.88156	444.22323	-591.87029	1
27563	H	65.80086	105.31174	65.06752	1228.43055	-4542.02615	2246.60399	1
27564	H	67.51310	105.80009	65.44473	-725.06547	-2837.91594	-7.42884	1
27565	S	67.29137	105.24996	62.94487	-231.26847	196.84101	-362.73500	1
27566	C	65.69167	105.42657	61.91040	79.09870	32.27219	301.56426	1
27567	H	65.64290	106.39274	61.25873	1557.54404	921.18119	-935.17262	1
27568	H	64.75731	105.48085	62.57678	-391.45313	1267.95927	-1211.14256	1
27569	H	65.52925	104.77673	61.05814	1627.62937	368.11406	178.75154	1
27570	C	67.04703	108.67498	66.33997	273.03484	484.13819	-401.21201	1
27571	O	67.00876	108.36322	67.51118	97.35977	-98.97455	-267.36347	1
27572	N	67.89128	109.50376	65.72092	148.70620	-471.13182	380.52334	1
27573	H	67.63665	109.85521	64.78940	-230.44712	-823.06740	749.44765	1
27574	C	68.93010	110.14013	66.47588	-50.38600	1090.82217	955.34078	1
27575	H	68.85571	111.26717	66.34672	-486.94086	3223.52077	-694.02976	1
27576	H	68.64501	109.88327	67.50625	-373.63719	-223.73014	3053.95904	1
27577	C	70.43341	109.66198	65.98486	-130.51819	1.98520	595.89741	1
27578	O	71.41591	109.95805	66.62177	218.49804	-339.43749	112.49189	1
27579	N	70.38921	109.08106	64.74005	386.30944	-200.40190	-419.52899	1

27580	H	69.46931	109.43979	64.38708	2365.24080	-1794.95550	-2190.17364	1
27581	C	70.39730	107.61342	64.70388	888.82692	-302.38806	127.27122	1
27582	H	69.62275	107.31782	65.42144	1945.48970	-823.24380	248.18720	1
27583	C	69.97281	107.20003	63.23152	-220.97712	530.26802	255.66956	1
27584	H	70.74593	107.53996	62.51368	2481.86928	-3570.12615	2553.53076	1
27585	H	69.95592	106.10516	63.11556	1388.23535	286.72610	-1260.53443	1
27586	O	68.88460	107.89964	62.52020	698.55035	744.68494	-159.90132	1
27587	H	68.29905	107.02116	62.33051	-868.76946	-2914.32541	-2135.14203	1
27588	C	71.84638	107.15161	65.14041	-362.93014	294.64800	-212.38341	1
27589	O	72.85823	107.70524	64.79197	226.56449	-56.13430	107.16415	1
27590	N	71.73378	105.93276	65.74629	72.23076	19.89212	877.88286	1
27591	H	70.83260	105.38329	65.91480	208.20998	2067.65387	779.53096	1
27592	C	73.03296	105.24379	65.94802	264.47329	-927.62190	118.41536	1
27593	H	73.72378	105.56776	65.14338	-1908.78538	-619.21173	-1023.88199	1
27594	H	73.36745	105.88288	66.83123	2100.95959	2403.37726	2513.86677	1
27595	C	72.80362	103.70915	66.12909	-480.39063	206.76901	403.40399	1
27596	O	71.71975	103.19626	66.15360	-776.11277	-168.22527	118.20391	1
27597	N	74.06756	103.14816	66.09391	328.03071	187.34677	-856.65269	1
27598	H	74.91306	103.75802	66.30106	96.48166	512.61071	1603.66050	1
27599	C	74.12172	101.78401	66.59805	218.49075	-571.99521	-668.34127	1
27600	H	73.17550	101.25533	66.25073	1927.18911	2662.00909	-1443.15836	1
27601	C	75.35905	101.06274	66.05433	-284.16525	-526.17303	119.58866	1
27602	H	75.51687	100.17416	66.68470	668.49145	-2247.84057	-360.85955	1
27603	H	76.32860	101.66235	66.20348	-778.99395	348.42006	324.10695	1
27604	C	75.06374	100.77460	64.47101	-614.05674	55.44362	633.42619	1
27605	O	76.00907	100.57883	63.69379	-274.65411	493.82418	413.13508	1
27606	O	73.89453	100.66342	64.18494	-76.44283	-199.33552	-304.40710	1
27607	C	74.13424	101.63093	68.25534	-32.01186	608.74474	-555.31373	1
27608	O	74.09199	100.52061	68.74017	379.08146	-35.01971	-360.89033	1
27609	N	74.53262	102.71392	68.93643	-88.69881	-539.27301	-231.13332	1
27610	H	74.56860	103.48247	68.24418	-4226.71136	2046.21713	-930.72712	1
27611	C	73.87585	102.92861	70.20251	-288.33496	-186.96562	-94.03623	1
27612	H	73.86034	101.85936	70.53595	-2285.88611	600.28537	660.65464	1
27613	C	74.64320	103.98812	71.11459	706.31911	-441.36690	-422.20644	1
27614	H	74.13956	104.18490	72.04517	-1134.71888	-1743.28699	-1618.29108	1
27615	H	74.83322	104.90198	70.56436	-1129.31256	1859.44426	-3723.21672	1
27616	C	75.99203	103.40244	71.68236	-200.84019	-146.17280	-616.13866	1
27617	C	76.07984	101.99309	71.87695	-87.53135	-513.56102	-764.07994	1
27618	H	75.29962	101.20009	71.62510	2050.18526	1777.68349	-4258.01178	1
27619	C	77.26188	101.60088	72.50850	682.88568	-85.31812	76.69527	1
27620	H	77.31927	100.51703	72.83062	670.96256	-3223.45233	47.92951	1
27621	C	78.31619	102.47831	72.86029	250.66719	-171.83556	880.25141	1
27622	O	79.43364	101.94048	73.55728	56.66098	178.47414	-1090.19632	1
27623	H	79.30450	100.89191	73.36909	-2412.15863	-193.41422	-1115.86199	1
27624	C	77.10303	104.28495	71.82871	-267.08562	-409.54277	-397.39178	1
27625	H	77.01909	105.39620	71.54749	-102.16545	350.29973	-1820.36300	1
27626	C	78.32953	103.77604	72.30199	-140.32924	227.69004	-206.33790	1
27627	H	79.18437	104.40559	72.49534	1117.56587	2553.39295	-1655.89301	1
27628	C	72.38887	103.52532	69.86608	-586.83371	-557.53834	-256.71338	1
27629	O	72.31022	104.77237	69.83914	457.25002	303.96276	611.99810	1
27630	N	71.42576	102.69672	69.64309	-185.68759	-473.62676	-657.45568	1
27631	H	71.67212	101.68671	69.53899	523.29513	287.96655	-533.86281	1
27632	C	70.07614	103.11636	69.52109	19.98506	70.15222	-12.71929	1
27633	H	69.91606	103.83246	70.34466	-986.96593	2041.50974	-1107.34422	1
27634	C	70.05163	103.70117	68.06738	-175.02775	-871.87974	105.14660	1
27635	H	70.89348	104.40890	67.99166	-784.31735	637.90294	1116.35198	1
27636	H	70.18199	102.83513	67.31010	-120.66136	-1169.53511	2425.44861	1
27637	C	68.75119	104.47008	67.66167	-185.18033	217.64341	-836.50951	1
27638	O	68.87751	105.20574	66.62363	379.64504	13.47381	2.29914	1
27639	O	67.61678	104.15904	68.08395	-1337.02779	546.66957	-767.11372	1
27640	C	69.26427	101.70360	69.81551	892.42279	767.39754	672.39013	1
27641	O	69.74031	100.60689	69.69243	512.45784	-683.85143	333.88159	1

27642	N	68.00711	102.01560	70.05620	433.85611	-1051.68528	562.14622	1
27643	H	67.80913	103.00788	69.90693	-340.41634	1363.77327	251.01077	1
27644	C	67.04710	101.19661	70.73761	-1252.13700	553.34480	802.23831	1
27645	H	67.66988	100.68320	71.52461	3124.35099	-1053.98323	-1685.71850	1
27646	C	65.89558	102.07649	71.27538	-402.69073	-183.36714	-239.01036	1
27647	H	65.51877	102.64844	70.45610	-1029.35888	-214.02369	2371.22842	1
27648	H	66.34210	102.85741	71.89127	1897.58146	-2742.86283	-3282.72814	1
27649	O	64.77695	101.35692	71.99035	-101.81684	399.70746	199.25586	1
27650	H	64.63290	100.62749	71.25053	-832.98419	1974.85276	792.47988	1
27651	C	66.32907	100.11639	69.74980	-138.83876	328.14624	109.11219	1
27652	O	65.12563	99.78206	69.86645	292.89187	317.90996	646.47527	1
27653	N	67.19877	99.62486	68.90001	527.97704	771.38349	-359.86606	1
27654	H	68.17925	99.90749	68.73205	-706.06908	-283.96809	-742.32701	1
27655	C	66.61494	98.71610	67.93810	382.68449	-130.60548	-731.77460	1
27656	H	65.61886	98.31512	68.24538	-638.37300	223.68465	1408.89791	1
27657	C	66.20927	99.50721	66.55274	-296.64027	661.42514	27.71497	1
27658	H	65.80885	98.75588	65.80492	-2538.51987	-1847.47989	-2032.46209	1
27659	H	65.44550	100.34970	66.72082	-1103.30489	-93.63865	-507.96715	1
27660	C	67.49611	100.11850	65.98003	86.50458	-1416.38965	50.83517	1
27661	H	67.98406	100.65828	66.86865	-1000.25118	-1814.66652	1108.30599	1
27662	H	68.30654	99.37115	65.68741	582.49469	3372.41900	-206.87016	1
27663	S	66.80207	101.07338	64.56511	223.20621	-170.74110	-273.51996	1
27664	C	66.22978	102.69758	65.36095	440.48687	-563.35539	-528.29040	1
27665	H	66.13052	103.54150	64.59308	-655.11317	2091.04234	2923.25903	1
27666	H	65.31101	102.68604	65.99605	1879.16581	-1132.79672	-1339.19170	1
27667	H	66.93059	103.03584	66.10183	-929.45657	800.71780	-3213.68109	1
27668	C	67.70262	97.65452	67.41647	-811.79940	-121.38767	-1032.62036	1
27669	O	68.93488	97.84738	67.37281	-50.02103	218.53927	107.02050	1
27670	N	67.01960	96.63738	66.98501	958.00426	113.70032	-452.31529	1
27671	H	66.01752	96.69937	67.11121	1012.81653	779.45055	-103.98149	1
27672	C	67.70375	95.35885	66.74478	321.51590	-20.85527	155.06359	1
27673	H	68.51263	95.30597	67.47827	1227.42758	-134.04882	-1417.67526	1
27674	C	66.58909	94.25105	66.80500	-397.12270	207.77095	553.27305	1
27675	H	65.69237	94.60869	66.21805	-134.76771	-388.54196	1890.39088	1
27676	H	66.91301	93.35210	66.26347	1693.50830	2008.29503	853.09863	1
27677	C	66.32341	93.98561	68.33802	850.81681	-774.22865	198.11195	1
27678	H	65.34422	93.44477	68.55589	-2261.44108	-3013.38021	-1404.49237	1
27679	H	66.39113	94.95734	68.94488	722.00825	1378.89471	-3716.34540	1
27680	C	67.51649	92.98932	68.70434	164.51443	-261.27940	-31.16714	1
27681	H	68.51659	93.36422	68.44542	1068.50648	-655.19001	-1772.56852	1
27682	H	67.41286	92.01687	68.11932	894.74682	-4011.99179	2056.76416	1
27683	C	67.61449	92.82741	70.26287	245.81773	168.38060	726.01760	1
27684	H	68.13397	91.92959	70.67381	856.25981	1067.74741	-2008.35420	1
27685	H	66.64268	93.00259	70.83361	-677.52176	-741.39795	-1658.16526	1
27686	N	68.63327	93.84394	70.77127	91.36634	-193.75125	84.21187	1
27687	H	68.86485	93.79166	71.80876	-1294.96255	-2444.03791	2634.65693	1
27688	H	69.71043	93.81487	70.25559	864.26321	5.01119	-1820.40307	1
27689	H	68.32566	94.92366	70.66707	670.41849	-909.44157	663.54086	1
27690	C	68.05109	95.52278	65.17227	440.60197	67.55067	429.70480	1
27691	O	67.44836	94.97888	64.30612	-173.44064	129.77826	333.58281	1
27692	N	69.19689	96.29555	65.15792	184.07508	662.43505	279.18571	1
27693	H	69.44004	96.89880	65.98848	-274.40895	-1276.26445	902.92225	1
27694	C	70.24240	95.93739	64.25560	237.20385	-487.23353	-472.46221	1
27695	H	70.44631	94.85855	64.33193	-2404.80900	1777.68893	-958.90601	1
27696	C	69.82448	96.30984	62.76939	272.73107	-284.96042	131.30754	1
27697	H	68.72733	96.13609	62.57509	1816.94507	1018.75519	761.49759	1
27698	H	69.91438	97.44876	62.55637	2272.32151	-1243.74826	-3870.00143	1
27699	C	70.73092	95.43596	61.90065	338.24360	128.72607	61.11215	1
27700	H	70.58829	94.31981	62.07847	-2572.21172	2500.68716	-337.84238	1
27701	H	71.78902	95.54632	62.14779	1088.95089	-479.23816	2557.13880	1
27702	C	70.41667	95.94673	60.35037	-11.95395	183.59999	-451.39570	1
27703	O	70.36445	95.18677	59.37231	523.55684	-392.98853	-113.46025	1

27704	O	70.44258	97.18043	60.19760	-357.31826	170.97641	560.50672	1
27705	C	71.57042	96.70814	64.80777	-653.81217	545.26736	-47.87465	1
27706	O	72.59817	96.11320	64.50389	-933.51113	282.95239	-635.98504	1
27707	N	71.45843	97.91236	65.32339	-57.15767	-731.57857	-289.19932	1
27708	C	70.61719	98.93555	64.69489	-838.05530	588.62086	653.24954	1
27709	H	69.63826	98.57264	64.69577	1938.47552	-1174.66204	2937.83007	1
27710	H	71.12097	98.97510	63.67066	754.19052	-1990.14706	2964.88929	1
27711	C	72.30135	98.42885	66.39025	201.40073	-643.40929	-212.33105	1
27712	H	73.20433	98.69957	65.75475	-522.36792	-1898.49963	-3654.97285	1
27713	C	71.38126	99.58638	66.99202	1139.59188	392.00219	-72.92185	1
27714	H	71.91198	100.19313	67.73862	330.33922	3733.79181	-702.85687	1
27715	H	70.52614	99.09229	67.53890	621.14474	-1605.02238	704.43964	1
27716	C	70.82133	100.18851	65.64633	-587.69556	-350.19185	-642.80369	1
27717	H	71.58476	100.82669	65.13040	2040.59791	-3119.15418	-358.89247	1
27718	H	69.93454	100.83076	65.75166	-775.33639	1168.08454	-1602.76520	1
27719	C	72.69337	97.33417	67.49268	-863.69338	369.88324	432.80122	1
27720	O	72.40877	97.56413	68.65935	54.84429	284.37558	628.11059	1
27721	N	73.53575	96.40604	67.04953	643.14977	515.27925	-142.58087	1
27722	H	73.62213	96.28807	66.03708	-2134.90327	1788.18594	-819.45980	1
27723	C	73.63499	95.17073	67.78692	-336.55657	-144.37719	-51.31331	1
27724	H	73.23056	95.41984	68.83784	-1771.61452	2821.32808	1733.80958	1
27725	C	72.79779	94.09237	67.01734	806.72652	-227.84483	-625.76875	1
27726	H	73.01532	94.13230	65.93050	432.77214	3224.05684	-4237.12525	1
27727	H	73.21492	93.10737	66.95472	-331.61758	172.34994	1064.01991	1
27728	S	71.07545	94.12620	67.56200	-147.43729	248.76325	-34.67316	1
27729	C	75.10935	94.48327	67.80117	781.26618	-166.42667	840.08210	1
27730	O	75.09829	93.31966	68.15023	-155.96390	-735.70107	304.84913	1
27731	N	76.14795	95.26980	67.43980	-59.88296	1226.32200	862.36476	1
27732	H	76.08639	96.27877	67.26447	52.00144	-373.06200	-2487.70932	1
27733	C	77.39129	94.79208	67.95508	-100.80205	-487.86537	640.51235	1
27734	H	77.48347	93.67675	67.66605	603.43968	-690.10476	-2051.05076	1
27735	C	78.52600	95.78193	67.45638	-142.41422	-430.62401	-833.88794	1
27736	H	79.55299	95.46953	67.76515	1258.52569	-1824.33337	1835.35782	1
27737	H	78.46417	96.85336	67.86575	-535.95345	-224.17568	4099.39870	1
27738	C	78.83703	95.83408	65.92973	-180.60528	-618.35993	-527.93225	1
27739	C	79.34909	94.76803	65.17347	-1109.10605	866.80233	-859.99417	1
27740	H	79.74901	93.89457	65.63810	-1408.11142	-3002.50407	2225.05034	1
27741	C	79.53174	94.96803	63.74226	467.14897	-166.75109	27.60598	1
27742	H	79.90735	94.12334	63.12493	-4618.33396	-2625.63671	2670.28756	1
27743	C	79.16430	96.20959	63.15229	644.46876	-173.62118	-321.19488	1
27744	H	79.35444	96.30842	62.07927	1198.21706	866.67432	2512.29350	1
27745	C	78.36625	97.00707	65.28022	3.29699	-157.41499	-336.33865	1
27746	H	77.81011	97.75056	65.93684	-91.81161	-118.65545	-744.01480	1
27747	C	78.61900	97.28428	63.91473	744.10312	573.14988	-676.73983	1
27748	H	78.26461	98.20970	63.41709	-1732.02786	-4112.84275	-42.85322	1
27749	C	77.37170	94.98509	69.62186	434.19397	462.17277	-627.56704	1
27750	O	77.25099	96.10464	70.10644	-1.27586	-399.28840	-535.57170	1
27751	N	77.66755	93.89550	70.28477	-309.72671	-49.02226	534.90503	1
27752	H	77.69643	93.12668	69.61112	2221.85827	1271.74432	1214.29882	1
27753	C	77.26318	93.75701	71.66453	427.60906	-414.20201	-607.45976	1
27754	H	76.54755	94.57806	71.77969	552.45828	4220.11714	-1580.46366	1
27755	C	76.58031	92.28980	71.84728	170.32943	333.92606	973.80602	1
27756	H	77.29952	91.51595	71.94213	-2977.97108	1793.65702	451.37123	1
27757	H	76.06151	92.02138	70.97104	671.15601	-1435.58213	-1689.01131	1
27758	C	75.72325	92.46418	73.11821	-697.49370	-524.06698	-357.10651	1
27759	H	76.32744	92.34976	74.01537	768.73194	1732.48949	457.59123	1
27760	H	75.41396	93.48952	73.26796	2652.92247	-1458.71520	-2668.46111	1
27761	C	74.42755	91.48726	72.92468	167.61277	228.27256	-493.48676	1
27762	H	74.65839	90.33396	72.93512	-2650.05357	2264.00922	2957.24902	1
27763	H	74.04408	91.74369	71.91862	3252.96295	-1363.42946	209.13287	1
27764	N	73.36596	91.90762	73.82418	-255.26887	-483.75342	-105.36239	1
27765	H	73.56098	92.54774	74.55473	-2345.04220	1100.74730	2588.42451	1

27766	C	72.12432	91.50145	73.78486	-9.57763	-193.95218	1258.51635	1
27767	N	71.61138	90.60692	72.81306	-887.79015	-330.23152	292.48400	1
27768	H	72.21967	90.39779	72.00961	-1140.19612	-1002.87676	-1549.89702	1
27769	H	70.61036	90.24869	72.69433	-3016.21990	-1071.27735	-58.55007	1
27770	N	71.28915	92.05837	74.78694	372.58092	647.21404	-275.40421	1
27771	H	71.67923	92.44906	75.66335	-1298.62020	911.32007	1655.55456	1
27772	H	70.38531	91.61024	75.03361	2475.73454	-1857.27760	1756.53534	1
27773	C	78.48054	93.86318	72.67045	524.09933	1007.27951	-561.25486	1
27774	O	78.27891	93.41916	73.82263	192.47672	153.80353	-375.99725	1
27775	N	79.62156	94.33812	72.20554	-560.16719	-323.87715	-333.09320	1
27776	H	79.57432	94.72260	71.24160	-387.23516	-3908.01421	48.64927	1
27777	C	80.41340	95.30294	73.00573	637.83199	-495.79331	250.62969	1
27778	H	81.18957	95.52398	72.25527	-1304.39284	-197.38083	-2772.51504	1
27779	C	79.53887	96.61078	73.20941	-423.54517	-696.08744	279.18072	1
27780	H	78.57289	96.41489	73.71120	3104.02381	-886.49988	-5845.83176	1
27781	H	80.12694	97.36441	73.79607	-1180.58524	-2057.31619	-1533.62050	1
27782	C	79.48213	97.27577	71.81063	545.55346	882.22770	-285.76376	1
27783	H	78.65389	96.81996	71.24148	-1366.07730	-632.44699	1162.64634	1
27784	H	80.44268	96.97052	71.33030	-3544.39242	477.30363	-2026.37262	1
27785	C	79.27912	98.85859	71.97293	-74.88382	440.02832	742.39353	1
27786	O	79.23831	99.29871	73.16340	-749.31250	214.15836	1128.80730	1
27787	O	79.11515	99.53886	71.00504	246.11651	-658.16201	-451.96685	1
27788	C	80.95157	94.70686	74.34695	-379.81965	214.65152	14.67682	1
27789	O	81.66461	93.71910	74.27767	519.09017	-372.57892	-1044.22852	1
27790	N	80.42519	95.23791	75.49071	453.83738	410.51854	331.76282	1
27791	H	79.79394	96.06477	75.47629	665.55012	-356.99481	-571.18453	1
27792	C	80.86827	94.64540	76.69654	251.17637	434.54833	-739.63878	1
27793	H	80.66976	93.56317	76.35319	-3497.52727	-3742.42001	2677.35003	1
27794	C	82.40686	95.02248	76.89963	-36.77292	-63.19661	-81.19314	1
27795	H	82.54727	96.07704	77.25257	1466.01514	1179.36940	3447.52834	1
27796	H	82.91565	94.94071	75.92066	-1371.11904	3736.74913	1881.73080	1
27797	C	83.12480	93.98022	77.82072	82.87924	-782.54457	217.21377	1
27798	H	82.85105	94.14172	78.86953	-634.83073	-491.85147	1919.37466	1
27799	H	84.23346	94.05418	77.88253	-609.22713	-2316.06221	-1577.05972	1
27800	C	82.80258	92.40679	77.59800	-417.70427	51.58739	189.23698	1
27801	O	83.47994	91.65887	76.90255	-707.87454	459.78499	151.07140	1
27802	O	81.75979	92.07256	78.19406	-362.66504	758.42600	-622.03507	1
27803	C	80.00366	95.29321	77.91571	-9.29101	70.26927	211.91904	1
27804	O	79.50342	96.39585	77.87500	-109.51075	-202.80190	134.82831	1
27805	N	80.05913	94.47220	78.98763	232.58050	-353.47772	-703.04832	1
27806	H	80.66888	93.65729	78.95487	-368.09452	1350.20709	-1197.21130	1
27807	C	79.61589	95.11820	80.17734	-226.96979	354.98569	-103.62332	1
27808	H	79.18964	96.05899	79.82646	-2817.55579	-1484.87926	3257.41800	1
27809	C	78.63226	94.12093	80.92211	-119.43236	-577.82408	13.64252	1
27810	H	78.95285	93.01925	80.82739	-312.52733	-2459.65930	1089.77081	1
27811	H	77.73553	94.18815	80.30161	-338.52104	-2435.24486	666.19838	1
27812	C	78.49870	94.36794	82.45309	-395.62755	1788.54028	406.45213	1
27813	O	78.07277	95.45092	82.89476	66.77105	-176.26598	266.63016	1
27814	N	78.70334	93.24237	83.18479	-237.62452	-520.19294	53.84649	1
27815	H	79.05618	92.27903	82.91021	-524.17950	-2897.83708	787.41856	1
27816	H	78.45644	93.30851	84.16760	1263.68600	-161.56889	-5.35389	1
27817	C	80.98389	95.19341	81.12386	-703.84443	-182.34947	31.33135	1
27818	O	81.75447	94.27360	81.44492	-295.77536	-582.83805	-18.14091	1
27819	N	81.32140	96.46084	81.25421	-367.00141	847.79726	51.00482	1
27820	H	80.48539	97.01179	80.98379	-1192.79630	78.80588	-564.18844	1
27821	C	82.60421	96.91430	81.67937	-754.63222	-105.57831	146.55241	1
27822	H	83.20810	96.04645	81.29594	937.61976	281.57393	731.15612	1
27823	C	82.67708	98.34299	81.09329	-241.23195	796.13730	-535.86804	1
27824	H	83.44886	98.99827	81.54726	-3497.33186	-967.63374	2722.37833	1
27825	H	82.87237	98.24835	79.96626	1074.25019	3687.06865	-1067.79673	1
27826	H	81.69501	98.92646	81.27963	-134.15954	398.94477	2195.51618	1
27827	C	82.42702	97.03505	83.39403	-132.51321	-776.97113	273.21176	1

27828	O	82.12762	98.09624	83.85170	706.84514	-76.64471	-294.51432	1
27829	N	82.74945	95.86428	83.93527	-3.61627	-314.79326	142.27717	1
27830	H	83.08875	95.19452	83.24964	2652.59298	564.11216	4250.51626	1
27831	C	81.90005	95.28926	84.95089	178.97056	-105.87566	-86.85472	1
27832	H	82.29902	95.73503	85.90338	-3104.58645	-1606.51107	3520.95918	1
27833	C	80.38323	95.58498	84.62967	-77.60620	116.60192	589.03584	1
27834	H	80.11358	95.09603	83.67964	1526.97971	-594.32882	-2578.23717	1
27835	H	80.33572	96.71769	84.32579	-1404.11865	974.15723	3171.83738	1
27836	C	79.49708	95.37421	85.87127	-724.86430	-200.16255	-414.05277	1
27837	O	79.84739	95.22546	87.05143	-200.25081	-401.42985	-533.96151	1
27838	N	78.19772	95.53272	85.47365	372.58514	-130.77679	351.18487	1
27839	H	77.70362	95.72674	84.56343	817.77657	2138.10611	1722.14726	1
27840	H	77.52381	95.23008	86.18470	2815.08061	-1175.83794	2139.04455	1
27841	C	82.09206	93.68300	84.85931	-48.15743	-565.98055	852.84132	1
27842	O	83.10998	93.27957	84.27914	1245.17389	408.40938	-634.16525	1
27843	N	81.23622	92.95830	85.54240	-757.30558	150.14221	-471.23446	1
27844	H	80.57014	93.55691	85.95543	794.69920	-1586.55147	196.87521	1
27845	C	81.59561	91.66893	86.05933	99.50776	275.49749	383.65107	1
27846	H	82.62099	91.82795	86.55978	317.83085	-2551.96813	-399.42931	1
27847	C	80.50641	91.19067	87.11018	152.33992	-20.42896	305.26671	1
27848	H	80.53121	91.87506	88.00435	-2856.98169	1166.84736	-740.77467	1
27849	H	80.84042	90.22114	87.49108	-266.17213	1216.31723	-1399.77209	1
27850	C	79.09613	91.01249	86.54863	35.27235	-423.99642	636.96138	1
27851	C	78.77236	90.83230	85.21379	-633.77465	-502.10302	-55.64670	1
27852	H	79.58915	90.53644	84.45733	-937.98640	3578.08109	-3.24519	1
27853	C	77.42876	90.77413	84.79624	-313.56653	-530.56022	-39.55433	1
27854	H	77.31762	90.65983	83.71552	199.35926	-1525.07609	970.15301	1
27855	C	76.30575	90.89276	85.68093	-145.44032	75.01651	623.95320	1
27856	H	75.29522	90.84269	85.38578	-2681.80244	-844.66685	166.33049	1
27857	C	78.02319	91.22277	87.47523	513.09401	-531.35980	528.84884	1
27858	H	78.24267	91.45560	88.57192	34.52267	-4350.85485	-1057.00841	1
27859	C	76.66657	91.05192	87.06248	-484.11432	34.24063	169.69292	1
27860	H	75.90192	91.18625	87.82803	162.83011	2336.74567	-1924.43500	1
27861	C	81.88007	90.52254	84.95769	560.90834	-53.64512	-357.05097	1
27862	O	82.23374	89.42009	85.37143	5.37113	96.04657	-561.77725	1
27863	N	81.60139	90.90178	83.67839	517.16545	64.53347	-91.05953	1
27864	H	81.52542	91.92612	83.77097	610.41127	-2235.89516	187.71822	1
27865	C	82.28425	90.20308	82.62599	-308.09170	-1313.51506	621.38960	1
27866	H	81.82024	89.21449	82.88396	-247.17268	-2900.32776	-3380.51957	1
27867	C	81.87475	90.79383	81.23050	-163.05613	84.84402	125.76588	1
27868	H	82.42629	90.31748	80.30935	371.94406	-3234.47474	2612.83152	1
27869	H	82.28487	91.85576	81.23469	-1008.15864	-3111.99153	-1270.41009	1
27870	C	80.35115	90.88524	80.96742	-257.84171	-601.72431	-1103.89911	1
27871	O	79.61242	91.08487	81.90555	-71.17593	-1379.49356	160.26937	1
27872	N	79.91492	90.80217	79.67960	-280.85323	-931.91862	-781.34849	1
27873	H	80.59859	90.95821	78.86281	-509.89069	3163.29697	1529.25767	1
27874	H	78.94091	91.09545	79.38745	-2125.19000	-792.61914	-2968.26137	1
27875	C	83.96120	90.21221	82.76626	596.87912	-19.01176	511.29717	1
27876	O	84.52420	89.30887	82.17248	-560.50798	-434.44677	-890.70729	1
27877	N	84.42227	91.09523	83.62220	-415.76605	-1008.44860	261.70297	1
27878	H	83.65893	91.73276	84.08419	2857.88464	45.98811	-59.61674	1
27879	C	85.86654	91.17845	83.85720	111.39564	89.06619	59.69723	1
27880	H	86.35394	90.57203	83.10043	-646.85839	2236.25588	3203.03332	1
27881	C	86.16612	92.69651	83.68239	-1694.38996	61.87300	-361.86219	1
27882	H	87.28304	92.84281	83.73498	-1512.42043	-2274.88065	1302.03247	1
27883	H	85.72878	93.25441	84.46722	-1073.03181	792.82656	1740.82632	1
27884	C	85.53818	93.28561	82.35216	-57.37471	53.98902	599.87314	1
27885	H	84.46818	93.40537	82.48246	1219.91838	4504.12427	3438.69631	1
27886	H	85.55351	92.49810	81.55568	896.67402	1211.40495	-807.13386	1
27887	C	85.99590	94.66559	81.81441	26.53420	-881.27369	-404.56340	1
27888	H	87.07406	94.75382	81.61798	-4775.26757	-560.76265	-905.29727	1
27889	H	85.72855	95.52811	82.54673	3526.66465	399.16757	631.82199	1

27890	C	85.25012	94.80502	80.38865	435.94916	-584.62334	496.76699	1
27891	H	85.77223	94.14859	79.61337	-241.53383	-1419.75881	-1693.91256	1
27892	H	84.17720	94.47970	80.40604	1101.33961	-90.55727	-1004.83268	1
27893	N	85.11623	96.15242	79.87709	457.78345	-42.60522	243.30071	1
27894	H	84.65154	96.38512	78.98972	1940.29293	646.91474	3514.54056	1
27895	H	86.00157	96.64705	79.79334	1787.85642	-1503.17419	-2687.49875	1
27896	H	82.14931	100.46160	79.07780	166.36720	1182.47200	1144.86071	1
27897	C	86.33523	90.74100	85.38394	-293.40600	409.32021	409.98541	1
27898	O	87.50310	90.99016	85.56846	341.02619	-656.09526	-662.00354	1
27899	N	85.33807	90.25681	86.12939	206.58323	-871.98542	734.19152	1
27900	H	84.40218	90.35947	85.70700	567.27487	-3242.51964	1214.34186	1
27901	C	85.53124	90.21997	87.52530	-439.25728	659.25069	-313.58975	1
27902	H	86.64502	90.27557	87.64742	1109.65689	170.52133	-702.63790	1
27903	C	84.76171	91.55092	88.05850	-190.27169	103.39809	-553.61123	1
27904	H	83.69006	91.55100	87.96509	-4321.52336	1014.64712	1282.38544	1
27905	C	84.84599	91.61060	89.62732	-1172.02914	-644.26190	-271.06653	1
27906	H	84.10260	92.38355	89.97462	754.70539	-2407.98759	331.95959	1
27907	H	85.82529	91.98526	89.96845	-164.04906	1133.19301	3065.65914	1
27908	H	84.62518	90.65347	90.10047	823.52918	-5058.10159	-589.37352	1
27909	C	85.49402	92.79703	87.52747	-61.08433	-418.53637	-458.97869	1
27910	H	86.33141	93.12295	88.18532	-3305.62237	1672.47093	2638.05354	1
27911	H	85.92215	92.62067	86.53998	-2143.86849	-161.27229	734.71165	1
27912	C	84.46051	93.98568	87.41303	-223.84969	-516.84925	544.00110	1
27913	H	83.59390	93.75486	86.76267	2598.49385	-4717.11650	460.18362	1
27914	H	84.06910	94.18108	88.47575	1870.57950	792.15935	-805.27474	1
27915	H	84.90820	94.96713	87.01982	229.74432	1151.46800	21.85222	1
27916	C	84.78377	88.95391	88.21514	-680.19064	-6.74133	736.09120	1
27917	O	85.27664	88.45111	89.24783	518.19642	874.40586	-411.65928	1
27918	N	83.49518	88.87208	87.90450	246.21192	-277.56790	101.90071	1
27919	H	83.20508	89.19550	86.94788	-1132.47449	-3194.01171	366.59404	1
27920	C	82.99007	87.54926	88.15613	529.79798	837.74656	230.42404	1
27921	H	83.44342	87.31176	89.11931	1814.03827	1939.42369	1369.51596	1
27922	C	81.40571	87.60354	88.10241	-524.90278	-1023.93560	310.26867	1
27923	H	81.00381	87.94441	87.13352	-2317.97700	-1371.43791	-438.14416	1
27924	H	81.04330	88.35025	88.81548	934.81243	-1367.27715	787.88444	1
27925	C	80.86272	86.19557	88.53589	-695.19811	-286.02746	-498.38975	1
27926	C	80.10256	85.50546	87.51193	18.76369	65.30462	-5.00926	1
27927	H	79.86901	85.87331	86.49616	946.81419	92.21565	832.25071	1
27928	C	79.40000	84.34180	88.00890	154.45790	-874.49142	-165.83350	1
27929	H	78.84100	83.76780	87.28590	-318.80834	-2946.15376	1011.64924	1
27930	C	79.47800	83.93480	89.35490	-632.41041	464.99289	-476.66066	1
27931	H	78.96900	83.02580	89.64090	-625.70790	-428.34926	3040.42916	1
27932	C	80.96312	85.85069	89.91547	-605.82934	599.61515	40.18883	1
27933	H	81.58735	86.49602	90.52873	-452.87996	-2851.72363	1301.71152	1
27934	C	80.30600	84.65280	90.26790	32.16816	-612.74824	-675.32755	1
27935	H	80.48200	84.28180	91.26690	-2365.96340	-1180.47132	-1697.01771	1
27936	C	83.56318	86.51864	87.01375	89.54771	971.84644	466.87680	1
27937	O	84.00451	85.44501	87.27949	125.10692	21.97534	201.66111	1
27938	N	83.54513	87.01467	85.71690	323.21954	-258.61779	1072.86374	1
27939	H	83.14982	87.95571	85.50399	931.31664	-39.43724	-3850.05213	1
27940	C	83.49683	86.02614	84.62068	-557.39378	814.15402	-264.78715	1
27941	H	83.02672	85.24698	85.28531	2524.82696	-425.67833	-3036.60245	1
27942	C	82.74093	86.53422	83.32124	-582.07465	160.62755	-224.73465	1
27943	H	82.94339	85.80275	82.54990	1466.04631	-794.43370	4666.02220	1
27944	H	83.17774	87.55897	83.03986	843.90596	-2917.71421	-1673.54465	1
27945	C	81.29611	86.85048	83.59531	465.62431	-131.54952	123.42351	1
27946	H	81.19449	87.82344	84.12121	410.44750	-1698.43534	-4389.43321	1
27947	C	80.63782	86.98350	82.23363	-371.83021	1290.75473	509.02535	1
27948	H	81.02537	87.80791	81.62379	1196.84677	-1404.28761	2742.16576	1
27949	H	79.48359	87.03989	82.33328	1243.88613	-478.00782	-2228.40578	1
27950	H	80.76355	85.99952	81.66193	1652.83243	-1387.35830	-3380.91725	1
27951	C	80.74804	85.68520	84.40285	-230.56388	-182.82457	-874.80699	1

27952	H	81.15100	85.62531	85.45374	-1922.65838	-216.55588	-2950.12611	1
27953	H	81.06767	84.69488	83.95823	-678.62841	290.91886	625.00448	1
27954	H	79.61721	85.72076	84.47489	1857.19402	-1483.12761	2446.10297	1
27955	C	84.93188	85.38774	84.29241	466.15084	341.65313	-114.29554	1
27956	O	84.87300	84.21580	83.92590	493.10536	-223.34454	560.01270	1
27957	N	86.01494	86.16923	84.25175	173.77894	-310.72454	526.64488	1
27958	C	85.91486	87.59870	83.97835	719.75410	-85.65731	96.46453	1
27959	H	85.61978	88.14213	84.89580	418.76820	-1132.47342	-1197.77892	1
27960	H	85.21427	87.72847	83.09723	-108.88844	401.73877	1163.71130	1
27961	C	87.27050	85.48903	84.24188	25.00915	-775.46986	14.41750	1
27962	H	87.36000	84.75980	83.39390	-1948.13834	-1717.88792	-1779.22688	1
27963	C	88.26182	86.72993	84.22287	-246.90369	750.51736	769.26946	1
27964	H	89.22017	86.56251	83.67500	-1762.71422	-2187.01932	-4157.00698	1
27965	H	88.43538	87.00925	85.28011	-604.59955	455.24299	505.03734	1
27966	C	87.41287	87.82755	83.51907	-489.96848	219.93887	-310.56103	1
27967	H	87.79305	88.80943	83.78194	-510.19672	-236.48497	-2238.46628	1
27968	H	87.61929	87.68063	82.49169	-458.41145	-1315.27456	-1308.92582	1
27969	C	87.49300	84.44880	85.47990	490.22796	-762.75021	-39.56190	1
27970	O	88.17500	83.43780	85.31690	670.73495	346.37402	-269.63289	1
27971	N	86.94800	84.79480	86.61690	-346.08892	369.05343	-692.97488	1
27972	H	86.29388	85.61054	86.50646	-1561.52745	-1313.26191	670.46364	1
27973	C	86.99100	84.05980	87.81290	758.19795	427.04437	-315.10757	1
27974	H	88.04200	83.90580	88.00490	-1276.60409	1362.86400	-2549.43866	1
27975	C	86.54200	84.90880	89.03390	429.07169	568.02755	-598.21509	1
27976	H	85.54368	85.46765	88.86106	903.53675	2552.88944	-3296.86263	1
27977	O	87.25871	86.29743	89.34913	714.11200	-26.70134	-264.90625	1
27978	H	86.58594	86.91033	89.59908	1361.35960	-2464.15186	714.11716	1
27979	C	86.58800	84.13880	90.31390	-272.92691	870.26609	87.40648	1
27980	H	86.42200	84.88380	91.12190	-1784.44574	1446.01936	2134.31421	1
27981	H	87.58000	83.65880	90.45790	-425.28022	1226.92280	2852.44042	1
27982	H	85.87300	83.28880	90.33790	857.51551	-2914.61989	777.81326	1
27983	C	86.28000	82.71080	87.71290	357.70829	-601.04106	-593.70962	1
27984	O	86.82200	81.66680	88.07090	496.10327	-359.09222	-512.27469	1
27985	N	85.01900	82.70380	87.12790	156.65224	126.10567	-836.13353	1
27986	H	84.59100	83.60380	87.13890	-2665.48952	1542.93597	-658.22644	1
27987	C	84.34600	81.49680	86.73990	-165.68046	905.43990	-29.18632	1
27988	H	84.30700	80.75780	87.52590	2634.21926	735.07951	-1580.22041	1
27989	C	82.88500	81.78680	86.44690	480.41095	499.91251	591.13603	1
27990	H	82.91900	82.67580	85.78090	-1559.48652	-1386.51348	2333.39472	1
27991	C	82.17700	80.62380	85.67890	-679.01659	-545.36355	-252.00280	1
27992	H	81.07800	80.71880	85.54690	605.49663	-2078.52793	-2284.95236	1
27993	H	82.70400	80.35880	84.73790	467.66253	2508.98557	-1866.81973	1
27994	H	82.32100	79.72080	86.31090	1411.42749	-2160.69640	1776.61210	1
27995	C	82.07000	82.12980	87.72690	838.60937	-248.75409	250.52121	1
27996	H	81.10200	82.37580	87.23990	2013.89467	-1834.10464	-1578.76846	1
27997	H	82.53400	83.06080	88.11890	2006.85685	-761.68449	2289.06679	1
27998	C	81.94500	81.05480	88.81990	-706.22984	307.31310	-499.28770	1
27999	H	82.88100	80.59980	89.20790	-582.56830	3062.15589	-500.59183	1
28000	H	81.31400	80.20680	88.47790	2823.60596	-497.02357	1289.51124	1
28001	H	81.40000	81.55980	89.64590	-688.73261	-1631.43098	2580.49272	1
28002	C	85.05200	80.71580	85.59890	-1.42936	127.12393	-918.27000	1
28003	O	85.24900	79.52680	85.71490	35.40890	795.06517	57.31549	1
28004	N	85.49400	81.43280	84.53190	-387.58000	-628.82032	-406.09573	1
28005	H	85.40200	82.42480	84.48490	-910.15699	-2996.72289	-183.76726	1
28006	C	86.03100	80.79380	83.32290	-678.79924	-501.56577	314.11558	1
28007	H	85.31500	80.12480	82.86790	2093.65569	-1740.96906	1552.35631	1
28008	C	86.55300	81.83280	82.24690	-279.04103	688.01826	-555.20774	1
28009	H	87.16500	81.34780	81.45690	-401.11554	1256.04783	2844.81843	1
28010	H	87.19100	82.46680	82.89890	-1413.18126	-2738.84749	574.25802	1
28011	C	85.50700	82.73980	81.58390	-380.76319	-508.74940	-660.31087	1
28012	C	84.15500	82.39380	81.53690	14.78335	746.50501	523.83204	1
28013	H	83.79200	81.55280	82.10890	-1970.53699	-494.48606	-2412.67322	1

28014	C	83.21100	83.32080	80.93390	-807.08979	360.04679	-250.42130	1
28015	H	82.15600	83.09880	80.98090	2042.22507	1778.14329	-1626.59391	1
28016	C	83.64600	84.52480	80.37890	779.43389	-19.73540	460.72376	1
28017	O	82.59601	85.41716	79.85340	-363.67648	-615.84005	-54.75398	1
28018	H	81.83700	84.81180	79.82390	-1073.05885	-2313.13104	1816.94513	1
28019	C	85.92600	83.94280	80.96390	13.06727	-896.06832	-123.25955	1
28020	H	86.96400	84.21780	81.07890	2836.47646	-592.18178	-1239.34454	1
28021	C	84.98800	84.82180	80.36790	-670.75937	504.10466	-382.18162	1
28022	H	85.30312	85.85768	80.09602	-28.55071	-1911.03383	1574.72173	1
28023	C	87.28100	79.90080	83.70090	-596.55663	666.12259	-219.81802	1
28024	O	87.52500	78.85780	83.08590	-544.31326	568.82749	97.93556	1
28025	N	88.11400	80.46780	84.61090	649.54969	520.49746	-192.01959	1
28026	H	87.81200	81.38580	84.85490	561.64598	2858.62954	1192.95931	1
28027	C	89.22100	79.75680	85.24590	-795.45105	444.49017	49.96568	1
28028	H	89.95300	79.50280	84.49390	-1458.48966	-2540.11249	1112.42314	1
28029	C	89.96200	80.65580	86.28690	-450.95317	-336.62819	694.59988	1
28030	H	90.83200	80.05380	86.62590	2290.22727	-329.85560	-2151.99105	1
28031	H	89.32800	80.96580	87.14490	939.17798	2264.55579	-1999.23999	1
28032	O	90.43900	81.84080	85.66990	618.05894	98.55423	469.59846	1
28033	H	89.67500	82.42080	85.62090	2377.04379	-1172.39585	1677.72604	1
28034	C	88.73400	78.47380	85.93690	-903.00649	109.16076	27.56711	1
28035	O	89.25800	77.41880	85.68690	457.50150	487.57046	413.64838	1
28036	N	87.62200	78.53080	86.72490	-695.57091	290.92291	-396.99625	1
28037	H	87.11900	79.38180	86.85290	1752.86221	2405.97445	-1058.88680	1
28038	C	87.01300	77.34680	87.36090	-107.27186	702.85918	565.29637	1
28039	H	87.78600	76.78980	87.87090	2157.44722	2275.38426	323.49462	1
28040	C	85.83700	77.64780	88.31690	-566.79865	-353.86260	-626.83551	1
28041	H	85.15200	78.26580	87.69790	2177.07729	963.61159	2050.17270	1
28042	C	85.23200	76.35180	88.91690	-578.35346	638.72920	-325.65642	1
28043	H	84.85900	75.70780	88.09290	1918.67343	876.96667	-2353.66145	1
28044	H	85.99500	75.79680	89.50290	-1842.13488	-1483.15902	2050.59499	1
28045	H	84.35600	76.61180	89.54990	-668.39830	3080.35667	114.88746	1
28046	C	86.39100	78.49780	89.48490	361.46628	781.86666	-340.99034	1
28047	H	87.06500	79.27980	89.07290	1435.53995	-2189.06132	-1753.63153	1
28048	H	87.08200	77.89680	90.11390	-983.71963	-1139.10588	2742.12937	1
28049	C	85.32100	79.24980	90.26490	556.26640	-635.23103	-349.96766	1
28050	H	85.66100	79.80480	91.16590	-1830.78279	-1084.58200	2293.78907	1
28051	H	84.50800	78.55480	90.56390	2596.84098	378.61303	-1758.88094	1
28052	H	84.81600	79.99880	89.61990	951.24663	-1644.81068	-2517.31716	1
28053	C	86.59100	76.33380	86.29590	42.23971	713.78948	-592.03544	1
28054	O	86.87600	75.13580	86.32990	267.81668	-238.61819	-716.40075	1
28055	N	85.94400	76.86980	85.20790	-710.84581	4.48208	439.02712	1
28056	H	85.63800	77.81680	85.14890	843.70432	1793.24327	-2465.20853	1
28057	C	85.54400	75.97380	84.09090	-585.86983	65.11588	-711.12977	1
28058	H	84.97100	75.16780	84.52390	-587.12490	-2283.37393	-2087.02836	1
28059	C	84.70500	76.68680	83.02590	815.94473	-144.97637	-389.37185	1
28060	H	85.34800	77.43880	82.51990	-2028.37090	-1161.06082	-2115.87436	1
28061	C	84.27500	75.71480	81.91990	388.97508	0.69857	810.15644	1
28062	H	85.09700	75.06980	81.54390	-1045.35130	1855.16217	-2338.83585	1
28063	H	83.47900	75.04880	82.31590	-1132.40933	2176.33542	1968.49803	1
28064	H	83.83700	76.40380	81.16690	-1218.57944	-1768.82503	-2305.47114	1
28065	C	83.45000	77.48980	83.55590	419.60996	394.50398	699.43664	1
28066	H	82.97200	77.88180	82.63290	2756.26863	509.65078	1419.06048	1
28067	H	83.89400	78.25780	84.22490	-2549.89391	-1003.83650	-1550.92548	1
28068	C	82.33100	76.72480	84.30590	-568.86443	-635.05095	-313.55255	1
28069	H	81.47300	77.36780	84.59690	626.62880	419.29995	3044.27828	1
28070	H	82.01000	75.87880	83.66190	-2555.16935	-322.74809	1793.43288	1
28071	H	82.78500	76.35380	85.24990	1987.14008	2434.85955	-285.29308	1
28072	C	86.82000	75.33080	83.39190	637.00700	14.94302	636.17295	1
28073	O	86.93000	74.10180	83.14490	-600.64060	522.36306	13.00956	1
28074	N	87.87300	76.12580	83.05390	-664.60713	298.98835	-449.06219	1
28075	H	87.78700	77.10580	83.21590	969.03204	2397.23374	1787.34319	1

28076	C	89.14600	75.69580	82.51290	629.67551	156.84010	-658.15556	1
28077	H	88.77200	75.17380	81.64490	1620.99100	-2054.24682	-1751.94346	1
28078	C	89.90200	76.92480	82.03590	428.28134	570.19656	-592.30451	1
28079	H	89.27500	77.50780	81.32890	-1807.53275	1041.20496	2342.67993	1
28080	H	90.24800	77.70980	82.74190	968.56855	-2100.23784	2107.82858	1
28081	C	91.23100	76.59480	81.38190	334.01530	-770.79250	319.01648	1
28082	C	91.21500	76.27080	80.01490	-26.05592	914.54890	67.74854	1
28083	H	90.34000	76.17680	79.38890	-470.67687	-1953.20109	-2433.38480	1
28084	C	92.38300	75.83580	79.33690	120.98455	110.17651	878.30028	1
28085	H	92.23500	75.47680	78.32890	1777.49859	-2556.74900	-409.73190	1
28086	C	93.59700	75.74780	79.99190	626.50663	-208.86124	-643.63027	1
28087	H	94.46100	75.44580	79.41890	-284.87963	2952.15028	1046.28094	1
28088	C	92.48600	76.63880	82.03490	850.64581	321.87138	-98.76369	1
28089	H	92.45700	76.91580	83.07890	1218.57156	-2329.02414	1700.72917	1
28090	C	93.65300	76.24480	81.37190	119.05896	625.38518	638.33017	1
28091	H	94.58100	76.33180	81.91690	2966.91080	-678.21337	766.66896	1
28092	C	89.91100	74.63880	83.25790	-900.41016	-90.23704	97.96802	1
28093	O	90.31700	73.58680	82.77890	111.42726	600.23109	-526.96562	1
28094	N	90.07200	74.84380	84.60690	-65.09389	771.33164	-370.93533	1
28095	H	89.75100	75.72580	84.94490	-1902.63814	2510.88162	82.64946	1
28096	C	90.99200	74.14780	85.47890	176.26922	840.54258	306.74208	1
28097	H	91.87600	73.95580	84.88990	-1939.25327	1237.50523	2131.56953	1
28098	C	91.44100	74.96580	86.68890	174.21619	901.68954	-43.62844	1
28099	H	90.54900	75.39680	87.18990	1721.12066	-1237.61042	-2340.04669	1
28100	H	91.98500	74.47680	87.52490	-139.40987	3120.38631	-445.71374	1
28101	C	92.29500	76.20180	86.29890	-747.79519	-247.90416	434.22363	1
28102	H	91.81200	76.81980	85.51190	2494.38928	796.35802	-1767.50321	1
28103	C	92.49600	77.08680	87.49090	618.51575	-34.87835	651.99494	1
28104	H	93.34000	76.67480	88.08490	-641.58908	2190.91568	-2189.68534	1
28105	H	92.75900	78.11980	87.17690	-2277.46442	-585.79530	-2104.47555	1
28106	H	91.62000	77.10680	88.17290	-2010.55765	1694.34159	1712.17882	1
28107	C	93.63900	75.80880	85.71290	-661.64940	-592.06903	166.94203	1
28108	H	94.39500	76.62280	85.73390	2426.76760	-1268.33368	-1567.01350	1
28109	H	94.08800	74.94380	86.24590	219.03612	-1958.80210	2427.48862	1
28110	H	93.51200	75.52980	84.64590	2280.66461	1364.96568	-1708.12171	1
28111	C	90.49500	72.83780	85.92890	-811.12081	-77.77506	390.23284	1
28112	O	91.27500	71.96380	86.38890	-129.72237	-262.35755	712.54881	1
28113	N	89.19100	72.60280	85.69690	-252.35301	129.19173	779.44895	1
28114	H	88.59100	73.30280	85.31790	42.93005	-3137.31584	-76.18310	1
28115	C	88.45900	71.35680	85.94490	725.72573	-364.36492	389.59401	1
28116	H	89.12800	70.64180	86.40090	2332.57931	-2073.20670	334.45166	1
28117	C	87.22600	71.64880	86.78490	631.66365	114.48076	633.12285	1
28118	H	86.71000	70.67580	86.92890	-1829.93245	1656.28553	1943.16775	1
28119	O	86.29500	72.52080	86.19690	721.95590	-286.10656	108.21924	1
28120	H	86.60700	73.42780	86.23990	273.02923	502.58455	-3110.48669	1
28121	C	87.61600	72.22880	88.17090	-734.90693	-487.23469	-226.45475	1
28122	H	86.73200	72.42180	88.81590	-1083.59082	2944.57383	301.95038	1
28123	H	88.12700	73.21380	88.10690	-33.64699	-1900.73002	2484.35189	1
28124	H	88.25200	71.51380	88.73390	1028.66700	2145.28904	-2083.94732	1
28125	C	88.17800	70.69480	84.65590	-49.07363	579.45998	-725.57271	1
28126	O	88.41700	69.53780	84.41390	233.00202	-353.15949	-678.23257	1
28127	N	87.69700	71.45480	83.66790	-644.00990	354.32760	-441.68354	1
28128	H	87.49600	72.42580	83.77290	2621.77794	500.70505	1649.26652	1
28129	C	87.33000	70.99180	82.32790	-518.22449	-521.16462	-550.37923	1
28130	H	86.87200	71.79880	81.77690	-1051.41400	-1579.82576	2489.64659	1
28131	H	86.53900	70.25880	82.39390	3134.17448	-185.05862	108.34011	1
28132	C	88.38800	70.38780	81.46990	-134.45764	-881.73444	-166.68237	1
28133	O	88.07800	69.34780	80.89690	-373.97637	-560.23070	388.73055	1
28134	N	89.50700	71.10180	81.21690	-382.31627	-566.44366	472.42766	1
28135	H	89.71200	71.85980	81.82990	-623.96899	-1569.54822	2633.12291	1
28136	C	90.54000	70.62380	80.30890	-326.41668	689.40592	494.60186	1
28137	H	90.04700	70.37080	79.38190	2545.13511	-1524.09663	1005.28892	1

28138	C	91.49700	71.77680	80.00190	-689.40157	-163.09392	558.83817	1
28139	H	90.87200	72.69580	80.01990	-279.39427	2912.02702	-1194.84033	1
28140	C	92.63800	71.97780	81.09890	358.35663	830.75539	125.23627	1
28141	H	93.11400	72.96780	80.93290	-1449.46793	-644.88039	2697.54576	1
28142	H	93.41500	71.18380	81.09390	-1779.25494	-138.79471	-2613.32095	1
28143	H	92.18000	72.00080	82.11090	2933.44960	-371.20895	1045.15464	1
28144	C	92.06200	71.74980	78.55590	277.34925	-283.92969	797.67264	1
28145	H	91.23500	71.68480	77.81690	-1773.78494	2098.12515	1531.04211	1
28146	H	92.43600	72.79180	78.45790	-1700.45139	2133.62028	1561.93717	1
28147	C	93.19900	70.75380	78.20890	620.39323	-555.28205	-371.24665	1
28148	H	94.09500	70.93880	78.83990	-2530.44445	391.14515	-1857.51078	1
28149	H	93.64100	70.73480	77.18990	895.77150	-2273.20041	1951.72837	1
28150	H	92.87200	69.72480	78.47090	-2543.87490	640.35358	1728.94438	1
28151	C	91.19200	69.33780	80.85890	-850.78767	47.81242	319.61574	1
28152	O	91.46200	68.34780	80.13890	-218.74698	682.56688	-367.79343	1
28153	N	91.48600	69.32480	82.18790	-417.20182	601.59414	-452.65598	1
28154	H	91.23100	70.17480	82.64090	2765.24017	-1184.24890	883.56449	1
28155	C	91.91500	68.12480	82.90290	670.69204	1.80269	-632.29933	1
28156	H	92.79300	67.74880	82.39990	1132.49441	2481.32632	1555.15893	1
28157	C	92.25100	68.54980	84.34890	-626.64967	-210.90559	609.40493	1
28158	H	91.36300	68.83680	84.95190	2028.60386	-2127.30605	-1122.46589	1
28159	C	92.93000	67.35280	85.13090	-41.12981	551.80014	709.89908	1
28160	H	93.39500	67.66780	86.08990	2814.72829	791.42608	-1180.39543	1
28161	H	93.59900	66.86780	84.38790	679.90348	2171.79798	2157.04109	1
28162	H	92.08600	66.72380	85.48590	-1300.36271	-2079.14996	-1985.07681	1
28163	C	93.12200	69.81780	84.36490	-85.06918	-707.31889	-581.50575	1
28164	H	92.59100	70.79080	84.28690	415.96983	-1818.60405	-2547.79010	1
28165	H	93.47800	69.79780	85.41690	-1801.45273	617.06534	-2527.14992	1
28166	H	93.92400	69.74080	83.59990	-2113.02464	-1552.35994	-1757.46789	1
28167	C	90.88500	67.01480	82.85490	-561.46284	648.82375	-349.31053	1
28168	O	91.19100	65.97680	82.31990	573.17608	282.10547	-480.43395	1
28169	N	89.59800	67.27880	83.21290	523.25846	515.03134	403.18812	1
28170	H	89.33800	68.17280	83.56890	-3104.68005	-442.16432	264.15926	1
28171	C	88.50800	66.28280	83.31090	-547.86210	562.57166	461.49133	1
28172	H	87.63400	66.81180	83.66190	-1062.66732	-2927.38533	382.24874	1
28173	H	88.77800	65.52880	84.03490	8.93346	2353.60871	2079.60135	1
28174	C	88.13700	65.55880	82.06790	308.48057	-553.38131	-662.61249	1
28175	O	88.04400	64.34280	82.03790	294.96319	-569.16094	430.05692	1
28176	N	87.94300	66.29480	80.94490	-139.42761	648.56090	-550.35862	1
28177	H	88.08700	67.28080	80.99990	-2818.32274	987.22325	-1030.89105	1
28178	C	87.72000	65.63780	79.67190	406.48535	-517.84704	-635.40502	1
28179	H	87.02600	64.82080	79.79990	1051.60674	215.28070	2939.43295	1
28180	C	86.96700	66.60780	78.71390	-99.63122	180.59688	-906.55763	1
28181	H	87.46400	67.58080	78.50890	3097.72287	89.30798	485.10087	1
28182	H	86.78100	66.01880	77.79090	2240.99069	368.16186	-2185.91712	1
28183	C	85.61000	66.79680	79.39290	250.27134	786.55772	-416.48197	1
28184	O	84.83300	65.81480	79.48890	34.22440	752.35528	250.79476	1
28185	N	85.34400	67.99780	79.87490	287.03502	785.99059	139.35399	1
28186	H	86.08300	68.66580	79.96190	-2091.98692	-1470.28973	1817.14185	1
28187	H	84.39500	68.15680	80.14790	-3080.07944	139.84286	642.17380	1
28188	C	88.89800	64.98780	79.03490	721.70059	384.15505	-414.21490	1
28189	O	88.72200	64.04280	78.34190	-702.32334	362.66611	-146.95869	1
28190	N	90.14400	65.40080	79.46790	202.69361	-784.26164	-221.84828	1
28191	H	90.25700	66.25580	79.96790	-1068.81255	2028.39635	-2182.73006	1
28192	C	91.31700	64.73480	79.05890	89.72030	522.95790	726.76392	1
28193	H	91.30700	64.62180	77.98490	-2935.77150	1158.21014	-94.04315	1
28194	H	92.21500	65.29480	79.27790	1054.48633	-1918.70401	2230.80482	1
28195	C	91.40100	63.43180	79.75790	302.77967	-789.81901	-334.89360	1
28196	O	91.82500	62.42080	79.26990	-585.86022	338.99517	405.46470	1
28197	N	91.02800	63.38680	81.05790	653.84063	161.57973	-520.40764	1
28198	H	90.80500	64.21680	81.56290	-2524.06541	1608.89934	-1015.82361	1
28199	C	90.91800	62.15580	81.79590	268.15943	-727.72465	-482.86823	1

28200	H	91.86200	61.64080	81.70190	-1073.65081	2396.75329	1727.08137	1
28201	C	90.82800	62.40680	83.27890	325.42931	-787.62330	281.31989	1
28202	H	90.54300	61.55180	83.92790	1671.63982	2651.92463	280.19405	1
28203	H	89.92600	63.04680	83.38890	-2291.78553	-1666.30648	1349.95496	1
28204	C	92.01900	63.17780	83.96190	-512.67023	-334.69939	-695.70824	1
28205	H	92.39400	64.07880	83.43090	2366.51489	464.31672	1996.17961	1
28206	C	91.67700	63.61180	85.38990	-432.00375	662.20059	448.78216	1
28207	H	91.21000	62.80180	85.98990	-2956.90848	-355.08276	-1042.76200	1
28208	H	92.58900	63.86880	85.96890	1880.12225	-741.64303	-2425.78053	1
28209	H	90.99500	64.48680	85.45990	-1867.13575	1331.55269	-2179.99712	1
28210	C	93.24800	62.26580	83.90690	389.86023	148.78501	788.96691	1
28211	H	93.04800	61.32980	84.47190	2314.17641	-1494.91627	1484.23197	1
28212	H	94.12500	62.84280	84.26990	-1444.21997	1880.78126	-2097.19841	1
28213	H	93.55700	61.98580	82.87690	1522.75985	1898.59281	1974.09120	1
28214	C	89.83700	61.22880	81.39190	-678.51139	397.56232	-497.03712	1
28215	O	90.05200	60.01880	81.38790	772.99757	-96.66008	29.55451	1
28216	N	88.67800	61.73480	81.04490	322.70469	-207.08847	729.29722	1
28217	H	88.46700	62.70780	81.09490	-1228.76098	-2116.41153	1956.12007	1
28218	C	87.67100	60.85880	80.39390	531.81909	469.08503	555.54941	1
28219	H	87.32000	60.08580	81.06090	-2118.36443	428.93297	-2311.93842	1
28220	C	86.36900	61.62080	80.15290	428.64517	387.32928	689.57978	1
28221	H	86.66700	62.53680	79.59990	-940.16048	-1897.00248	2307.55889	1
28222	C	85.41000	60.79180	79.24990	-49.64048	149.13754	-915.13852	1
28223	H	85.78800	60.71980	78.20790	-347.88803	2242.84454	2174.67503	1
28224	H	84.42100	61.27980	79.11590	-2241.76490	1466.52007	1656.83482	1
28225	H	85.21300	59.82180	79.75490	-1565.22592	-954.93084	-2573.73210	1
28226	C	85.66900	62.05280	81.46790	52.47096	173.96395	879.74916	1
28227	H	84.86800	62.78280	81.22090	2281.63667	-965.75841	-1940.00842	1
28228	H	85.26400	61.20280	82.05790	1411.05962	-202.26383	-2815.08006	1
28229	H	86.41700	62.61580	82.06690	1679.94079	1804.64591	-1972.20181	1
28230	C	88.14800	60.21080	79.10090	-470.40345	416.20329	656.22135	1
28231	O	87.98300	59.02080	78.84890	-689.09523	370.29163	-195.87772	1
28232	N	88.93200	60.97080	78.26790	593.18899	-476.41987	-355.03563	1
28233	H	88.88200	61.95180	78.43890	940.48310	-2002.49271	-2242.82448	1
28234	C	89.63900	60.42180	77.09990	714.24102	373.99708	396.18193	1
28235	H	88.99200	59.82980	76.46890	-2648.72128	-770.16176	-1546.58881	1
28236	C	90.13200	61.55680	76.21090	-256.54453	336.20744	-832.47005	1
28237	H	90.77500	62.20780	76.84090	2377.57761	1982.80805	-559.79790	1
28238	C	91.04800	61.07380	75.04890	-466.42691	-398.34301	-697.27267	1
28239	H	91.94600	60.50580	75.37390	-1651.30017	-2665.30198	246.23287	1
28240	H	91.50200	61.91580	74.48490	2366.17923	2042.75739	294.21510	1
28241	H	90.55600	60.35680	74.35590	-897.35464	-321.17988	-3019.67884	1
28242	C	89.00800	62.48180	75.66090	-4.11286	575.13852	696.78191	1
28243	H	88.47400	61.93980	74.85190	2600.89096	-1676.37286	-499.92892	1
28244	H	88.14100	62.60780	76.34490	-2641.77470	-1482.01111	-884.97305	1
28245	C	89.53000	63.78780	75.11390	-564.17527	-407.18269	576.64718	1
28246	H	90.19400	63.52080	74.26490	931.26531	-2993.11035	48.43409	1
28247	H	88.68400	64.35180	74.66590	-2117.37220	2274.62612	-587.31441	1
28248	H	89.97900	64.42080	75.90890	-2582.55385	1663.06860	-753.36763	1
28249	C	90.77300	59.45680	77.46190	321.61981	-602.12345	-609.51982	1
28250	O	90.96700	58.38780	76.89490	-45.12124	745.73069	259.17854	1
28251	N	91.47500	59.73380	78.58890	-216.30865	-454.61066	657.12123	1
28252	H	91.42900	60.64380	78.99590	1666.93926	1718.58246	2020.11581	1
28253	C	92.46700	58.82380	79.17890	-735.18206	-468.95599	-302.24164	1
28254	H	93.13400	58.59180	78.36190	-2165.42203	2204.92666	-670.26739	1
28255	C	93.39400	59.54580	80.25190	-736.74887	-60.44056	525.46063	1
28256	H	93.67500	58.93680	81.13790	-486.38816	1906.32222	2441.07505	1
28257	H	92.68800	60.32980	80.60090	-1894.30994	2446.11103	-645.08247	1
28258	C	94.60100	60.20980	79.64990	-9.34708	141.88751	-922.66208	1
28259	H	94.23900	60.46180	78.62990	-1504.26995	2215.09368	-1689.58302	1
28260	C	95.06300	61.43480	80.47190	172.90107	822.61958	-383.13079	1
28261	H	95.28300	61.04180	81.48790	-1719.69230	-2397.89678	1070.38304	1

28262	H	94.26400	62.20680	80.47790	-1646.98097	-1983.09286	-1825.30487	1
28263	H	96.00300	61.82780	80.02690	781.11060	-1749.53616	2467.21924	1
28264	C	95.76500	59.20580	79.52190	-733.80263	520.24648	183.62918	1
28265	H	96.08900	58.91780	80.54590	-2589.02162	1684.90442	627.36802	1
28266	H	95.53700	58.21280	79.07790	1387.32958	-2448.29342	1365.19879	1
28267	H	96.53300	59.68580	78.87890	581.74892	-2902.12889	1024.89315	1
28268	C	91.86500	57.57880	79.69390	-593.02800	-296.36710	-651.89200	1
28269	O	92.42900	56.49880	79.48290	524.73613	-18.29702	-599.34976	1
28270	N	90.65400	57.56080	80.28190	-391.50102	-689.14031	268.11773	1
28271	H	90.21300	58.42780	80.50190	-2083.71505	2034.79785	-1237.27944	1
28272	C	89.92200	56.39580	80.60690	-279.63664	-25.14970	-888.63107	1
28273	H	90.56100	55.73180	81.16890	2599.67311	-676.62688	-1636.81146	1
28274	C	88.72200	56.64380	81.52490	-265.58573	826.23980	-327.89780	1
28275	H	88.11700	57.51680	81.19890	-2210.03128	-863.78927	2055.66312	1
28276	C	87.81900	55.37180	81.65790	-280.12478	317.11001	-831.10384	1
28277	H	87.24900	55.30580	80.70590	-1690.04081	2614.21740	521.37691	1
28278	H	88.39100	54.44580	81.87890	2314.77873	1317.87646	-1683.55201	1
28279	H	87.10100	55.43280	82.50390	1532.11441	-1887.68138	-1997.56711	1
28280	C	89.30500	57.08480	82.90890	-343.71352	794.83744	-333.26503	1
28281	H	89.91800	58.00280	82.78290	2323.99366	617.14832	-2039.71293	1
28282	H	89.92900	56.23680	83.26390	-1977.37561	1716.07195	1743.46658	1
28283	H	88.39800	57.27180	83.52290	-1988.28875	-1718.66287	-1747.70541	1
28284	C	89.44700	55.63980	79.32990	-370.76351	584.15171	590.65417	1
28285	O	89.89800	54.49180	79.18290	-461.72519	655.94445	15.27234	1
28286	N	88.71500	56.24380	78.37590	-699.42666	370.06510	-347.36749	1
28287	H	88.39800	57.18380	78.48190	-1693.74516	-201.91012	-2667.30115	1
28288	C	88.13600	55.43780	77.35890	468.73961	-506.79843	-594.91622	1
28289	H	87.98700	54.42380	77.69790	2154.38979	1553.27492	-1694.35310	1
28290	C	86.80000	55.99480	76.89190	505.48273	-60.55365	730.85680	1
28291	H	86.79700	57.04880	76.53890	-1156.71311	2804.20846	-897.06713	1
28292	H	86.30400	55.48680	76.03690	1241.22141	2542.64825	-1395.92392	1
28293	C	85.67600	55.90280	77.97190	-496.76177	-141.16177	742.37360	1
28294	H	86.01400	56.61080	78.75890	1860.48459	1236.98597	2195.07512	1
28295	H	85.62800	54.90080	78.44890	-2231.20200	1011.83499	1977.21546	1
28296	S	83.95900	56.24880	77.57990	-417.37037	-134.63999	341.17869	1
28297	C	84.12800	58.00880	77.20090	-209.15388	-499.70267	-744.07932	1
28298	H	83.24300	58.67880	77.24590	-425.70864	-2969.84438	905.61370	1
28299	H	84.54900	58.20380	76.19090	398.95230	2092.74618	-2336.25532	1
28300	H	84.85200	58.45580	77.91490	2076.17325	1042.89387	-2129.68819	1
28301	C	89.02800	55.25480	76.12090	438.24514	-395.53778	-698.87022	1
28302	O	88.67300	54.33880	75.34490	-497.05183	225.05426	-603.76090	1
28303	N	90.17100	55.99680	75.92590	-681.04892	-214.95638	448.24138	1
28304	H	90.45000	56.78180	76.47390	1334.96930	2734.49259	-821.52364	1
28305	C	91.03600	55.84080	74.74190	-904.26683	198.86292	-73.24142	1
28306	H	91.33000	56.77180	74.28090	-1601.23895	304.16835	-2719.34462	1
28307	H	90.59400	55.18780	74.00390	-587.47725	2949.30196	938.85860	1
28308	C	92.32500	55.26980	75.05690	622.49286	-633.93388	103.65726	1
28309	O	92.92800	54.78180	74.07790	-214.58636	-692.22184	289.05720	1
28310	N	92.85900	55.28180	76.31390	-433.88650	-720.11135	69.58835	1
28311	H	92.39700	55.80080	77.02990	-2192.48745	-314.62696	2226.27108	1
28312	C	94.18600	54.76780	76.54990	-529.95396	742.79317	-169.36137	1
28313	H	94.42000	54.19980	75.66190	2031.97478	2187.55999	-996.14718	1
28314	C	95.24000	55.87480	76.84190	-416.42281	774.49635	-299.91679	1
28315	H	96.23400	55.39980	76.97990	1630.74082	999.18790	-2513.82470	1
28316	H	94.96800	56.43880	77.75990	1795.15835	-532.65629	-2539.73141	1
28317	C	95.32500	56.83880	75.67490	645.41977	605.02043	-216.65612	1
28318	C	94.57400	58.04680	75.56990	722.78223	-399.40116	333.64495	1
28319	H	93.81100	58.35680	76.26890	1613.32237	-2625.70905	552.60356	1
28320	C	94.76300	58.89280	74.47790	-434.11815	-262.72903	-784.28561	1
28321	H	94.19800	59.78980	74.27190	-2223.36429	878.63299	2041.18908	1
28322	C	95.64700	58.60780	73.44990	403.09801	586.86039	543.32932	1
28323	O	95.87200	59.44180	72.41690	-569.53331	-358.96270	405.62564	1

28324	H	96.32200	59.00280	71.69190	1945.37758	-1690.04113	1761.13338	1
28325	C	96.26800	56.58880	74.66090	-721.35779	-522.53848	-252.13508	1
28326	H	96.92000	55.72780	74.64290	-1406.62000	233.59813	-2834.85367	1
28327	C	96.40200	57.42980	73.55890	229.31113	-858.13584	-185.54474	1
28328	H	97.07000	57.15380	72.75690	1800.15240	1090.58769	-2351.73750	1
28329	C	94.25100	53.70880	77.63690	503.92665	688.03024	-334.99672	1
28330	O	94.75800	52.60880	77.40090	-430.12468	-617.52861	-270.40334	1
28331	N	93.66100	53.96080	78.80590	244.28722	-665.94167	421.01394	1
28332	H	93.27600	54.86780	78.95390	-1246.06241	-2598.01889	1241.81877	1
28333	C	93.44100	53.00680	79.89090	-611.74241	607.01131	-353.65185	1
28334	H	94.35700	52.47780	80.10790	1815.62811	1581.03871	1997.70412	1
28335	C	92.94400	53.62880	81.25290	434.74374	-390.21683	-709.71902	1
28336	H	92.05600	54.20480	80.91490	1517.55532	1908.99186	1966.13856	1
28337	H	92.64800	52.84180	81.97990	1206.93876	903.32940	2738.76239	1
28338	C	93.94700	54.46080	82.04690	-403.54980	821.59500	85.75598	1
28339	H	94.47900	55.07880	81.29190	-1526.98798	-2744.45688	165.36984	1
28340	H	94.64500	53.84780	82.65590	2432.83857	-1922.22247	441.51423	1
28341	C	93.27700	55.39580	83.02990	-576.35835	49.00822	692.32572	1
28342	O	92.47900	54.97380	83.85390	269.76400	-648.20252	322.94924	1
28343	N	93.52300	56.72180	82.88790	-595.97997	-80.19627	579.82874	1
28344	H	94.41900	57.02380	82.56290	-2105.96006	51.18228	-2365.81974	1
28345	H	92.86000	57.35880	83.28190	1721.61098	370.81856	-2622.52386	1
28346	C	92.57700	51.86780	79.50590	296.34519	602.53029	596.96352	1
28347	O	92.78500	50.65780	79.79990	-599.83033	401.56875	-371.38816	1
28348	N	91.47300	52.18080	78.75590	347.82678	369.28638	652.35637	1
28349	H	91.20800	53.14080	78.70990	2016.06534	270.44841	2370.97669	1
28350	C	90.61600	51.17280	78.07990	611.18318	-481.45342	430.16434	1
28351	H	90.80800	50.23680	78.58390	-2158.57346	-1353.94248	-1875.41741	1
28352	C	89.08300	51.53180	78.20090	463.51199	-642.07161	407.68790	1
28353	H	88.90900	52.51580	77.71390	-2997.94955	-805.98719	557.31575	1
28354	H	88.49600	50.75480	77.66490	373.07110	2818.23485	1343.55164	1
28355	C	88.66600	51.54680	79.65090	-29.39620	735.84789	531.76601	1
28356	H	89.15400	52.39480	80.17690	1400.71442	2464.68859	-1383.72596	1
28357	H	89.07300	50.61780	80.10390	2457.70716	-1047.06986	-1655.00991	1
28358	C	87.13900	51.48180	79.68990	-445.50741	-787.26841	-119.84949	1
28359	H	86.76700	52.34880	79.10290	809.04252	-1650.27837	2527.41691	1
28360	H	86.88900	50.48680	79.26190	-2973.57162	813.87537	682.88567	1
28361	C	86.57500	51.74980	81.08890	614.39152	591.46520	-332.02139	1
28362	H	86.92000	52.73180	81.47690	-1481.84431	2547.16315	-1152.92936	1
28363	H	86.98500	50.92780	81.71390	416.46154	-2555.85624	-1787.66933	1
28364	N	85.12500	51.68880	81.07790	-337.81971	643.61311	-467.14848	1
28365	H	84.77400	50.75480	80.78390	2048.84644	2262.28543	-772.98653	1
28366	H	84.69900	52.02580	81.96490	-2265.29941	-2161.72169	-334.82773	1
28367	H	84.83800	52.34680	80.32490	2690.56484	856.60779	-1384.58703	1
28368	C	90.95300	50.94980	76.60790	-807.13571	422.34025	159.93149	1
28369	O	90.98900	51.89480	75.82090	-492.36392	-336.44991	-546.08096	1
28370	N	91.05100	49.72080	76.17790	-665.55952	405.37265	344.56023	1
28371	H	90.96200	48.97080	76.82890	1442.30907	2355.66186	-1521.39727	1
28372	C	91.29900	49.34780	74.85290	-213.52954	859.70684	237.83150	1
28373	H	91.82800	50.10280	74.28990	793.20039	-477.58175	-3020.69137	1
28374	C	92.38200	48.18380	74.82990	-250.05268	674.85422	-595.32394	1
28375	H	92.07000	47.34480	75.48790	1980.26708	900.42084	2240.56480	1
28376	H	92.30400	47.74580	73.81190	-1480.36954	-2622.76325	899.75509	1
28377	C	93.85500	48.62380	74.83190	-441.68292	623.25146	499.22849	1
28378	H	94.07900	49.05780	73.83490	-1551.20324	-1549.47734	-2285.34090	1
28379	H	94.46100	47.69280	74.87390	-1030.58371	-903.23766	-2857.83656	1
28380	C	94.33100	49.57380	75.99790	-139.62115	755.22636	483.54835	1
28381	H	93.81300	50.55380	75.93290	2501.00392	1870.93166	273.47697	1
28382	H	94.18600	49.06480	76.97490	-1102.46374	2945.50039	-297.47796	1
28383	C	95.82100	49.84980	75.84490	645.92773	340.16174	507.93599	1
28384	H	96.00100	50.55280	75.00390	1593.12527	-835.29974	2546.96236	1
28385	H	96.33200	48.90480	75.56290	-1882.74949	2260.31593	1130.83546	1

28386	N	96.36400	50.35680	77.12790	68.77608	-834.91780	-27.90790	1
28387	H	95.93900	49.92380	77.97290	352.06442	-1842.45155	-2542.14141	1
28388	H	96.24700	51.38080	77.26290	-227.26609	-2412.96226	-2023.87272	1
28389	H	97.39300	50.20580	77.11590	2205.71917	1042.66206	1948.72805	1
28390	C	90.00100	49.00580	74.10290	-663.76463	-425.76074	457.02755	1
28391	O	90.08300	48.49180	72.98190	-127.70645	638.10412	444.57691	1
28392	N	88.81000	49.29580	74.67490	628.17863	-283.40440	441.99410	1
28393	H	88.70200	49.78880	75.53390	-1353.02095	-682.33870	2745.59799	1
28394	C	87.55400	48.97680	74.08890	793.05496	341.17643	235.66176	1
28395	H	87.68600	49.00780	73.01690	1242.82668	-2801.22024	624.90922	1
28396	C	87.15200	47.53380	74.50490	177.73078	-363.24730	-825.65445	1
28397	H	87.00100	47.55280	75.60590	610.43385	-2721.94284	1414.16521	1
28398	H	88.03400	46.90580	74.25790	-313.33462	1846.71417	2519.07078	1
28399	C	85.88800	46.98380	73.78190	-533.26062	-666.75881	-346.46170	1
28400	H	85.04600	47.70380	73.87690	2141.25873	2137.56504	825.71964	1
28401	C	86.19700	46.73680	72.27590	493.62684	-380.99977	628.67154	1
28402	H	86.97300	45.94380	72.21590	737.45170	1561.86777	-2645.74915	1
28403	H	86.79000	47.58380	71.86990	-2389.69886	11.64969	2052.80258	1
28404	H	85.32100	46.35980	71.70490	1399.72155	2209.83334	-1759.33026	1
28405	C	85.44900	45.69380	74.43390	-591.56735	-678.53865	157.14214	1
28406	H	86.17400	44.86080	74.31090	-2615.68367	1304.57427	1199.98104	1
28407	H	84.50200	45.40480	73.93090	-2917.49780	-252.73516	-1210.27578	1
28408	H	85.30700	45.81980	75.52790	-2876.02913	-593.57569	1153.32930	1
28409	C	86.58300	49.95080	74.48290	453.42690	44.98935	764.21854	1
28410	O	86.54200	50.31480	75.64190	-604.63646	478.38241	-254.80898	1
28411	N	85.76300	50.38280	73.53390	57.03341	-803.83282	198.06615	1
28412	H	85.97600	50.05580	72.61690	1787.53361	1554.55617	2045.93074	1
28413	C	84.62100	51.21080	73.67290	-182.34987	-433.19456	-794.32327	1
28414	H	84.52300	51.36680	74.73690	-1683.31259	2612.08870	-604.62227	1
28415	C	84.88700	52.61880	73.07790	854.28666	233.55172	-165.08085	1
28416	H	83.94100	53.16780	72.88390	1354.25118	593.22148	2756.81940	1
28417	H	85.25400	52.43280	72.04590	-1956.54738	-76.90707	-2491.24807	1
28418	C	85.88700	53.42880	73.88690	629.15694	-631.57424	50.56340	1
28419	H	86.80800	52.87480	74.16590	-308.96163	2781.20607	-1474.75847	1
28420	H	85.38700	53.70380	74.83990	-236.04273	2924.88007	-1177.34438	1
28421	C	86.28500	54.67180	73.14490	-62.36114	-642.79523	-651.40403	1
28422	H	85.41500	55.31380	72.88890	956.32491	2330.38395	-1903.86709	1
28423	H	86.96800	55.30180	73.75390	1551.44630	2009.37450	1839.10287	1
28424	N	87.02500	54.16280	71.89790	-625.96051	361.34410	450.35111	1
28425	H	86.52100	54.27380	71.04090	2238.31299	2197.77550	-157.05820	1
28426	C	88.26400	53.66480	71.80990	-587.06887	371.93100	-629.20634	1
28427	N	89.10000	53.50980	72.82190	561.03556	618.34810	-99.11113	1
28428	H	88.79100	53.70980	73.75190	-343.79495	2644.30135	1668.41486	1
28429	H	90.04200	53.23980	72.62390	2807.38407	638.48628	1216.22440	1
28430	N	88.74400	53.35480	70.59690	225.70736	-456.37641	643.80082	1
28431	H	88.15000	53.32880	69.79290	575.04941	-1069.05184	-2912.56325	1
28432	H	89.71700	53.20780	70.42090	1537.06485	2705.84297	429.75688	1
28433	C	83.32200	50.61480	73.20590	-645.07893	-468.50601	-470.23693	1
28434	O	83.24600	50.07780	72.10590	139.62546	86.95801	756.04690	1
28435	N	82.30300	50.67980	74.02090	271.66047	-347.02789	-721.22722	1
28436	H	82.47000	51.01780	74.94390	-1333.44928	2091.10896	1945.09595	1
28437	C	80.90500	50.41080	73.69990	196.33547	873.29287	195.13613	1
28438	H	80.90700	49.61780	72.96590	2603.79563	1237.98405	1220.30987	1
28439	C	80.09800	49.91280	74.88890	874.33762	111.18718	154.18296	1
28440	H	80.65700	49.07480	75.35590	-627.09511	2749.85102	-1435.98716	1
28441	H	79.13500	49.50380	74.51390	-1351.29826	-2443.03627	-1456.98842	1
28442	O	79.93000	50.94380	75.84990	389.31338	689.25063	13.60092	1
28443	H	80.78600	51.10580	76.25190	2029.82635	-1922.75384	1392.92826	1
28444	C	80.20200	51.63780	73.09290	-307.99423	472.52124	719.34700	1
28445	O	80.82500	52.67380	72.89290	-10.70658	-658.72379	405.38123	1
28446	N	78.90600	51.49280	72.63190	786.57145	-232.83882	65.91513	1
28447	H	78.46200	50.61780	72.45690	1948.43052	2044.35528	1368.66700	1

28448	C	78.10900	52.61380	72.12490	-56.27022	-510.54261	-756.21032	1
28449	H	78.62900	53.02480	71.27190	553.42774	3050.13663	576.07300	1
28450	C	76.74700	52.13880	71.62190	-19.64090	699.69816	590.62661	1
28451	H	76.16900	52.99880	71.21990	942.82897	-1441.18635	2609.90452	1
28452	H	76.18700	51.79780	72.51890	-1780.38202	-2477.76268	-773.81852	1
28453	C	76.84800	51.01580	70.56590	-694.96463	344.64043	505.02540	1
28454	H	75.93000	51.16180	69.95690	945.54010	1605.81791	2527.07957	1
28455	H	77.66100	51.23680	69.84290	2338.17225	477.56021	2020.49877	1
28456	S	76.94200	49.31380	71.19890	321.89148	421.36201	157.81853	1
28457	C	75.79700	48.59480	69.95690	806.63777	258.66977	286.31438	1
28458	H	75.35400	47.67380	70.39290	2044.24435	-2356.92010	-128.11922	1
28459	H	76.40800	48.33680	69.06590	-381.28376	-2311.72198	2079.18495	1
28460	H	75.08300	49.32480	69.51890	1716.52622	1360.77018	-2259.50478	1
28461	C	77.92300	53.80080	73.01490	-233.18361	649.87850	604.93159	1
28462	O	78.11000	54.94380	72.61990	495.46300	-563.50869	-183.25892	1
28463	N	77.71000	53.58280	74.34390	100.65679	-787.32945	232.92340	1
28464	H	77.59800	52.67680	74.74290	-1372.79735	-1220.06447	2546.63198	1
28465	C	77.68700	54.67680	75.33990	-692.86238	-96.71184	-609.48792	1
28466	H	76.94800	55.38980	75.00390	-1221.10306	2918.36097	24.42064	1
28467	C	77.20500	54.32980	76.79390	458.85473	23.54970	-789.51871	1
28468	H	77.72800	53.41580	77.14590	2359.85022	-1285.98696	-1615.57935	1
28469	O	75.76300	54.21780	76.78490	236.24222	-461.17558	-588.35400	1
28470	H	75.63300	53.42280	76.26290	3015.46709	-789.56478	-279.23609	1
28471	C	77.39900	55.42680	77.81890	-578.41851	437.98999	564.98504	1
28472	H	76.81700	55.15480	78.72490	2368.46184	2051.34901	266.49152	1
28473	H	78.42900	55.46880	78.23490	211.56592	3120.06031	-446.41509	1
28474	H	77.11100	56.36280	77.29590	-20.58772	-3016.18027	840.67074	1
28475	C	78.99300	55.41280	75.48290	687.58594	-564.76564	-89.68756	1
28476	O	79.01200	56.64380	75.52890	-72.80808	-763.43108	-147.16472	1
28477	N	80.04200	54.60680	75.54790	-413.03926	522.57987	-552.73081	1
28478	H	79.91100	53.62580	75.42390	-2363.99488	2078.31403	319.20582	1
28479	C	81.45000	55.05880	75.60490	192.77057	648.32466	-631.12515	1
28480	H	81.54600	55.60980	76.52890	618.85499	-631.37854	-3026.83569	1
28481	C	82.49400	53.85080	75.62690	583.99387	407.75279	-574.91718	1
28482	H	83.54200	54.17680	75.80090	-2246.75540	-1651.00346	-1481.88230	1
28483	H	82.40300	53.30880	74.66190	661.38133	2412.49974	-1929.45429	1
28484	C	82.13700	52.85880	76.75290	-384.31801	48.69163	-845.59085	1
28485	O	82.51800	51.66580	76.56390	-366.33450	32.11052	693.53208	1
28486	O	81.53100	53.20380	77.76190	273.46739	85.69504	719.27429	1
28487	C	81.81100	55.96680	74.36290	191.07950	711.94610	-558.54295	1
28488	O	82.31600	57.09180	74.51690	397.33695	427.86500	516.55973	1
28489	N	81.46000	55.58180	73.12090	215.06256	-730.25778	-343.62400	1
28490	H	80.97900	54.71980	72.97790	2561.49609	1058.46481	1456.86121	1
28491	C	81.68400	56.29980	71.95890	373.29787	-158.63586	-819.48279	1
28492	H	82.73300	56.54780	72.03390	-1985.35951	1760.62315	-1733.09934	1
28493	C	81.30300	55.39580	70.72990	-598.86198	334.82489	-635.78727	1
28494	H	81.29600	56.08680	69.85890	-2360.06664	-2021.26807	515.86011	1
28495	H	80.24900	55.09180	70.90490	-2718.56326	1295.70398	964.41133	1
28496	C	82.34400	54.32980	70.40590	27.33623	-668.74167	592.97615	1
28497	H	82.91800	54.03380	71.31090	-1081.80021	1995.99786	2182.82970	1
28498	H	83.11200	54.74680	69.71990	-630.04658	-2629.10792	1584.89821	1
28499	C	81.85800	53.05580	69.67590	641.70834	-556.51804	256.83039	1
28500	H	81.45300	53.35580	68.68590	-2536.46237	-597.54559	1774.03053	1
28501	H	81.02700	52.73880	70.34090	-304.91608	-1808.74736	-2562.40301	1
28502	C	82.96900	51.98280	69.53090	-534.38564	-505.31660	534.04030	1
28503	H	83.51800	51.86480	70.48990	1838.09856	1404.12533	2109.15433	1
28504	H	83.71600	52.20480	68.73890	1281.99051	-1523.49474	2404.62216	1
28505	N	82.51400	50.65680	69.16890	515.04050	538.95473	370.53903	1
28506	H	82.10400	50.74380	68.21690	-190.13789	2212.70846	-2254.23781	1
28507	H	83.32800	50.00980	69.15490	-713.26160	2027.10241	2299.52432	1
28508	H	81.81100	50.26080	69.82490	-1911.04524	-2324.52589	917.80348	1
28509	C	80.96500	57.63780	71.82890	815.72317	-325.03234	152.35509	1

28510	O	81.52700	58.63680	71.43890	512.93415	56.94395	-597.54262	1
28511	N	79.66900	57.69580	72.21290	52.01670	417.06737	-748.87031	1
28512	H	79.23700	56.80280	72.31390	1037.09729	-1311.13104	2642.06455	1
28513	C	78.91900	58.95380	72.34290	659.22263	16.59755	603.41964	1
28514	H	79.04000	59.54580	71.44790	-1811.21228	2281.86435	1222.59432	1
28515	C	77.45800	58.71880	72.77690	802.61771	-336.57817	-213.58723	1
28516	H	76.82600	59.62580	72.87990	-1473.59856	-649.11244	2697.99846	1
28517	H	77.44500	58.21880	73.76890	-2764.66404	1072.38694	1090.25763	1
28518	C	76.64300	57.82380	71.87090	555.18718	-72.68911	696.67511	1
28519	C	76.58300	58.10480	70.48090	180.27908	-831.79968	-289.55149	1
28520	H	77.12200	58.96280	70.10690	-2038.49597	1455.90393	-1940.08797	1
28521	C	75.81100	57.35880	69.59390	-637.89380	-130.97257	643.41760	1
28522	H	75.76500	57.60680	68.54390	-1792.66235	-1771.61723	-1895.69226	1
28523	C	75.22600	56.17080	70.00690	490.56358	-701.95528	238.57098	1
28524	O	74.53900	55.28780	69.16190	618.55470	38.41979	458.30495	1
28525	H	74.41500	54.44180	69.59890	-1247.53161	-2714.61327	-977.93117	1
28526	C	75.90500	56.70580	72.30390	-453.76185	-205.99898	760.18277	1
28527	H	75.83900	56.41280	73.34090	-1404.29579	2317.70838	1621.90511	1
28528	C	75.30900	55.81680	71.36490	-155.15144	500.59058	-766.93871	1
28529	H	74.94300	54.87280	71.74090	1858.48372	1919.08140	-1667.12813	1
28530	C	79.49600	59.91880	73.36590	301.23976	-614.19446	572.10292	1
28531	O	79.75100	61.08780	73.13790	153.03038	46.03056	-782.42903	1
28532	N	79.82100	59.45580	74.55290	-654.16877	-328.94787	-442.05920	1
28533	H	79.68400	58.49580	74.78390	2756.67813	-1441.96957	-345.16050	1
28534	C	80.44200	60.30880	75.56290	-742.01508	370.52257	-423.77706	1
28535	H	79.90500	61.24580	75.55490	-2799.54192	-889.18705	-1157.80006	1
28536	C	80.24100	59.73180	76.98690	321.60341	563.36220	-656.67806	1
28537	H	80.77400	60.48080	77.61190	2455.51025	135.91841	1937.63519	1
28538	H	80.74600	58.75980	77.17490	-1139.33646	2494.61413	-1580.45329	1
28539	C	78.72500	59.53680	77.40490	-666.56659	482.30459	-435.95067	1
28540	H	78.16700	60.42180	77.03090	2651.55890	1573.63102	-619.58722	1
28541	H	78.24300	58.62080	77.00190	-2111.54911	-1935.06133	1292.25797	1
28542	C	78.50600	59.36680	78.91590	21.72689	210.99136	878.89821	1
28543	H	78.94700	58.43680	79.33590	-84.79430	2305.11921	2142.04037	1
28544	H	77.42800	59.16480	79.09190	-1980.64394	-1060.00602	2195.92775	1
28545	N	79.05000	60.55680	79.71390	-238.88839	508.04631	632.57090	1
28546	H	79.41200	61.35180	79.22890	823.89614	-2912.76770	-817.54633	1
28547	C	79.10800	60.62180	81.05290	116.27213	-635.85154	-640.31617	1
28548	N	78.65600	59.79180	81.93890	-685.83957	-266.79913	408.43758	1
28549	H	78.00100	59.08680	81.66790	-1764.50460	-2212.02277	1356.22867	1
28550	H	78.68000	60.11080	82.88590	-1990.69027	-1557.58192	-1881.56193	1
28551	N	79.61200	61.72080	81.54490	-342.21461	-573.53169	-519.19126	1
28552	H	79.92100	62.44280	80.92490	-1569.90436	1503.25521	2276.22913	1
28553	H	79.73600	61.78780	82.53490	-1802.59164	1804.81454	-1870.79647	1
28554	C	81.91100	60.65180	75.26890	604.68752	451.14598	-519.84544	1
28555	O	82.34700	61.74380	75.64890	397.51844	684.78385	-59.07697	1
28556	N	82.63500	59.80580	74.56990	-203.18848	80.81452	-832.64986	1
28557	H	82.35300	58.85480	74.46790	-2543.02997	1473.73080	1152.81748	1
28558	C	83.96700	60.27580	74.06590	567.40208	-672.47994	154.58031	1
28559	H	84.51900	60.58080	74.94290	-2027.90668	-260.23289	2386.22520	1
28560	C	84.76500	59.15580	73.29790	793.40391	-153.07117	-405.62790	1
28561	H	84.27400	58.99080	72.31490	-1319.37419	1435.52047	-2497.10734	1
28562	H	84.62400	58.26080	73.94190	-1624.04533	2711.81323	61.77102	1
28563	C	86.25700	59.33680	73.14890	-750.89967	206.78175	483.97336	1
28564	H	86.42000	60.38280	72.81090	2268.82818	-2071.01965	-615.61842	1
28565	C	86.99400	59.10380	74.43890	-146.10957	767.61783	-504.18482	1
28566	H	88.03400	59.42780	74.21690	2302.95279	2068.15433	522.81187	1
28567	H	86.66200	59.73080	75.29390	1752.20163	-1713.06114	1938.23251	1
28568	H	86.94000	58.03480	74.73590	1604.56783	1956.19797	1851.63044	1
28569	C	86.78800	58.36680	72.08090	-48.22492	299.45066	847.80643	1
28570	H	86.63600	57.36080	72.52590	-1378.47833	2403.96486	-1534.07063	1
28571	H	87.88400	58.53880	72.02790	-277.69766	2658.91755	1658.31499	1

28572	H	86.34700	58.51580	71.07190	-2558.43979	1751.94101	613.96782	1
28573	C	83.83400	61.42680	73.15390	-362.71848	-402.29179	-748.11878	1
28574	O	84.63000	62.37580	73.26490	640.61715	417.09596	-190.34929	1
28575	N	82.85300	61.48880	72.22890	-710.43106	-433.01478	-187.86893	1
28576	H	82.23800	60.70680	72.16490	2542.85674	1728.83900	-652.21695	1
28577	C	82.51100	62.67080	71.40490	-188.53906	903.91366	-71.58609	1
28578	H	83.43700	63.02080	70.97290	2728.07422	947.22861	1211.86944	1
28579	C	81.45100	62.39580	70.30990	639.91855	643.08901	49.46190	1
28580	H	80.52300	61.97280	70.74890	-1139.26346	1226.96498	2663.46704	1
28581	H	81.11100	63.34480	69.84290	-1251.90463	-1022.28711	2689.56949	1
28582	N	83.07400	62.04880	68.49190	-81.66189	-813.53402	156.70630	1
28583	C	81.94000	61.60380	69.18490	537.95340	-711.61713	36.33552	1
28584	C	83.07900	61.30880	67.38090	-173.13829	811.54290	-420.68446	1
28585	H	83.93400	61.31080	66.70590	2689.75906	1611.42785	61.66388	1
28586	N	82.06700	60.43080	67.32990	10.26186	702.73093	-496.16498	1
28587	H	81.96900	59.68080	66.67590	2105.04890	2331.30333	-98.63259	1
28588	C	81.28500	60.67180	68.46190	735.32528	355.41164	-396.58890	1
28589	H	80.30900	60.21780	68.57990	2022.51039	202.40779	2376.57246	1
28590	C	81.99700	63.82580	72.29390	-173.03965	-881.25334	-110.37601	1
28591	O	82.45800	64.95180	72.13090	-754.64678	62.90660	-277.63139	1
28592	N	81.10700	63.58780	73.24290	-519.18868	-344.75678	561.45998	1
28593	H	80.64000	62.70880	73.29990	2248.83001	594.45047	-2119.91690	1
28594	C	80.62600	64.63480	74.15290	529.65895	431.64015	590.30548	1
28595	H	80.25900	65.41980	73.50690	1093.26837	2687.52873	-1243.49964	1
28596	C	79.51400	64.01580	75.02690	476.46596	691.14087	353.21247	1
28597	H	78.93200	63.32680	74.37890	1769.73449	-1438.98637	2138.56033	1
28598	H	80.05900	63.34980	75.72990	2036.79934	2149.96755	-1076.11436	1
28599	C	78.65200	64.92580	75.86790	140.97685	905.52865	-114.22640	1
28600	H	79.32500	65.43280	76.59190	1568.07336	-152.99894	-2727.91909	1
28601	C	77.84300	65.91680	75.11090	392.77156	407.55035	-726.16503	1
28602	H	78.40300	66.58380	74.41990	-2091.47387	-2117.92781	-1024.27187	1
28603	H	77.04300	65.37980	74.55790	1416.42658	-2267.79191	1621.53912	1
28604	H	77.34800	66.57180	75.85890	465.08608	689.66527	-3045.07112	1
28605	C	77.73700	63.96780	76.62590	168.36482	-623.48541	-638.28996	1
28606	H	78.25600	63.31880	77.36390	-2278.52532	-1434.00913	1620.31779	1
28607	H	77.23500	63.24180	75.95090	-2040.99628	-458.20412	-2366.16769	1
28608	H	77.01400	64.60180	77.18190	1027.60192	2981.43455	-114.18648	1
28609	C	81.76100	65.29180	74.99290	333.22464	310.75678	777.23595	1
28610	O	81.80900	66.50180	75.10190	437.31409	539.52976	367.53266	1
28611	N	82.73700	64.49880	75.49490	-444.22640	397.93849	-625.04323	1
28612	H	82.74800	63.51180	75.35190	2656.56263	-1423.62131	-864.91767	1
28613	C	84.02000	64.94880	76.06590	565.02296	-670.30737	180.94191	1
28614	H	83.77900	65.63080	76.86790	-1572.78517	1475.60702	2289.65810	1
28615	C	84.77200	63.73480	76.76590	585.89305	-672.89193	-116.52896	1
28616	H	85.81700	64.05580	76.96690	-1299.61019	2335.23294	1665.51197	1
28617	H	84.71000	62.84780	76.09990	2115.90920	2044.05967	-1126.94525	1
28618	O	84.15300	63.55380	78.01490	476.96398	-32.95950	-634.90335	1
28619	H	84.37800	64.25280	78.63390	-1795.72106	2073.85870	1549.15124	1
28620	C	84.93100	65.67980	75.13190	-673.68724	-278.74273	540.48053	1
28621	O	85.56500	66.64980	75.53790	-597.57678	-503.82375	-134.54697	1
28622	N	85.05100	65.29680	73.86190	-270.70807	751.85478	293.05525	1
28623	H	84.70800	64.42780	73.51290	-2118.45158	-129.69826	2318.13927	1
28624	C	85.69500	66.04380	72.82190	561.45053	376.20020	-622.14849	1
28625	H	86.70800	66.33380	73.05990	2753.48780	-1492.24392	-23.37662	1
28626	C	85.74100	65.15480	71.54090	-145.83835	-859.63305	-256.35246	1
28627	H	84.87900	64.46080	71.44990	135.50247	2098.86734	-2362.34690	1
28628	C	85.79600	65.94080	70.19390	441.26739	-353.98463	686.79908	1
28629	H	84.86900	66.50480	69.95490	2538.64818	-1356.58861	1217.81602	1
28630	H	85.96200	65.21880	69.36590	-1490.56290	-25.35099	-2793.18732	1
28631	H	86.63500	66.66980	70.17690	-1305.06859	2554.44327	1307.66197	1
28632	C	87.01400	64.26180	71.59490	-405.64969	631.87518	522.10195	1
28633	H	86.82200	63.39980	72.26990	-904.72875	-2476.78989	1693.98109	1

28634	H	87.92700	64.84480	71.84190	302.92711	-2964.45510	962.84788	1
28635	H	87.23900	63.84180	70.59090	-3037.53330	-809.79689	276.64244	1
28636	C	84.98600	67.39680	72.55390	-393.32703	-797.51248	-197.79958	1
28637	O	85.69000	68.41580	72.40690	199.36775	-506.32084	544.82362	1
28638	N	83.64700	67.48780	72.47490	204.78337	-304.06268	-766.66159	1
28639	H	83.09500	66.66380	72.57690	1581.85373	338.96549	2679.65555	1
28640	C	82.92000	68.76280	72.32790	-526.60786	267.78538	-719.66092	1
28641	H	83.22900	69.31680	71.45390	2013.32391	1701.52348	-1728.01662	1
28642	C	81.43200	68.40580	72.15790	637.44865	-290.80037	553.27639	1
28643	H	80.91900	69.33580	71.83390	-1736.41116	1327.30820	-2289.76061	1
28644	H	80.92200	68.18880	73.12090	-1767.57737	-1732.65182	1929.63341	1
28645	H	81.28100	67.60480	71.40290	-749.70618	1530.46326	2642.46123	1
28646	C	83.14400	69.72080	73.44490	-405.09772	822.85031	110.40997	1
28647	O	83.43900	70.90080	73.25090	530.46652	569.80595	-152.49182	1
28648	N	83.00700	69.24380	74.69190	-43.27364	584.07962	-631.63512	1
28649	H	82.62000	68.33680	74.84090	2957.51904	983.95912	373.06830	1
28650	C	83.27700	70.00580	75.90190	865.76783	34.81644	246.54996	1
28651	H	82.61000	70.85480	75.90990	-2620.10542	-274.61727	1716.83608	1
28652	C	83.12800	69.09680	77.13590	-196.61834	-620.89654	616.97021	1
28653	H	83.48300	69.52780	78.09690	-436.56227	1747.49376	2574.16073	1
28654	H	83.61800	68.12180	76.92790	544.35223	-3038.46759	-559.81073	1
28655	C	81.58900	68.79880	77.42290	498.91951	757.18393	-147.69318	1
28656	O	80.75700	69.59680	76.91990	627.15544	480.22106	22.23409	1
28657	O	81.33500	67.81580	78.15690	-688.35649	-118.13729	-390.35566	1
28658	C	84.71100	70.58080	75.95190	710.28357	62.14943	545.51439	1
28659	O	84.86800	71.75680	76.30490	-399.90626	-417.59084	521.09529	1
28660	N	85.74100	69.79480	75.67590	-423.22044	274.82805	-700.42962	1
28661	H	85.60700	68.83480	75.43990	2128.32981	-2190.93500	684.71940	1
28662	C	87.13300	70.09780	75.63590	-196.72757	-880.46224	-86.11464	1
28663	H	87.32400	70.52680	76.60790	1084.61033	-2107.91929	2039.74509	1
28664	C	87.91400	68.77880	75.41390	480.85260	-584.28204	473.82004	1
28665	H	87.59900	68.21680	74.50790	690.51699	2659.24696	1527.46952	1
28666	H	87.63200	68.11480	76.25890	-2490.50283	1391.59668	1334.80473	1
28667	C	89.44000	68.82480	75.48290	684.11273	578.34543	-178.96211	1
28668	H	89.72900	69.58180	74.72290	289.29758	-1738.75085	2582.22371	1
28669	C	89.94100	69.29480	76.88690	174.38105	689.19533	560.16841	1
28670	H	89.75800	68.53080	77.67190	2535.90943	1857.66092	-105.84251	1
28671	H	91.05200	69.32680	76.88190	1539.02314	717.62985	2627.65635	1
28672	H	89.44900	70.26980	77.09490	2906.56806	815.37650	852.77664	1
28673	C	89.95100	67.43480	75.03090	-444.50546	-432.26796	652.07167	1
28674	H	89.65900	67.25180	73.97490	-2239.97514	-1197.87058	1846.04092	1
28675	H	91.05800	67.51580	75.08490	-2356.10899	2044.79560	-508.57009	1
28676	H	89.58900	66.62280	75.69590	2308.54338	2123.01573	209.09856	1
28677	C	87.46200	71.14180	74.60090	234.95944	-506.52872	695.86758	1
28678	O	88.19800	72.07180	74.83790	234.35813	-365.26392	635.72529	1
28679	N	86.84400	71.04980	73.39090	-215.36365	-781.64143	196.43057	1
28680	H	86.17000	70.32580	73.26190	-2338.92391	-1636.53352	1312.76193	1
28681	C	87.01800	71.85880	72.20590	-806.88972	-376.02903	-233.72847	1
28682	H	88.03400	71.65880	71.90090	-1378.42024	-1171.78121	-2591.61169	1
28683	C	86.05600	71.26180	71.07990	-555.16034	-632.00221	336.31036	1
28684	H	85.03600	71.30180	71.51890	1888.63044	-2208.57001	1156.46511	1
28685	H	86.42000	70.23180	70.88090	-1167.34001	-2070.03045	2043.27270	1
28686	C	86.06000	71.96180	69.68690	-568.74987	626.10426	-389.78315	1
28687	H	85.52600	72.93580	69.71790	1886.27144	-321.80314	2473.19221	1
28688	C	87.48200	72.28980	69.17990	210.98311	-621.34433	-636.20499	1
28689	H	88.21400	71.45680	69.22790	746.15447	3053.56996	212.05655	1
28690	H	87.92000	73.10780	69.79090	-684.62915	2382.48548	-1967.98936	1
28691	H	87.44600	72.71180	68.15290	1926.43750	1436.71787	2009.53204	1
28692	C	85.20100	71.16880	68.59090	61.11321	-580.92244	676.17695	1
28693	H	85.60800	70.14180	68.47390	346.11036	-2851.62702	1243.02934	1
28694	H	84.15200	71.20580	68.95590	-2370.25080	2039.63274	-481.60652	1
28695	H	85.20300	71.73380	67.63390	1731.23255	-17.59462	-2632.89556	1

28696	C	86.64900	73.30080	72.42790	163.28429	-748.51710	461.82059	1
28697	O	87.45100	74.21280	72.17190	113.86102	-360.95213	-702.78116	1
28698	N	85.50800	73.52580	73.11090	153.99283	-278.72627	-791.25266	1
28699	H	84.97100	72.71180	73.31890	2613.17707	-1503.53325	-871.33234	1
28700	C	85.11500	74.80280	73.59690	619.57897	-467.29983	444.62417	1
28701	H	85.32400	75.60080	72.90090	1523.05296	1543.69951	-2295.20525	1
28702	C	83.55300	74.85180	73.84290	668.54820	215.29355	563.47643	1
28703	H	83.38800	74.05380	74.59790	-1792.45025	-1107.39065	2323.78595	1
28704	H	83.04800	74.70080	72.86490	-1457.58158	-2327.13776	1514.13478	1
28705	C	83.06600	76.20680	74.31390	-323.03519	801.24789	312.75377	1
28706	C	83.49400	77.39480	73.61290	-689.97272	365.06017	475.19578	1
28707	H	84.09300	77.25680	72.72490	-734.23668	2303.08153	-2041.40415	1
28708	C	83.02700	78.64780	74.04590	587.49427	-643.17893	-241.28433	1
28709	H	83.34500	79.53480	73.51790	2485.51139	418.75734	1864.67758	1
28710	C	82.11700	78.73280	75.12690	-71.89238	806.18347	-453.24246	1
28711	H	81.80600	79.73380	75.39090	-2027.94785	295.00080	2380.23334	1
28712	C	82.25700	76.31380	75.36790	510.48864	702.47055	-306.69678	1
28713	H	81.88900	75.42480	75.85690	-289.18882	3139.61089	-184.24328	1
28714	C	81.80600	77.52180	75.83390	156.06689	-637.24516	-632.74150	1
28715	H	81.02300	77.59480	76.57490	1612.26280	1961.78209	1854.02292	1
28716	C	85.85600	75.28680	74.89890	551.95939	-309.91492	631.47376	1
28717	O	86.21200	76.46780	74.94090	-622.98865	-320.39066	351.38957	1
28718	N	86.17100	74.39980	75.83690	359.64670	191.00978	723.75952	1
28719	H	86.02200	73.41680	75.76590	-970.43444	631.97442	2914.49181	1
28720	C	86.82000	74.75980	77.14490	87.69195	-698.96611	551.73209	1
28721	H	86.15300	75.48880	77.57990	-2695.54495	380.20029	1572.31070	1
28722	C	86.94000	73.58780	78.11590	405.86190	710.47600	-428.31252	1
28723	H	87.14500	72.68280	77.50590	2422.59196	1815.12457	843.57357	1
28724	C	88.11000	73.73880	79.17790	428.61189	-776.20205	-185.22671	1
28725	H	89.11200	73.50380	78.75790	-2806.92243	16.83858	-1447.14204	1
28726	H	87.89000	73.00680	79.98390	1685.23580	-2012.55682	1704.33945	1
28727	H	88.01200	74.79180	79.51590	-2368.79835	1465.10246	-1493.42098	1
28728	C	85.60400	73.41880	78.88190	484.62585	400.59295	647.95356	1
28729	H	85.67200	72.50580	79.51190	2300.79418	1928.88099	-962.90899	1
28730	H	85.36200	74.27280	79.54890	1146.40760	-2914.76946	-169.78304	1
28731	H	84.74200	73.40480	78.18090	843.78006	-2259.07019	1993.41069	1
28732	C	88.17300	75.40380	76.92690	264.77688	-690.54514	-536.01145	1
28733	O	88.54300	76.32780	77.61390	218.61823	-465.92783	-607.38923	1
28734	N	88.89700	74.85580	75.91890	-243.42236	-506.67748	-642.29400	1
28735	H	88.53000	74.08180	75.40890	-407.67356	2264.76943	2138.82319	1
28736	C	90.29200	75.32580	75.66290	-234.40314	-237.15189	830.43962	1
28737	H	90.89600	75.29980	76.55790	2240.78219	1868.00603	-1197.47755	1
28738	C	90.95300	74.41080	74.56690	334.29043	772.11828	342.51084	1
28739	H	90.23300	74.14880	73.76190	2546.44324	1660.15825	784.80284	1
28740	C	92.24400	75.00980	73.95790	-645.07261	646.62843	104.52492	1
28741	H	92.97600	75.11480	74.78690	-1458.79765	1645.51120	2239.52190	1
28742	H	92.67300	74.27880	73.23890	1794.58241	-2161.55303	1376.27765	1
28743	H	91.99400	75.90680	73.35290	2247.46825	-2185.05023	-116.54220	1
28744	C	91.30800	73.01580	75.20290	573.33390	-205.85473	-688.57652	1
28745	H	90.39500	72.66380	75.72790	-1260.53149	2450.10615	1518.60766	1
28746	H	92.16300	73.06880	75.90890	-2573.04807	-1163.32955	-1412.85416	1
28747	C	91.58000	71.93880	74.11790	-553.14185	730.58761	87.31651	1
28748	H	92.58900	72.13780	73.69690	-1858.08883	1933.12470	1643.90721	1
28749	H	90.83500	71.82580	73.30090	3072.52870	564.95627	285.29521	1
28750	H	91.68900	70.94580	74.60390	1163.99858	2856.99260	-652.47489	1
28751	C	90.27000	76.76580	75.16090	38.30557	537.61062	-758.33933	1
28752	O	91.26100	77.50980	75.35290	-674.55837	-410.81316	-48.72602	1
28753	N	89.15800	77.21180	74.50990	-191.70675	-537.10239	-634.09308	1
28754	H	88.43600	76.60280	74.19090	1194.56770	1551.73528	2448.10681	1
28755	C	89.12800	78.59280	74.10490	378.96849	511.12210	639.29392	1
28756	H	90.03400	78.84180	73.57190	1470.69278	-1255.36802	-2491.77053	1
28757	C	87.93400	78.86780	73.12990	-27.84526	-728.51622	520.24415	1

28758	H	88.03500	79.86580	72.65290	876.40526	-2359.39646	-1890.10186	1
28759	O	86.60800	78.75480	73.78290	495.95419	-516.54046	293.91090	1
28760	H	86.49900	77.90180	74.21090	3134.28441	37.17456	177.07715	1
28761	C	87.97000	77.75680	72.01390	-720.89828	-534.08487	-182.72049	1
28762	H	87.68400	76.74380	72.36890	1930.46344	2477.82300	-230.55865	1
28763	H	87.16200	78.06680	71.31790	1557.93958	-1305.16330	-2407.19683	1
28764	H	88.96600	77.83780	71.52890	194.85999	-1555.74549	2705.57919	1
28765	C	88.96700	79.58880	75.24390	-550.58253	-590.12663	-435.39817	1
28766	O	89.33600	80.75080	75.13190	-477.31486	-507.99957	-382.19602	1
28767	N	88.46200	79.15180	76.40990	-47.42215	-808.61943	-224.71508	1
28768	H	88.27300	78.17780	76.50590	-1756.36428	-1459.09255	-2178.40565	1
28769	C	88.07500	80.00680	77.54090	-25.15273	197.34172	875.68303	1
28770	H	87.30100	80.66680	77.17790	2299.28682	339.27316	-2134.39597	1
28771	C	87.30500	79.28680	78.65090	-597.13852	191.94809	-682.03055	1
28772	H	87.05400	79.85480	79.57290	-2000.43677	1725.52346	-1734.54222	1
28773	H	87.98500	78.45680	78.93890	45.74815	-2579.97166	1771.68714	1
28774	C	85.94700	78.73980	78.20890	-393.93245	323.11955	746.86611	1
28775	H	86.02600	78.13580	77.27990	-2806.97186	1422.60668	-221.13972	1
28776	C	85.44800	77.83980	79.37790	-898.42423	-1.33234	-183.55856	1
28777	H	86.11200	76.94880	79.37190	224.49532	-2785.13879	-1442.62808	1
28778	H	85.48900	78.35180	80.36290	-2612.37491	1759.50386	-153.13173	1
28779	H	84.39600	77.56880	79.14390	-3048.83379	-117.47447	762.98199	1
28780	C	84.96300	79.87180	77.92290	-898.94532	94.24828	130.46834	1
28781	H	85.05400	80.27480	76.89190	2456.03826	1971.53293	28.66630	1
28782	H	85.04300	80.76780	78.57490	-1999.64707	-1887.74570	-1532.91368	1
28783	H	83.95600	79.43980	78.10290	829.36633	-1446.17845	-2675.20727	1
28784	C	89.17800	80.94580	78.08890	-713.45087	499.54925	272.56908	1
28785	O	88.80600	82.04980	78.42590	648.80847	456.07285	-2.94969	1
28786	N	90.47200	80.68380	78.13390	-571.30315	-11.82846	605.53011	1
28787	C	90.96500	79.30680	78.36890	-411.78602	-441.37848	-698.25945	1
28788	H	91.18800	78.92780	77.34790	-1622.97689	1662.22752	2111.58483	1
28789	H	90.26700	78.62680	78.90290	-1442.24204	-1849.69777	-2109.49779	1
28790	C	91.54100	81.64680	78.45690	-30.70912	-442.96606	-810.87662	1
28791	H	91.23900	81.98780	79.43590	1755.55944	-1801.73556	-1900.06920	1
28792	C	92.73700	80.82480	78.49790	-844.24673	150.74586	-336.96245	1
28793	H	93.63600	81.30280	78.94390	414.48463	-1803.38382	2520.14860	1
28794	H	93.12400	80.48380	77.51490	13.66557	-2362.14001	-2090.16911	1
28795	C	92.24000	79.53580	79.14890	-349.04111	-205.26436	797.25696	1
28796	H	92.99800	78.74380	78.96890	-2029.62439	2409.71880	-131.22772	1
28797	H	92.10900	79.69280	80.24090	1906.94672	925.88891	-2345.24323	1
28798	C	91.62700	82.88080	77.58990	246.80872	696.13406	-561.31701	1
28799	O	92.02600	83.95080	78.05690	148.41707	-164.22806	737.78931	1
28800	N	91.29900	82.78080	76.30590	-333.75937	603.45044	-515.50931	1
28801	H	91.10600	81.91780	75.84690	1442.67546	2799.43946	-125.39753	1
28802	C	91.14300	83.99380	75.47590	609.73468	-311.55412	-613.73001	1
28803	H	92.02900	84.60980	75.52090	339.46346	2842.33107	1301.19709	1
28804	C	90.89300	83.53080	73.98690	513.78702	-491.63094	-578.72229	1
28805	H	89.88900	83.05780	73.93690	2124.91896	1644.82028	1621.81200	1
28806	H	90.85600	84.47980	73.41090	-1260.19752	2235.62675	-1849.36340	1
28807	C	92.01000	82.69580	73.39690	-551.87153	500.28007	518.45896	1
28808	C	93.29400	83.19280	73.34590	782.08915	-194.34887	396.18078	1
28809	H	93.55400	84.19180	73.66590	2078.36162	1136.63265	-2089.78906	1
28810	C	94.39900	82.58680	72.68290	-623.44556	-283.99407	583.82605	1
28811	H	95.32400	83.13780	72.59590	651.14999	2027.78267	2298.48005	1
28812	C	94.10100	81.35380	72.07090	594.22044	415.06221	531.46264	1
28813	H	94.80900	80.81280	71.46190	2038.53133	-1252.23848	-2053.53216	1
28814	C	91.83500	81.41480	72.88390	-375.96232	-308.42326	-789.59499	1
28815	H	90.85900	80.95880	72.95990	2815.39528	1345.06334	-407.59520	1
28816	C	92.82900	80.73080	72.21990	272.08127	875.04754	-25.69892	1
28817	H	92.53500	79.82280	71.71490	659.96160	-2796.00586	1245.05429	1
28818	C	90.05300	84.85580	75.95490	650.87763	572.87026	-310.32920	1
28819	O	90.14587	86.11234	75.77375	-124.01111	-678.17334	177.28012	1

28820	N	88.89800	84.23980	76.38290	-70.42080	-678.34391	470.04024	1
28821	H	88.83200	83.24980	76.48090	1529.10648	549.43358	-2710.99196	1
28822	C	87.77100	84.95680	77.05290	-792.30918	77.85748	432.24572	1
28823	H	87.51159	85.75114	76.30439	148.08212	1495.59116	-2578.30328	1
28824	C	86.55800	84.09580	77.20590	168.73112	505.48003	730.74729	1
28825	H	85.74200	84.75480	77.57290	-13.96029	1997.90591	2423.59123	1
28826	H	86.63600	83.28580	77.96190	-1440.86034	-2239.20863	1649.65174	1
28827	C	85.94200	83.48480	75.94290	-437.56689	-524.43407	-612.24198	1
28828	C	86.43200	82.68380	74.93490	-341.74798	788.44006	316.37283	1
28829	H	87.49000	82.51880	74.79890	2681.02996	-1067.97892	1221.95974	1
28830	N	85.42800	82.11980	74.20990	-289.74452	729.39974	321.89520	1
28831	H	85.59200	81.26780	73.76190	-660.60189	1792.30253	-2522.39122	1
28832	C	84.25200	82.63580	74.59690	744.98951	-439.36109	-276.04899	1
28833	C	84.51500	83.48880	75.69290	565.29046	483.32508	520.06192	1
28834	C	83.41000	84.02980	76.41090	-683.06443	157.81169	575.13206	1
28835	H	83.66700	84.57280	77.30890	-3136.55166	-233.37395	-102.04177	1
28836	C	82.13800	83.76480	75.96090	-657.41259	-454.69968	418.70917	1
28837	H	81.32000	84.18880	76.52390	2397.64680	-848.48622	1832.92438	1
28838	C	82.96000	82.40980	74.11690	-620.77357	-646.41178	126.94814	1
28839	H	82.82800	81.82880	73.21690	3099.47862	-406.92692	281.51623	1
28840	C	81.86200	82.98280	74.83290	-46.44835	664.97202	622.10919	1
28841	H	80.85600	82.74780	74.51690	1528.18771	-1254.33206	2427.89416	1
28842	C	88.13183	85.68674	78.46632	49.40242	-77.90216	694.16675	1
28843	O	87.66123	86.74919	78.77297	117.15638	-349.01017	-538.65717	1
28844	N	88.88700	84.89880	79.22090	-37.98239	148.65045	-847.99748	1
28845	H	89.17100	83.95280	79.08290	-2208.41131	-2223.07313	-227.87872	1
28846	C	89.46148	85.47798	80.41173	-317.03098	-1168.30876	363.86974	1
28847	H	88.57344	85.88963	80.95953	2237.08556	337.44443	-1611.39337	1
28848	C	90.14400	84.27080	81.25390	381.71611	-496.37928	640.64734	1
28849	H	90.98300	83.74980	80.74590	2224.94998	1546.72725	-1624.49596	1
28850	H	89.46800	83.42280	81.49390	-1276.76834	889.99227	-2753.08297	1
28851	H	90.53800	84.71780	82.19190	-2538.47142	-1847.50412	-73.64145	1
28852	C	90.49868	86.71988	80.13821	-535.35754	413.05951	-20.10553	1
28853	O	90.96327	87.37099	81.06055	-1011.31959	721.22617	-15.35339	1
28854	N	90.85491	86.89254	78.81553	-128.02360	-542.94757	56.72784	1
28855	H	90.33414	86.16697	78.32807	1689.44873	-1299.50938	1486.46512	1
28856	C	91.33968	88.10425	78.28857	461.60987	86.82200	305.51018	1
28857	H	91.76726	88.57189	79.16613	1415.61853	-3690.52459	-174.15243	1
28858	C	92.56679	87.76788	77.30550	-846.97015	666.31839	-290.36652	1
28859	H	92.07037	87.25587	76.41631	-3972.95428	-1124.50905	-610.37065	1
28860	C	93.53013	88.94203	76.97683	-452.39175	405.43898	-303.38794	1
28861	H	92.96278	89.57347	76.28521	388.39493	-650.28449	-395.58364	1
28862	H	93.85319	89.55619	77.85998	-1542.06265	-2158.54899	-2547.38201	1
28863	H	94.39399	88.55149	76.39124	867.08179	-39.24035	-611.54887	1
28864	C	93.41216	86.63382	77.97906	-8.66450	466.34136	-431.67196	1
28865	H	93.61607	86.86424	79.11007	2861.30695	-195.51492	3641.46853	1
28866	H	94.43994	86.60557	77.50552	1230.03216	6306.08375	-2627.79040	1
28867	H	92.93367	85.64948	77.96022	542.15539	2176.78359	2106.78364	1
28868	C	90.10889	88.97329	77.67209	-325.80993	-168.63665	641.52630	1
28869	O	90.11072	90.19216	77.91799	-81.49334	-960.18814	-55.62084	1
28870	N	89.44859	88.35777	76.73412	147.17131	506.67903	-110.25850	1
28871	H	89.40664	87.31824	76.48855	-1494.37267	2590.88491	645.97974	1
28872	C	88.80090	89.30996	75.79381	1322.72369	-143.46107	558.77570	1
28873	H	89.46044	90.15183	75.55005	-2533.40774	3672.50099	-2409.23530	1
28874	C	88.68132	88.45355	74.50127	820.37772	957.42621	98.91166	1
28875	H	88.79861	89.06256	73.52193	3297.53790	-7903.70120	1464.28512	1
28876	H	89.46465	87.65417	74.42804	1047.41645	-298.62993	192.76730	1
28877	C	87.15237	87.88955	74.28574	-1055.62731	-1033.51998	212.08451	1
28878	O	86.68699	87.11148	75.11816	245.18416	797.79711	-84.85104	1
28879	O	86.44709	88.23890	73.34106	4.73418	-878.04030	-506.09658	1
28880	C	87.41919	89.76281	76.46129	-683.07293	268.50895	-345.94626	1
28881	O	86.81258	90.61201	75.83591	429.37569	143.57949	217.79148	1

28882	N	87.07499	89.33629	77.69339	517.76150	-606.73502	-10.85161	1
28883	H	87.39113	88.39721	78.03735	-27.96393	-977.73105	3421.55378	1
28884	C	85.94777	90.07455	78.26343	1254.59867	-846.85207	-170.50525	1
28885	H	85.25159	90.42395	77.51018	-315.68510	1054.61233	-2782.10345	1
28886	C	85.00133	89.11373	79.15231	-150.12034	83.98725	262.62385	1
28887	H	84.80008	88.12390	78.65622	-3816.77343	-4347.05648	1278.58686	1
28888	H	85.38240	89.00095	80.19943	-1060.65748	873.86640	-1567.94131	1
28889	H	84.04627	89.60471	79.10180	1475.64127	-1639.27964	2233.98856	1
28890	C	86.43752	91.20155	79.24224	640.23304	-111.89438	-17.39216	1
28891	O	85.58033	91.96011	79.67544	-12.31455	-389.15858	-38.74513	1
28892	N	87.79422	91.26841	79.42741	282.44975	-476.98450	82.02895	1
28893	H	88.16277	90.39364	79.01841	-3773.19350	-1465.95608	-919.59129	1
28894	C	88.47139	92.02150	80.37842	366.49475	-339.06382	-4.34869	1
28895	H	87.71656	92.37914	81.08372	-1362.75270	2100.87273	1024.28263	1
28896	C	89.61944	91.15635	81.08322	-107.66655	683.06735	-74.03182	1
28897	H	90.50511	91.17384	80.46147	-111.54739	878.25100	-346.32535	1
28898	C	89.93229	91.86475	82.44857	-1.51201	825.02303	-464.06746	1
28899	H	90.79273	91.32720	82.94174	-291.03755	602.75534	-1312.24292	1
28900	H	90.15482	92.92155	82.45320	972.70399	645.74753	-1835.93164	1
28901	H	89.05585	91.72040	83.16753	3594.93929	2013.34574	2734.12274	1
28902	C	89.11917	89.72147	81.41996	407.65526	-337.78766	-616.29882	1
28903	H	89.36560	89.06382	80.53510	-1444.54670	1696.77040	1167.17274	1
28904	H	88.05048	89.65295	81.65799	-96.84439	803.46974	-1361.19199	1
28905	H	89.67341	89.22839	82.21828	-2910.81457	-1001.04651	-2040.28499	1
28906	C	89.36106	93.27167	79.76389	193.25270	-715.56775	-281.86899	1
28907	O	89.59381	94.27509	80.42027	-217.05435	14.06951	-254.14269	1
28908	N	89.93174	92.84992	78.65053	-340.66212	-33.23452	465.63413	1
28909	H	89.77462	91.88859	78.22966	-6.52526	-3345.91301	1110.94243	1
28910	C	90.83209	93.81514	78.07052	240.73886	-181.34341	-102.69880	1
28911	H	90.54583	94.80283	78.57064	1307.70249	-366.25459	-1386.92901	1
28912	C	92.32290	93.43797	78.53502	81.40172	632.23073	261.97246	1
28913	H	93.03410	94.22024	78.34472	-3486.02716	-476.28150	-291.86938	1
28914	H	92.43540	93.21727	79.60639	2620.16881	-1283.42464	-2300.97693	1
28915	H	92.67178	92.54840	77.95497	1959.01740	2722.46436	238.30055	1
28916	C	90.65856	93.68129	76.48594	678.99435	-458.77553	-557.09987	1
28917	O	90.33703	94.66655	75.85942	-242.49030	-518.90281	-388.44051	1
28918	N	91.04615	92.47166	75.99842	-87.95934	-540.82073	50.29642	1
28919	H	91.38700	91.63425	76.43590	-3281.49823	487.57229	2332.81096	1
28920	C	90.88459	92.39731	74.57105	1073.33079	-135.69870	432.99716	1
28921	H	89.96109	92.94356	74.19138	-416.19946	-80.51822	-2151.60272	1
28922	C	92.19623	92.98623	73.91618	697.59800	657.98233	313.08226	1
28923	H	92.61472	93.73072	74.67121	1138.71912	2153.92655	2351.45543	1
28924	H	92.98062	92.27789	73.81917	1498.40849	-915.80176	2985.15101	1
28925	C	91.85987	93.72634	72.54063	-325.92402	280.03593	-246.03307	1
28926	O	91.06057	94.66237	72.45364	456.61969	-115.89507	-86.52346	1
28927	N	92.59710	93.25536	71.54385	323.19387	-145.80454	-156.63710	1
28928	H	93.22224	92.40673	71.54337	-1526.05140	631.47524	-1209.51931	1
28929	H	92.49249	93.52496	70.52840	118.94815	-2977.50971	-1547.28359	1
28930	C	90.92524	90.82607	74.09069	-120.20309	154.71057	944.73911	1
28931	O	91.70063	90.00086	74.59177	-439.68880	-684.73590	598.63062	1
28932	N	90.18239	90.59986	72.98729	263.86901	422.76992	182.59628	1
28933	H	89.72733	91.50180	72.72269	373.21992	1852.29787	2282.18100	1
28934	C	90.53883	89.60885	72.05512	31.49920	-593.69435	-181.03769	1
28935	H	90.62401	88.65650	72.69490	2473.10538	-833.07884	1123.06119	1
28936	C	89.42084	89.52841	70.91958	-369.34327	328.71634	-272.28899	1
28937	H	89.51655	90.43882	70.31795	-1823.35073	-1842.89762	-1222.44939	1
28938	H	88.36775	89.68230	71.34899	1476.63657	-2646.61166	1788.74932	1
28939	C	89.53066	88.24351	70.15264	-514.91291	-929.33763	-235.40536	1
28940	C	89.91359	88.10962	68.79490	-156.51342	-368.68042	-194.47824	1
28941	H	90.02132	88.90453	68.03621	-1528.56275	1951.34516	804.63982	1
28942	N	90.09364	86.82751	68.50868	-108.35168	472.93793	-561.37635	1
28943	H	90.41690	86.44013	67.60413	1976.62297	269.47734	-50.69802	1

28944	C	89.71442	86.00322	69.52674	559.05985	-287.90164	389.66464	1
28945	C	89.25296	86.89295	70.64898	2043.21790	270.24624	151.46571	1
28946	C	88.62511	86.42724	71.84784	994.44930	-89.95925	151.02129	1
28947	H	88.39955	87.07983	72.70796	0.25085	2932.00147	-827.87079	1
28948	C	88.64077	85.05455	71.95907	315.26452	184.26450	71.55458	1
28949	H	88.40421	84.63172	72.98212	2526.10569	165.48025	-46.02765	1
28950	C	89.56154	84.59272	69.68460	213.78325	575.26256	-127.30969	1
28951	H	89.64257	83.77791	68.82792	2714.69233	705.39367	-3576.68223	1
28952	C	89.08951	84.16888	70.96388	212.26509	-1010.61453	490.07193	1
28953	H	89.06416	83.07005	71.22607	747.27133	-560.26087	-1622.09449	1
28954	C	91.93294	90.01785	71.27680	781.60877	-690.88617	487.79152	1
28955	O	92.04327	90.38689	70.12776	101.85503	-153.72926	153.44150	1
28956	N	92.93788	89.75375	72.08268	-31.77593	284.45256	549.10246	1
28957	H	92.80637	89.46907	73.06335	498.11512	-1569.62860	1413.78792	1
28958	C	94.30640	89.90973	71.71775	-557.46125	90.40278	248.36040	1
28959	H	94.40319	90.96987	71.30364	3163.78892	1496.24239	-18.47989	1
28960	C	95.23468	89.74664	73.02474	-274.89317	447.90848	486.74031	1
28961	H	94.77435	89.00068	73.65269	-2762.38708	1115.50245	-1286.17637	1
28962	H	96.27005	89.38712	72.79891	-2999.30461	-1307.19516	2126.26936	1
28963	C	95.09920	91.11478	73.71906	376.16264	38.59088	-325.19978	1
28964	C	94.72344	91.10860	75.06422	-411.49544	-614.21531	-882.95761	1
28965	H	94.50442	90.19156	75.64790	-792.46997	-2161.43418	1233.61950	1
28966	C	94.69386	92.25321	75.85655	387.73033	6.97664	149.47668	1
28967	H	94.42507	92.18915	76.93324	3157.70139	613.20761	-3264.94224	1
28968	C	95.02121	93.48279	75.30595	-503.68092	-298.60371	194.30885	1
28969	O	94.72603	94.61953	76.05328	-52.85764	395.79874	-348.10853	1
28970	H	95.28935	95.33052	75.74470	690.54064	107.33970	342.45579	1
28971	C	95.49654	92.37099	73.16133	-75.73926	-610.30284	31.25134	1
28972	H	95.90702	92.38319	72.11495	-449.02884	-4870.14775	-2616.14663	1
28973	C	95.49994	93.49854	73.96097	-5.02199	-631.34047	-288.94796	1
28974	H	95.70404	94.45550	73.48926	-2699.66230	303.92906	-763.35834	1
28975	C	94.84457	88.83353	70.68633	-1216.41435	-399.93626	-2.86929	1
28976	O	96.04285	88.52234	70.68193	361.30888	-768.92458	-573.69949	1
28977	N	93.93267	88.48496	69.72418	-481.97883	-130.44523	165.82859	1
28978	H	92.98169	88.80193	69.84150	1525.29923	469.67075	-539.63687	1
28979	C	94.16742	87.17142	69.21015	290.05868	322.54179	24.13828	1
28980	H	95.21603	87.05475	69.54349	1739.52437	-2331.90194	468.67234	1
28981	C	93.09422	86.11525	69.74355	312.53194	54.89978	471.01334	1
28982	H	93.40670	85.07158	69.31530	-208.04149	-2270.33312	-3377.63179	1
28983	H	92.03511	86.23770	69.44603	-314.06818	-472.10723	1459.81006	1
28984	C	93.12343	86.13735	71.25187	-80.64746	451.52072	-364.65939	1
28985	C	94.41764	85.85822	71.87858	548.57958	2095.13644	30.40132	1
28986	H	95.22776	85.55837	71.21149	-812.40673	1669.75846	2309.16165	1
28987	C	94.48283	86.03169	73.28716	-389.24080	-8.51887	1.53072	1
28988	H	95.52029	85.84208	73.66275	1931.74895	2434.39196	-1669.36677	1
28989	C	93.31885	86.41368	74.08191	152.42183	-746.07415	-258.16258	1
28990	H	93.34994	86.44573	75.18101	1423.47101	-1849.85235	-829.01987	1
28991	C	92.03070	86.62014	72.01794	-60.57382	-180.12718	-51.17209	1
28992	H	91.11035	87.04208	71.59235	-64.02363	-4590.98466	1393.53831	1
28993	C	92.12652	86.76631	73.42653	-44.61035	-151.51755	-250.20162	1
28994	H	91.15381	87.12645	73.97415	-2092.84634	-156.54250	-3188.12668	1
28995	C	94.15208	87.26211	67.58189	-1130.27475	28.40839	471.82855	1
28996	O	95.04368	86.75294	66.91716	26.73706	804.73707	449.72717	1
28997	N	92.94461	87.66614	67.15117	-256.55254	815.55847	-1409.29794	1
28998	H	92.25425	88.02373	67.87551	-1737.34688	-4426.08681	-3348.54008	1
28999	C	92.85370	88.24074	65.79729	-726.78838	569.59501	1206.89922	1
29000	H	93.77368	87.85581	65.22280	-1231.72200	-192.70816	4306.29850	1
29001	H	92.89099	89.32761	65.87339	-1627.56348	376.45135	1663.07800	1
29002	C	91.47359	87.80621	65.20106	-7.75062	298.17957	250.47851	1
29003	O	90.61298	87.06424	65.80272	-324.48108	561.68809	-320.09661	1
29004	N	91.26064	88.32305	64.03173	110.99306	672.83240	331.30264	1
29005	H	91.94660	88.86887	63.53401	-2993.89870	-1023.53465	2729.97631	1

29006	C	89.99508	87.99373	63.41090	177.71408	-412.89825	-144.04033	1
29007	H	89.26792	88.03753	64.26705	2322.49325	2189.22769	251.54913	1
29008	C	89.65327	89.13627	62.40960	948.62122	210.29686	-785.54391	1
29009	H	89.99091	88.86949	61.38575	-2293.88296	-227.42527	-1315.54158	1
29010	H	90.23761	90.10777	62.61768	1471.17024	1378.67618	1691.36655	1
29011	C	88.09746	89.34212	62.35416	700.36725	394.31858	-236.71873	1
29012	O	87.61504	90.42761	62.13086	146.54938	734.94310	116.98537	1
29013	N	87.43318	88.17441	62.68370	-52.25101	131.22670	341.61422	1
29014	H	87.82138	87.27419	62.50499	-1833.99093	-732.62543	1094.61289	1
29015	H	86.38002	88.14646	62.55205	-455.56918	-1252.79543	-826.57095	1
29016	C	90.12268	86.47329	62.74320	-110.11522	32.16948	315.79286	1
29017	O	89.09477	85.95561	62.32991	-425.37835	-132.00356	218.94896	1
29018	N	91.35009	86.02762	62.69250	141.50596	-437.39453	284.65114	1
29019	H	91.99963	86.61442	63.22634	3.29442	1772.74554	-1989.29057	1
29020	C	91.51800	84.51480	62.52590	-314.75420	335.51957	-812.91684	1
29021	H	90.87200	84.13680	61.74790	641.53811	1483.60040	-2718.49567	1
29022	C	92.98800	84.28580	62.01190	-250.03390	376.38662	779.54344	1
29023	H	93.08100	84.82880	61.04690	1073.49440	-2915.84025	-440.92626	1
29024	H	93.75600	84.78580	62.63890	1117.83600	-2197.71093	1920.81051	1
29025	C	93.37900	82.83780	61.76390	596.64009	-547.02170	-412.17673	1
29026	C	93.09300	82.24380	60.53090	-482.12258	-649.23028	-444.68798	1
29027	H	92.55800	82.73080	59.72890	-1620.99405	-1769.41926	-2058.01546	1
29028	C	93.42400	80.89180	60.32490	-639.65420	-646.77170	92.61830	1
29029	H	93.07600	80.44380	59.40590	-1060.27761	1150.19237	2718.84927	1
29030	C	94.15700	80.14080	61.27890	566.18948	672.59670	-247.55101	1
29031	H	94.35300	79.09980	61.07090	1110.81349	-367.04161	2894.08018	1
29032	C	94.09900	82.07280	62.66490	450.75172	-770.66016	-136.44283	1
29033	H	94.24300	82.65980	63.55990	-96.84269	-3121.07343	311.32347	1
29034	C	94.50800	80.76380	62.47290	663.20746	112.50901	-623.35631	1
29035	H	94.97700	80.15980	63.23490	1548.24887	-1612.82019	-2221.17541	1
29036	C	91.15900	83.68080	63.73290	-522.17613	29.28783	736.38351	1
29037	O	90.49700	82.62580	63.60990	154.26357	366.51651	-701.51367	1
29038	N	91.54500	84.08880	64.97890	401.35571	-697.89705	197.19177	1
29039	H	92.25500	84.78180	65.07190	2440.00443	-1684.01106	1001.13196	1
29040	C	91.05900	83.46380	66.12890	-641.25608	226.60788	-637.36024	1
29041	H	90.97300	82.39880	65.96990	-1287.90673	-1115.61662	-2664.08902	1
29042	C	91.97900	83.68480	67.32190	671.05753	299.07159	515.33943	1
29043	H	92.00800	84.76880	67.56390	98.30172	2285.56388	2148.47433	1
29044	H	91.54900	83.17080	68.20790	2783.36854	1233.42514	-796.03260	1
29045	C	93.41300	83.09980	67.07090	455.49992	789.34110	39.76926	1
29046	H	93.86800	83.56380	66.16990	27.52891	2139.69222	2292.38368	1
29047	C	94.41000	83.62580	68.14990	-608.22320	-664.44252	-164.77433	1
29048	H	94.13600	83.23380	69.15290	1334.97407	-1099.20299	-2642.04858	1
29049	H	94.50000	84.72780	68.25790	-2091.73346	2352.82445	-232.94978	1
29050	H	95.41400	83.22980	67.88390	-2821.95305	-43.56368	-1426.82008	1
29051	C	93.41700	81.60480	66.91190	-596.48470	-410.77268	539.28204	1
29052	H	92.78300	81.17580	66.10690	59.69900	-2202.01703	2220.05103	1
29053	H	93.12900	81.18280	67.89790	-696.26524	1512.93045	-2694.60177	1
29054	H	94.45700	81.21880	66.84390	-1165.67874	-2820.92881	733.76870	1
29055	C	89.61400	83.83780	66.42890	-560.13732	-566.34368	-461.04472	1
29056	O	88.85000	83.03980	67.01290	267.22989	-622.04227	370.85715	1
29057	N	89.10548	85.03432	66.01109	-951.77683	-32.71581	100.81715	1
29058	H	89.87497	85.68501	65.50203	-872.94364	-892.82159	3377.37636	1
29059	C	87.73388	85.46142	66.34729	615.66477	-1411.99228	91.42702	1
29060	H	87.65604	85.32950	67.45758	-2555.75568	-1088.89413	-156.44518	1
29061	C	87.61209	86.96068	66.00400	-196.99878	238.28476	442.27302	1
29062	H	87.44109	86.97043	64.93867	990.64507	4087.40527	586.92624	1
29063	H	88.57123	87.57638	66.23238	-877.45165	121.79335	-1938.15756	1
29064	S	86.13029	87.46331	66.98106	200.45651	-45.14521	185.91083	1
29065	C	86.67300	84.54580	65.53490	459.65089	-768.67590	-95.81165	1
29066	O	85.70400	84.06480	66.09490	-63.65564	-661.46119	398.00099	1
29067	N	86.85900	84.23180	64.25690	56.29141	-760.31313	325.29955	1

29068	H	87.68800	84.53680	63.79390	-145.69376	1077.37095	-2971.78216	1
29069	C	86.09400	83.32380	63.49490	119.75204	-820.68955	-368.08107	1
29070	H	85.03600	83.53880	63.49790	2357.73500	-1139.85416	-1736.33261	1
29071	C	86.54900	83.31080	62.03090	101.09807	646.12400	-658.01716	1
29072	H	86.13700	82.48080	61.41790	-316.92654	-3112.28596	-256.57201	1
29073	H	87.65600	83.22380	61.99490	2925.29305	-909.00857	639.21911	1
29074	C	86.19500	84.62180	61.36690	-508.98543	-278.03084	-722.71392	1
29075	H	86.48957	85.53124	61.90275	-1034.14997	-1269.71604	-418.70581	1
29076	H	85.09100	84.55380	61.26190	-2310.68590	-1774.10927	1181.57548	1
29077	C	86.79500	84.65480	59.96290	647.73023	313.02320	-565.89955	1
29078	H	86.34400	83.82380	59.38090	2413.48801	-1982.87521	-211.53547	1
29079	H	87.86800	84.41480	60.12190	-1399.92916	-1531.99702	-2381.91169	1
29080	C	86.42062	86.05862	59.30259	970.86058	487.80615	360.59085	1
29081	H	86.43847	85.95832	58.17197	-1570.30679	-68.89051	-2076.31971	1
29082	H	87.05905	86.92060	59.63359	3092.75375	1933.25699	-2021.07004	1
29083	N	84.90022	86.35130	59.73542	-438.46896	253.43058	282.80383	1
29084	H	84.50115	87.02390	59.00454	-1747.51197	715.73154	-1906.96210	1
29085	H	84.81849	86.74455	60.70017	-1499.41882	673.04767	-115.94933	1
29086	H	84.29122	85.49169	59.68122	1036.05386	-71.66730	1356.01706	1
29087	C	86.02200	81.92880	64.05690	-36.14440	-721.25895	529.85840	1
29088	O	84.99900	81.30480	64.09590	-680.76804	-135.13578	378.61133	1
29089	N	87.20100	81.39480	64.42590	653.55558	332.90465	-423.37012	1
29090	H	88.05400	81.83980	64.16690	1863.78489	1579.80210	-1994.90000	1
29091	C	87.36500	80.09380	65.00890	-817.71895	415.18936	-141.50449	1
29092	H	86.88200	79.29380	64.46790	-852.02340	752.26439	-2954.74868	1
29093	C	88.86800	79.76980	65.00690	372.96045	420.96874	700.15288	1
29094	H	89.28500	79.59280	63.99190	230.48155	2849.36191	-1346.67745	1
29095	H	88.98400	78.87080	65.64790	-2634.03934	1517.97694	843.41933	1
29096	H	89.43500	80.62280	65.43790	-681.60451	321.95242	-3074.66922	1
29097	C	86.72700	79.92780	66.35090	437.58794	-656.89183	417.28328	1
29098	O	85.95200	79.01880	66.54290	7.60325	-524.26126	566.86387	1
29099	N	86.90000	80.80780	67.33590	43.02177	7.80744	-857.87037	1
29100	H	87.40500	81.66380	67.25290	-644.48772	3083.61991	-218.63852	1
29101	C	86.19000	80.52680	68.62890	-53.66316	-736.53044	507.54342	1
29102	H	86.32400	79.48480	68.87990	2480.58912	-1403.66198	-1320.58335	1
29103	C	86.84000	81.26180	69.83390	890.25605	-100.83009	-131.76747	1
29104	H	86.44200	80.90480	70.80790	1401.28768	2484.31516	1322.77548	1
29105	C	88.33400	81.07680	69.72290	-589.97745	641.40019	-319.13742	1
29106	H	88.48300	79.98080	69.82890	-1218.10724	2657.99058	1172.72723	1
29107	H	88.82500	81.27280	68.74590	-2167.77382	-2200.49371	579.09454	1
29108	H	88.77100	81.69980	70.53290	-2082.21516	-2096.19584	1061.21092	1
29109	C	86.58200	82.78080	69.82590	-590.28178	-472.08202	494.16361	1
29110	H	86.96400	83.25980	70.75290	2207.52573	-170.42095	-2243.79780	1
29111	H	85.55100	83.08380	69.54390	617.83991	2765.42721	1369.15654	1
29112	H	87.13100	83.11580	68.91990	-251.85312	3134.12273	-284.76701	1
29113	C	84.70900	80.73080	68.63990	-632.47023	-110.98013	639.85384	1
29114	O	84.02200	80.17280	69.49290	-246.49725	582.01804	476.43335	1
29115	N	84.24600	81.55880	67.65790	-160.34488	-799.74567	169.52707	1
29116	H	84.91200	81.97480	67.04290	1968.56210	1883.31701	1560.40628	1
29117	C	82.80800	81.69580	67.40890	490.93992	-237.06480	708.69857	1
29118	H	82.37200	81.78180	68.39290	-356.46806	-207.93187	-3131.39383	1
29119	C	82.41500	82.92780	66.52990	733.80009	-19.94493	515.83835	1
29120	H	81.41600	82.87480	66.04590	886.90616	-2272.61089	-1980.86487	1
29121	H	83.13300	83.04280	65.69090	-1156.19101	1818.25082	2292.97681	1
29122	N	83.14181	85.32901	67.40120	-974.69353	211.50290	-336.03231	1
29123	H	83.79970	85.62706	66.73885	-1150.21840	2545.05699	-2327.20345	1
29124	C	82.39900	84.15480	67.43290	894.19674	-113.75176	-59.81169	1
29125	C	82.96860	86.19465	68.38132	-205.47965	-238.10845	124.77750	1
29126	H	83.39460	87.27011	68.43688	-2184.12388	3667.59010	-402.69914	1
29127	N	82.00719	85.60206	69.12905	-119.62659	300.17744	-677.23057	1
29128	C	81.65600	84.41580	68.51590	138.70665	-471.88251	-771.14416	1
29129	H	80.87200	83.84280	68.99590	-3028.41535	358.63753	-816.35034	1

29130	C	82.16700	80.46780	66.77990	715.89326	121.84692	-553.17027	1
29131	O	81.09700	80.01880	67.19390	469.40566	-443.29027	421.21686	1
29132	N	82.89000	79.89280	65.78590	177.50581	745.85722	-382.98874	1
29133	H	83.69400	80.36680	65.43590	1904.16028	-538.57247	2421.99504	1
29134	C	82.59700	78.59880	65.20790	42.59755	780.71335	-498.45925	1
29135	H	81.57800	78.58580	64.84890	-1060.79809	2437.97326	1693.97790	1
29136	C	83.57500	78.33080	64.01290	584.55072	-676.32729	42.35095	1
29137	H	84.59400	78.72480	64.21390	-509.02153	2048.78513	-2358.14493	1
29138	C	83.59900	76.78780	63.77490	219.01998	-869.69153	-62.79012	1
29139	H	84.31500	76.28780	64.46290	233.75217	212.34865	-3143.67829	1
29140	H	83.98300	76.51480	62.76890	-2351.85702	292.35276	2072.91317	1
29141	H	82.64600	76.27180	64.01990	-2680.91119	273.54349	-1659.71999	1
29142	C	83.00400	79.04680	62.75690	-691.63615	269.74188	538.48069	1
29143	H	81.91100	78.88580	62.63890	3106.72221	-297.43568	-275.74660	1
29144	H	83.47200	78.73680	61.79890	-205.35964	3032.97874	-866.30069	1
29145	H	83.14800	80.14080	62.88390	1759.65178	-2399.32431	-986.87686	1
29146	C	82.54300	77.54080	66.30590	-642.35477	156.25674	629.38149	1
29147	O	81.51500	76.91780	66.54690	-141.39339	591.96453	507.46589	1
29148	N	83.59100	77.46180	67.16990	116.20034	-106.80078	813.09872	1
29149	H	84.39600	78.01380	66.96890	1946.35085	-1106.66354	-2209.41941	1
29150	C	83.61000	76.47880	68.21290	162.44742	-874.68325	-147.26198	1
29151	H	83.48300	75.48980	67.79590	1990.29978	-2180.58454	-1057.92268	1
29152	C	85.03500	76.38780	68.80890	-558.47487	-696.65599	-191.36467	1
29153	H	85.44800	77.41780	68.87090	-1713.42504	1690.48571	2027.70215	1
29154	C	85.07400	75.72080	70.18590	-549.06400	-529.93080	484.56262	1
29155	H	86.10000	75.62280	70.60190	-2620.98947	1749.61040	-235.05377	1
29156	H	84.55100	76.30080	70.97590	-505.49626	-1161.10275	2863.56417	1
29157	H	84.66100	74.69080	70.12890	2358.54625	-2046.62751	228.83899	1
29158	C	85.97700	75.72480	67.76590	-100.73507	-235.82610	858.74691	1
29159	H	85.69100	74.65480	67.67490	-1519.62965	2278.55637	-1588.25482	1
29160	H	85.74100	76.16480	66.77290	1459.87339	1877.37216	2045.72517	1
29161	C	87.47200	75.97180	67.95890	387.72153	408.46859	700.46295	1
29162	H	88.05300	75.45780	67.16290	1573.19929	-2590.85975	-809.22022	1
29163	H	87.73000	75.66880	68.99590	1398.62915	5.47557	2797.06993	1
29164	H	87.69600	77.04780	67.79490	1750.88087	-1721.47652	-1965.75038	1
29165	C	82.51700	76.61280	69.28290	-621.76613	91.76000	-683.51406	1
29166	O	81.96700	75.61980	69.76790	-710.20191	246.70939	266.11614	1
29167	N	82.13600	77.82380	69.67790	-406.05985	-486.73167	541.92372	1
29168	H	82.59400	78.62980	69.31090	643.08892	2528.25733	1758.42892	1
29169	C	81.05000	78.07380	70.56590	646.00238	-578.92773	-245.76258	1
29170	H	81.27600	77.50580	71.45590	-385.33273	-3105.13403	-219.23294	1
29171	C	81.05200	79.58980	71.00790	-121.67052	874.37231	260.17681	1
29172	H	80.98000	80.15680	70.05590	935.56818	-561.09253	-2957.68417	1
29173	H	82.02300	79.80180	71.50490	-1755.13888	667.79685	-2544.00401	1
29174	C	79.92200	80.03280	71.97990	446.04165	540.10097	578.95054	1
29175	C	79.38500	79.12780	72.88490	748.35587	212.00830	-481.62875	1
29176	H	79.82100	78.13980	72.84190	2338.02134	-2078.22912	167.99388	1
29177	C	78.46300	79.55580	73.85390	-198.72221	811.13546	-404.94322	1
29178	H	78.13700	78.88380	74.63390	504.64662	2855.93033	1236.81142	1
29179	C	77.98700	80.85580	73.88990	704.91000	202.95130	-549.24763	1
29180	O	76.96700	81.12580	74.81990	330.00824	-625.40281	-331.81572	1
29181	H	77.08100	82.02380	75.14090	1603.10196	-1698.04147	2086.29834	1
29182	C	79.47200	81.38480	72.01490	-509.94864	750.96974	166.95448	1
29183	H	79.94600	82.09480	71.35290	1999.62592	-788.07983	2277.46291	1
29184	C	78.48900	81.79280	72.93090	686.34858	418.16866	-444.10744	1
29185	H	78.06400	82.77980	73.03490	46.49858	770.03332	-3062.57698	1
29186	C	79.67300	77.54080	70.07190	-600.28347	-259.56790	-649.16781	1
29187	O	78.96500	76.79380	70.76590	472.05566	-460.47372	-421.35703	1
29188	N	79.39400	77.68380	68.75890	-751.68453	-390.10308	-4.46157	1
29189	H	79.95300	78.19680	68.11190	-1162.54948	-973.54607	2745.65451	1
29190	C	78.20500	77.02080	68.19390	51.67565	808.57374	431.06762	1
29191	H	77.43900	76.92980	68.94890	2947.50593	324.73349	1018.36531	1

29192	C	77.48800	77.80880	67.07390	354.61150	-628.55193	-544.34277	1
29193	H	76.97700	77.12180	66.36490	1477.87575	-2362.72318	1417.67952	1
29194	O	78.48200	78.54080	66.33890	-440.52771	-390.39757	-535.63147	1
29195	H	77.96600	79.06380	65.71990	-585.08432	2177.80209	2200.04692	1
29196	C	76.51200	78.84980	67.67590	687.71131	572.03929	172.87574	1
29197	H	76.14500	79.53180	66.87990	2239.48995	-1703.60362	-1382.65247	1
29198	H	77.06600	79.47580	68.40790	2625.50466	-1587.83832	618.90347	1
29199	H	75.64300	78.39980	68.20290	-723.14487	1863.64828	2434.81753	1
29200	C	78.36700	75.56380	67.75190	-18.09878	-784.55656	432.69192	1
29201	O	77.49200	74.70580	67.73790	228.63785	739.07188	-206.40446	1
29202	N	79.64800	75.13880	67.41590	-420.05019	735.43670	139.68933	1
29203	H	80.37000	75.81880	67.31490	479.16378	-2719.44449	-1493.56577	1
29204	C	79.99100	73.68980	67.21490	84.76523	915.90931	-82.13045	1
29205	H	79.38000	73.32380	66.40290	1623.16420	92.24308	2675.55099	1
29206	C	81.38900	73.44280	66.61790	740.63510	-131.81556	481.49987	1
29207	H	82.10200	74.18380	67.03690	-10.83933	-3117.96690	314.18145	1
29208	C	81.96200	72.04380	66.97190	577.02974	174.70395	663.39653	1
29209	H	82.88300	71.83080	66.38890	1721.01895	-1897.15353	-1815.45484	1
29210	H	81.18600	71.31880	66.64490	2489.88841	-872.17172	-1700.07277	1
29211	H	82.34400	71.99180	68.01390	412.65092	-1847.55910	-2515.19738	1
29212	C	81.32400	73.80080	65.10990	458.23590	446.42192	636.07484	1
29213	H	80.97800	74.84980	64.98990	2733.82052	-1505.29931	-237.14152	1
29214	H	82.37400	73.66580	64.77390	-1765.79034	1447.28425	-2195.71929	1
29215	H	80.63300	73.08980	64.60990	668.70388	-2971.41108	717.99914	1
29216	C	79.75400	72.79980	68.47990	-623.31026	631.78440	-281.70777	1
29217	O	79.20000	71.70380	68.33390	527.57885	401.94167	414.24377	1
29218	N	80.08100	73.22380	69.70090	169.78437	-489.88253	643.39832	1
29219	H	80.50800	74.12280	69.76890	-633.54456	-2677.46234	-1520.58824	1
29220	C	79.61600	72.58280	70.91190	-768.40093	89.91084	-511.25518	1
29221	H	79.83700	71.53080	70.80090	-2399.38882	-655.95008	1924.58301	1
29222	C	80.32000	73.15880	72.15090	164.48410	898.01489	114.61105	1
29223	H	80.52000	74.24680	72.04990	-496.11756	2929.19019	-1083.09252	1
29224	H	81.33400	72.70680	72.18690	-1951.92865	-1092.97973	-2226.58165	1
29225	C	79.57500	73.06880	73.50490	-7.74470	-698.39683	560.94810	1
29226	O	78.59100	73.73680	73.79790	495.34131	-57.99487	-614.60405	1
29227	N	80.05400	72.13480	74.36090	389.04132	-690.98479	236.09360	1
29228	H	80.91400	71.64380	74.22290	2435.04735	1931.13259	-504.21407	1
29229	H	79.62900	72.06180	75.26290	-1611.49912	-1813.64402	1987.42900	1
29230	C	78.06400	72.62880	71.06090	-133.27219	914.95547	-56.52673	1
29231	O	77.44500	71.63380	71.38190	-397.43538	295.79632	618.11912	1
29232	N	77.42000	73.74480	70.75490	-516.95427	-654.63096	-108.31337	1
29233	H	77.98600	74.52280	70.49790	-2044.24602	-2295.19176	647.81796	1
29234	C	76.00300	73.97580	70.88590	-855.75586	113.48541	-333.20694	1
29235	H	75.75900	73.92180	71.93690	1773.95093	-2446.86498	807.65784	1
29236	C	75.56400	75.38480	70.54190	-262.48749	-857.47951	83.45713	1
29237	H	75.41200	75.53680	69.45190	2137.40929	1438.33514	1797.05657	1
29238	H	76.35700	76.10880	70.82590	2118.80727	-2275.90707	-369.80283	1
29239	C	74.25900	75.91580	71.28290	-533.70505	558.55911	502.22058	1
29240	H	73.50300	75.10180	71.26190	-1675.23337	-2285.84956	1346.12679	1
29241	C	74.54200	76.24980	72.74990	-625.40159	-471.24451	455.45137	1
29242	H	74.82100	75.38380	73.38690	-358.79049	2879.49283	-1257.80928	1
29243	H	73.69400	76.78080	73.23390	-1927.73382	2256.78986	1079.79745	1
29244	H	75.40100	76.95280	72.71390	-596.86305	-2934.71846	918.08664	1
29245	C	73.71700	77.15380	70.58690	-96.27846	495.45238	762.97552	1
29246	H	72.74800	77.35680	71.09090	-1284.43475	2240.66576	1814.65642	1
29247	H	73.66100	76.90080	69.50690	-2213.14032	948.77564	2035.08798	1
29248	H	74.31300	78.05480	70.84590	-1242.76986	-2549.69975	1334.55763	1
29249	C	75.09600	73.04480	70.08690	-833.74293	400.61601	-73.08523	1
29250	O	74.19500	72.43780	70.57690	515.98404	469.05771	-380.86176	1
29251	N	75.58000	72.79280	68.84390	432.46405	-699.06949	-94.43471	1
29252	H	76.37800	73.29880	68.52390	590.39305	1459.40292	-2737.17852	1
29253	C	75.03800	71.79380	67.92590	28.34672	-536.14562	-733.77106	1

29254	H	73.97500	71.68380	68.08490	-956.06147	2279.60452	1961.90793	1
29255	C	75.21300	72.27780	66.44590	-12.83589	-897.22372	-41.50797	1
29256	H	74.68000	71.57580	65.76990	-404.87950	2233.32930	2188.16526	1
29257	H	76.30400	72.25780	66.23490	1239.19433	1677.64867	-2366.54047	1
29258	C	74.58800	73.64280	66.30190	13.68064	875.22084	291.74143	1
29259	C	73.40500	74.05580	66.90090	-633.73150	181.77163	-652.58102	1
29260	H	72.87400	73.31580	67.48090	2133.58228	2101.65790	-975.54514	1
29261	C	72.89700	75.36980	66.79290	-869.53013	259.05330	-196.26919	1
29262	H	72.03100	75.61380	67.39190	1591.85880	2189.20643	1607.45046	1
29263	C	73.59500	76.30480	66.07290	-551.09754	466.90045	-586.45630	1
29264	O	73.11000	77.58880	66.04690	448.93375	-240.44343	582.40657	1
29265	H	73.77800	78.08480	65.56790	2095.58498	-2252.73228	556.88039	1
29266	C	75.25300	74.59480	65.48390	-697.87107	94.99356	-604.28267	1
29267	H	76.17700	74.26580	65.03190	39.50013	-2916.07200	1137.07158	1
29268	C	74.76400	75.91180	65.39090	323.12990	480.17923	700.86076	1
29269	H	75.26000	76.67480	64.80990	2034.82926	-721.53513	-2280.47982	1
29270	C	75.55000	70.36280	68.08790	-743.65347	239.76953	-504.59009	1
29271	O	74.98700	69.48580	67.47890	478.81347	-453.30402	-411.06207	1
29272	N	76.64500	70.10980	68.85690	319.48086	-561.50195	-530.39402	1
29273	H	77.20900	70.81580	69.27890	-344.28608	-1600.08821	2671.35134	1
29274	C	77.21400	68.74780	68.93090	-696.55456	-54.13208	-609.07947	1
29275	H	76.76200	68.11280	68.18290	-2613.78597	1623.58777	729.44126	1
29276	C	78.76800	68.59680	68.72990	590.04657	460.73938	505.97380	1
29277	H	78.91700	68.76980	67.64290	2131.96913	-2287.33800	56.33228	1
29278	H	79.12100	67.55780	68.90390	-2653.33095	-686.45954	1551.93362	1
29279	O	79.43400	69.45380	69.61290	748.55044	223.22457	2.50025	1
29280	H	79.36600	70.29480	69.15390	-3059.88770	-652.65500	399.49406	1
29281	C	76.83600	68.12980	70.21990	493.07107	606.96772	-481.66569	1
29282	O	76.31600	67.01880	70.22490	-318.31322	543.03291	-508.61205	1
29283	N	76.90800	68.88580	71.39690	71.55352	483.24532	-705.35942	1
29284	H	77.09200	69.86380	71.34290	-1877.32710	2147.57682	1354.26978	1
29285	C	76.65900	68.29280	72.72790	489.24708	476.25399	-614.79260	1
29286	H	77.37300	67.49480	72.86990	-362.71215	-34.88673	-3135.48595	1
29287	C	76.99100	69.27280	73.89690	716.13688	85.93258	-556.39227	1
29288	H	78.08900	69.43780	73.90890	357.56702	3135.61524	-110.83097	1
29289	H	76.72300	68.86880	74.89590	2921.03508	91.37787	1134.12277	1
29290	O	76.37400	70.60180	73.75590	270.67969	533.30825	-533.00046	1
29291	H	76.99100	71.20580	73.33690	525.33849	2609.39653	-1703.62152	1
29292	C	75.22200	67.71180	72.98090	191.50267	-536.04545	690.72336	1
29293	O	75.04700	66.54180	73.22690	533.67450	-295.16206	-488.92685	1
29294	N	74.23400	68.54880	72.77190	-762.75217	-367.49152	-42.72514	1
29295	H	74.49300	69.49780	72.60890	1257.72421	2621.23652	1214.44142	1
29296	C	72.81700	68.20780	72.84690	699.36357	-413.43164	-385.79876	1
29297	H	72.69700	67.79180	73.83690	-696.78864	-1485.78076	-2684.98420	1
29298	C	71.92400	69.42580	72.75590	198.82039	-21.07117	881.03811	1
29299	H	72.28100	70.22380	73.44090	-2094.80380	2299.04240	570.69798	1
29300	C	71.88500	70.06880	71.32090	488.82914	-477.60549	-587.82946	1
29301	H	72.95400	70.30580	71.12690	2768.36114	754.60424	1268.79256	1
29302	H	71.46800	69.35080	70.58190	1512.92861	-1873.15201	-2007.26076	1
29303	H	71.31100	71.01980	71.33190	2627.09780	-1615.08620	-536.85857	1
29304	C	70.59100	69.04780	73.37790	-382.80592	-720.13681	383.80642	1
29305	H	69.91400	69.92780	73.42990	1615.46874	2277.84087	1458.80339	1
29306	H	70.01500	68.20180	72.94690	-874.82960	-1991.33842	2258.72528	1
29307	H	70.85600	68.68180	74.39290	-478.94811	2035.83386	2360.50859	1
29308	C	72.36900	67.11980	71.85690	617.65767	373.38601	-560.03701	1
29309	O	71.52900	66.26080	72.13090	-601.64107	378.38902	-385.15092	1
29310	N	72.91100	67.09180	70.61690	-462.01505	182.83367	-701.09622	1
29311	H	73.50900	67.85780	70.39290	1952.31412	-640.29952	-2375.22676	1
29312	C	72.45400	66.06380	69.71790	455.05176	-447.32674	624.68307	1
29313	H	71.39000	65.90280	69.80790	2177.99818	1261.12915	-1887.89042	1
29314	C	72.66000	66.54280	68.23090	-184.69736	-598.57329	646.34850	1
29315	H	72.52100	65.61380	67.63890	-2077.03837	-942.45905	2168.59276	1

29316	H	73.68700	66.96680	68.24990	1991.31318	423.10810	-2396.39789	1
29317	C	71.72500	67.59780	67.72090	114.28259	-712.45476	528.33626	1
29318	C	71.74100	68.95780	67.92090	880.89085	-14.28887	168.69695	1
29319	H	72.58600	69.44280	68.38690	2017.08762	2073.12225	1234.98479	1
29320	N	70.70500	69.55680	67.31790	713.51501	436.68426	-85.90161	1
29321	H	70.35400	70.42880	67.57890	-1987.01410	-1636.03126	1804.60087	1
29322	C	69.94900	68.58180	66.73890	228.76522	-47.23946	-880.98093	1
29323	C	70.55000	67.30580	66.99790	-205.85219	188.64238	869.78910	1
29324	C	69.90800	66.17080	66.61990	-109.47294	-644.34995	617.06658	1
29325	H	70.39900	65.26380	66.93990	2033.19004	-2000.81934	1272.87692	1
29326	C	68.76100	66.27480	65.85090	-393.20845	-601.14118	550.82680	1
29327	H	68.26800	65.37480	65.51390	1714.06115	-2311.89111	1212.99476	1
29328	C	68.83000	68.69180	65.97190	715.52184	-287.84191	-456.59949	1
29329	H	68.33200	69.62280	65.74690	-2335.23502	1355.82151	1646.09844	1
29330	C	68.20200	67.49880	65.54590	-260.29628	-624.94458	596.41941	1
29331	H	67.29300	67.52580	64.96390	-1281.81872	2134.60263	-1955.50298	1
29332	C	73.19300	64.74780	69.88990	-496.88788	-396.40926	-661.96662	1
29333	O	72.67800	63.69780	69.58190	-241.86928	531.65506	-558.71192	1
29334	N	74.40600	64.73880	70.51790	292.99711	457.36682	-657.36989	1
29335	H	74.96100	65.55880	70.63090	528.13801	-2249.24033	-2125.23298	1
29336	C	74.94700	63.53980	71.09390	197.74805	682.30820	575.15861	1
29337	H	75.05800	62.74180	70.37490	1178.91628	-1512.70486	2470.51181	1
29338	C	76.44200	63.74480	71.56290	-177.74957	-864.12960	-194.63638	1
29339	H	76.37000	64.76080	72.00790	-1643.01498	2157.83651	1616.32610	1
29340	C	76.85300	62.73380	72.62490	-621.66809	-634.99322	193.15001	1
29341	H	77.96400	62.74180	72.63890	2683.24955	-1608.09309	-47.34691	1
29342	H	76.59800	61.68380	72.36590	1166.01066	2744.09273	1015.14671	1
29343	H	76.41300	62.97180	73.61690	-1490.55430	1618.02243	-2275.60700	1
29344	C	77.39100	63.63880	70.36590	-5.96114	278.59097	862.68963	1
29345	H	76.79400	64.06380	69.53090	448.13655	-2921.25008	-1044.93942	1
29346	H	77.58600	62.57880	70.09590	-1530.99539	1481.76781	2323.02801	1
29347	C	78.55700	64.57680	70.48490	825.87728	-342.58200	-31.59529	1
29348	H	79.21500	64.35480	71.35190	-449.85290	-2973.69877	-900.64016	1
29349	H	78.21700	65.63480	70.49190	2162.74271	-1937.01925	1156.98040	1
29350	H	79.23400	64.48180	69.60890	-345.91227	2208.73191	2217.20068	1
29351	C	74.09700	62.96180	72.24090	636.37074	652.50533	38.86666	1
29352	O	73.82900	61.77480	72.30290	-152.07116	191.67824	-764.26245	1
29353	N	73.51000	63.84680	73.06590	344.09450	-522.39898	538.36963	1
29354	H	73.79600	64.80180	73.04790	592.51929	2830.75155	1258.05575	1
29355	C	72.53000	63.56280	74.09690	-379.31015	834.36126	150.82837	1
29356	H	72.92800	62.80480	74.75590	-2242.41451	-2189.26837	-260.57337	1
29357	C	72.31300	64.68880	75.09590	-724.18194	548.86503	-198.91745	1
29358	H	71.43000	64.41080	75.70990	727.61949	-1431.77997	2688.80116	1
29359	H	71.98400	65.56780	74.50090	977.65107	-2608.73224	1421.40397	1
29360	C	73.46500	64.97780	76.06990	305.73784	824.68291	-281.28929	1
29361	H	74.37300	65.14780	75.45290	-1417.96528	-134.82035	2802.14456	1
29362	C	73.19900	66.08480	77.11390	-694.91394	-482.69543	-343.51268	1
29363	H	74.07700	66.31080	77.75590	166.91416	-2529.93738	-1849.98486	1
29364	H	72.87400	67.00380	76.57990	-2618.51597	-1487.29011	905.33431	1
29365	H	72.38300	65.70780	77.76590	1607.44606	-2440.45802	-1128.23698	1
29366	C	73.79100	63.67480	76.88490	641.59147	188.16037	-621.05184	1
29367	H	74.66400	63.90280	77.53190	1920.86341	-1997.12630	1451.18917	1
29368	H	72.87900	63.35080	77.43090	-547.39857	2898.95510	1128.91913	1
29369	H	74.16100	62.87780	76.20390	833.08868	-2790.84613	-1155.78527	1
29370	C	71.22700	62.91880	73.51690	175.37332	-374.51263	-808.13545	1
29371	O	70.71800	61.98380	74.14690	564.94096	-27.81404	531.89615	1
29372	N	70.70300	63.40180	72.34790	115.24727	647.84694	539.38764	1
29373	H	71.10300	64.26580	72.05290	174.09009	113.76305	-3144.44771	1
29374	C	69.73400	62.58180	71.58590	640.27159	-562.53126	-267.04601	1
29375	H	68.87900	62.38480	72.21590	1284.75015	-2796.68798	-551.35069	1
29376	C	69.26800	63.38280	70.33890	-424.11427	470.68431	671.80712	1
29377	H	68.28800	62.96680	70.02090	2091.53948	-2261.67343	517.21090	1

29378	H	69.96100	63.29480	69.47590	-2178.26464	41.18536	-2288.84361	1
29379	H	69.03900	64.45180	70.53990	993.70684	964.86977	-2829.56078	1
29380	C	70.21000	61.21680	71.12590	476.54509	614.10727	-486.87038	1
29381	O	69.50700	60.27980	71.39790	-547.58014	-387.31911	-425.23599	1
29382	N	71.39700	61.10080	70.48690	-240.39950	-761.67007	235.28611	1
29383	H	71.96500	61.91780	70.43290	2152.12498	707.11625	-2179.47232	1
29384	C	71.91600	59.80780	70.10590	-141.89557	590.96465	689.67830	1
29385	H	71.21400	59.26580	69.48990	-706.79395	-1774.27767	-2499.30406	1
29386	C	73.26300	60.01580	69.27590	207.85591	199.10790	-871.35284	1
29387	H	73.86400	59.08180	69.30890	-1636.11255	-2109.22268	-1670.45624	1
29388	H	73.85400	60.81780	69.76790	1897.82176	-1726.92681	-1797.38188	1
29389	C	73.07700	60.37180	67.86290	-639.31348	-248.88951	605.39498	1
29390	C	71.99300	61.12680	67.38390	-171.10750	-677.55341	-578.58208	1
29391	H	71.19200	61.52980	67.98490	-1068.20851	-1852.22056	2297.42879	1
29392	C	71.80300	61.37380	66.02090	-126.47382	-445.36158	-785.30275	1
29393	H	70.93800	61.91180	65.66190	-2714.81127	583.87189	-1522.77408	1
29394	C	72.70500	60.88880	65.10690	539.93130	-571.69802	411.81921	1
29395	H	72.48900	61.01780	64.05590	-1412.98112	1814.15602	-2178.93089	1
29396	C	73.97600	59.87980	66.90290	-686.35659	-277.88340	-554.46816	1
29397	H	74.74700	59.17780	67.18090	-537.82180	-1935.20329	-2422.11094	1
29398	C	73.75000	60.08480	65.52790	326.43879	-750.54189	348.79959	1
29399	H	74.35200	59.44180	64.90390	1597.04518	-2414.64838	1169.09766	1
29400	C	72.12500	58.72180	71.18490	-319.37285	871.04649	-87.00105	1
29401	O	71.74000	57.56280	70.96290	-461.74365	532.60497	-402.89018	1
29402	N	72.61100	59.07480	72.37390	609.74416	-26.88695	560.01804	1
29403	H	72.89000	60.02280	72.50490	-2048.45752	-287.90352	-2387.57865	1
29404	C	72.68100	58.14080	73.49390	699.28323	-419.20585	359.22946	1
29405	H	73.09600	57.19180	73.18990	-1648.63924	668.94453	-2614.82328	1
29406	C	73.64600	58.74880	74.51190	246.80312	-3.93243	866.47462	1
29407	H	74.62300	58.87080	73.99490	-2081.34823	-1929.86584	-1366.02044	1
29408	C	73.16700	60.07580	75.15390	427.60107	-528.05411	-592.90128	1
29409	H	72.36900	59.90880	75.90790	-1747.25852	-1824.14202	-1878.62629	1
29410	H	72.74200	60.71680	74.35090	2063.57255	1160.16381	-2074.25942	1
29411	H	73.98700	60.55380	75.73090	49.42166	-1989.04614	-2432.60798	1
29412	C	74.00800	57.66680	75.58290	-420.92743	579.08917	-595.78415	1
29413	H	74.22300	56.72280	75.03790	-1807.91594	1581.56640	-2062.63924	1
29414	H	73.10600	57.48480	76.20490	-1538.53947	1854.39441	-2052.72844	1
29415	C	75.17000	58.18180	76.40990	752.77662	243.38693	-447.84550	1
29416	H	76.07100	58.47080	75.82890	2374.24312	-190.18960	2030.62679	1
29417	H	74.83000	59.07680	76.97390	-1849.58533	2231.99326	-1272.88633	1
29418	H	75.49500	57.43180	77.16290	2546.61485	743.51621	1670.12790	1
29419	C	71.27200	57.86480	74.12990	-487.66772	561.63517	-561.29589	1
29420	O	71.00500	56.75880	74.66690	-283.62694	354.07219	654.96007	1
29421	N	70.33700	58.79980	73.99790	632.56668	550.17573	91.54139	1
29422	H	70.55600	59.61580	73.46790	767.32572	-2082.35285	-2215.73883	1
29423	C	68.93700	58.59380	74.35490	579.78259	584.69550	-399.46939	1
29424	H	68.88800	58.26980	75.38390	194.35220	2093.60329	-2357.82329	1
29425	C	68.03700	59.88580	74.21290	-230.60440	-800.48705	337.74631	1
29426	H	66.94500	59.71580	74.32590	-672.22769	-2518.91707	1738.61853	1
29427	H	68.26200	60.32580	73.21790	-1046.98488	-2139.64603	-2048.41347	1
29428	O	68.38100	60.83480	75.21390	-266.09557	762.46427	47.38163	1
29429	H	69.14200	61.29780	74.85590	791.18150	3037.27204	-358.97255	1
29430	C	68.26600	57.55280	73.49690	-44.64990	-609.40941	-666.07878	1
29431	O	67.62400	56.66180	74.00890	-161.84997	781.09397	-136.84894	1
29432	N	68.41900	57.71580	72.14690	-303.26697	-12.46717	-796.90566	1
29433	H	68.91000	58.48880	71.75390	1130.24598	-2406.71399	1643.44506	1
29434	C	68.00800	56.73880	71.10290	143.21043	-387.09213	-805.38270	1
29435	H	66.93000	56.69380	71.05990	-2645.89074	1733.12346	-203.44868	1
29436	C	68.42200	57.32980	69.74790	-577.37324	-671.55300	-213.55790	1
29437	H	68.40100	56.60980	68.90190	687.48060	2187.33253	-2169.22075	1
29438	H	69.46400	57.71380	69.75790	-2193.66017	995.35861	2045.22913	1
29439	C	67.53700	58.48480	69.21390	-520.23272	94.51965	753.21796	1

29440	H	67.35400	59.16180	70.07590	1486.72880	-2746.04679	66.07898	1
29441	C	68.30300	59.44180	68.21290	-906.68541	104.19287	-184.74276	1
29442	H	67.50000	60.12880	67.86990	-484.52412	2732.94448	-1521.00795	1
29443	H	68.58400	58.83980	67.32290	3121.05735	-182.94605	-66.81040	1
29444	H	69.13000	60.00380	68.69590	-2166.73404	642.35615	-2214.19176	1
29445	C	66.27600	58.00980	68.50990	-873.28746	285.87171	-167.85780	1
29446	H	66.46300	57.26280	67.70990	-3000.47059	-552.77308	822.59740	1
29447	H	65.65900	58.82780	68.07890	785.19618	-1263.02768	-2761.17646	1
29448	H	65.59800	57.65380	69.31590	1193.03099	2504.00554	-1502.67718	1
29449	C	68.65300	55.42080	71.41890	374.42243	-364.67484	-734.21406	1
29450	O	67.96100	54.39280	71.36790	438.46429	561.93266	-348.24397	1
29451	N	69.99700	55.34680	71.65690	334.81259	579.09419	516.56250	1
29452	H	70.50300	56.19780	71.54090	-1995.91961	-2325.81409	699.64347	1
29453	C	70.66600	54.11680	71.95390	418.69627	189.26775	-787.42549	1
29454	H	70.37400	53.43580	71.16790	845.85705	2374.54226	-1899.65661	1
29455	C	72.21100	54.42880	71.99990	374.39037	692.27009	-475.22627	1
29456	H	72.41300	55.16980	72.80390	335.84462	-471.98686	-3094.82102	1
29457	H	72.52700	54.79380	70.99990	-2891.54356	-475.46478	-1188.43438	1
29458	C	72.99600	53.16680	72.28990	-175.18698	912.09501	26.96025	1
29459	O	73.09800	52.74080	73.45190	-336.40478	-22.30506	713.98534	1
29460	O	73.42800	52.48280	71.30890	3.62019	-557.82922	536.31042	1
29461	C	70.16900	53.41580	73.19190	730.44268	27.49475	517.82262	1
29462	O	70.09800	52.19680	73.28190	-338.98626	-285.42318	649.93782	1
29463	N	69.80300	54.19280	74.24790	-550.03502	-427.82792	474.66002	1
29464	H	69.85400	55.18780	74.23790	-113.50087	2195.68367	2261.65105	1
29465	C	69.17300	53.66180	75.45390	474.35535	650.59435	430.97096	1
29466	H	69.73600	52.83980	75.86990	-2544.20665	-1764.29433	-580.84021	1
29467	C	69.09800	54.71380	76.61790	-522.22856	619.88521	-460.76932	1
29468	H	69.19700	55.75280	76.23590	-2719.84796	536.24120	-1522.07036	1
29469	H	68.12200	54.60580	77.13890	1655.92099	1361.33859	-2306.61292	1
29470	C	70.26100	54.47080	77.66490	615.74512	-220.38302	611.56908	1
29471	H	70.11000	55.20080	78.48890	-1958.36255	1929.58321	1559.46625	1
29472	H	70.18700	53.40880	77.98390	-1782.52816	-2189.83819	1374.63265	1
29473	C	71.68300	54.73580	77.10590	309.86227	743.38769	437.26604	1
29474	H	72.30700	54.92680	78.00490	1713.14981	1894.23961	1834.02724	1
29475	H	71.52300	55.67780	76.53890	1217.49611	-691.06016	2801.99703	1
29476	N	72.29500	53.58780	76.26790	-660.52098	-467.05110	244.23785	1
29477	H	72.33300	53.71780	75.27790	-2312.27078	1225.63618	-1782.65551	1
29478	C	72.51900	52.36480	76.67390	647.26313	252.68095	573.64640	1
29479	N	72.45100	51.90980	77.92390	509.12341	601.77331	300.69319	1
29480	H	72.43900	52.51280	78.72190	-1800.54236	2484.09126	771.57210	1
29481	H	72.53400	50.92280	78.06190	605.10983	50.78793	3077.59353	1
29482	N	72.86300	51.48580	75.77490	-515.28073	380.14536	566.88064	1
29483	H	72.93300	51.87680	74.85690	412.60337	-2744.67268	-1456.40159	1
29484	H	73.24600	50.61580	76.08390	2872.64718	39.89041	-1254.35596	1
29485	C	67.78400	53.02580	75.23090	404.15345	-685.17088	400.05021	1
29486	O	67.57600	51.90080	75.66890	724.16851	9.04000	-280.20726	1
29487	N	66.94800	53.66880	74.42790	256.66799	-509.72332	-603.88690	1
29488	H	67.26800	54.51680	74.01190	-130.13703	587.26005	3088.71573	1
29489	C	65.70600	53.17180	73.94890	786.40618	-324.57604	-267.62692	1
29490	H	65.24000	52.91680	74.88890	-789.13568	2952.99787	825.19994	1
29491	C	65.01600	54.39180	73.21590	-530.22118	-555.49007	-489.83947	1
29492	H	65.75700	55.08780	72.76690	569.99946	-1154.09451	-2862.56459	1
29493	H	64.48300	54.96280	74.00590	-1933.68752	-1931.97011	-1555.41645	1
29494	C	63.96000	54.00580	72.20890	572.61672	-632.67822	-246.23310	1
29495	C	62.81500	53.27380	72.56890	65.25153	-883.20719	104.90922	1
29496	H	62.64500	52.99980	73.59990	-1384.12650	-1977.31026	2010.47784	1
29497	C	61.86200	53.00680	71.55590	-417.30699	314.59678	764.87131	1
29498	H	60.98800	52.51080	71.95090	-310.35988	-3069.79902	-517.10905	1
29499	C	62.07000	53.38380	70.23690	-291.92299	98.48302	866.44083	1
29500	O	61.17200	53.02380	69.23190	476.41208	-55.23612	-609.43969	1
29501	H	61.57000	53.06280	68.35890	831.84284	-2227.98231	2030.80902	1

29502	C	64.22300	54.25280	70.86090	632.63922	-287.65141	-562.41550	1
29503	H	65.19200	54.70680	70.71490	1332.08516	2791.30538	-622.27282	1
29504	C	63.28000	53.95980	69.85490	-296.23735	553.80008	683.50105	1
29505	H	63.50300	54.29180	68.85190	1256.30861	-1210.12910	-2601.09485	1
29506	C	65.83400	51.91380	73.11590	556.92574	159.88021	-696.36489	1
29507	O	65.14200	50.94680	73.39390	535.01553	538.19400	-220.53748	1
29508	N	66.72600	51.85580	72.13990	404.25962	591.77573	-455.10516	1
29509	H	67.18100	52.70080	71.86790	1185.54700	-1013.52919	2715.00121	1
29510	C	67.06100	50.73780	71.34590	771.48529	441.17136	-168.04741	1
29511	H	66.18800	50.37980	70.82090	-2281.29349	-433.92167	-2142.11801	1
29512	C	68.18900	50.95680	70.27890	593.65038	662.49591	192.65161	1
29513	H	68.49600	49.97580	69.85790	1427.92864	1590.91159	2303.06100	1
29514	H	69.07300	51.42780	70.75990	-541.14784	3117.21600	95.43952	1
29515	C	67.74500	51.90280	69.18490	-410.86180	-798.79128	110.63539	1
29516	H	67.22000	52.78380	69.61290	-1795.49656	1378.46496	2207.95612	1
29517	C	68.90400	52.46280	68.26490	490.17772	656.81448	-405.66699	1
29518	H	69.21300	51.65180	67.57190	-835.68160	2436.15343	1833.65022	1
29519	H	69.81900	52.69180	68.85290	2287.63570	-1560.21714	-1450.65686	1
29520	H	68.67000	53.44480	67.79890	-532.83512	2276.23622	2124.05922	1
29521	C	66.79800	51.18780	68.16290	92.96459	262.92868	-873.74311	1
29522	H	67.28100	50.33580	67.63890	-1982.37956	-2083.35853	-1284.10753	1
29523	H	66.50300	51.92080	67.38290	-1887.29411	494.89760	-2490.08973	1
29524	H	65.90400	50.68680	68.59190	-1270.46405	1262.07688	-2607.69284	1
29525	C	67.57100	49.59980	72.22890	-528.80305	-738.75032	9.05302	1
29526	O	67.16500	48.45580	72.05690	150.83461	-378.39494	-665.37440	1
29527	N	68.39700	49.92080	73.24090	626.54943	425.79231	-364.58448	1
29528	H	68.72700	50.85680	73.34190	1461.92908	-31.24706	2771.99468	1
29529	C	69.08400	48.91580	74.02090	-288.62854	-751.06639	406.91597	1
29530	H	69.46000	48.13080	73.38090	1779.20058	451.11523	2540.24198	1
29531	C	70.26000	49.50580	74.88190	451.31701	-754.84863	130.46984	1
29532	H	69.96200	50.21280	75.68490	2038.17934	1382.86690	1946.66416	1
29533	H	70.89000	50.10780	74.19090	-2163.85049	1298.12498	-1914.80397	1
29534	H	70.83600	48.64580	75.28590	1442.48995	2755.42722	-516.44639	1
29535	C	68.12500	48.26380	75.04290	738.85576	522.63343	-63.87598	1
29536	O	68.45400	47.23480	75.64590	278.89964	-686.91240	198.75853	1
29537	N	66.89700	48.82080	75.37790	80.71654	416.61786	734.10977	1
29538	H	66.81100	49.74780	75.01990	-1528.00014	45.51326	-2762.28151	1
29539	C	65.93700	48.35880	76.39690	-640.92064	518.45635	-438.79472	1
29540	H	66.38800	47.45080	76.76890	-1527.62301	-1823.40126	2053.08314	1
29541	C	65.75500	49.42180	77.42890	-356.94903	-678.94741	476.93139	1
29542	H	65.76800	50.45180	77.01090	-1477.89510	1170.75989	2533.11004	1
29543	C	64.37800	49.29580	78.19190	-263.61743	780.72023	-434.79422	1
29544	H	64.35700	50.15180	78.89890	1458.40810	2781.43741	304.49970	1
29545	H	63.54600	49.42280	77.46690	1372.35221	-2544.83110	-1185.33817	1
29546	H	64.34900	48.32980	78.73890	2090.79010	-2022.35620	1139.40808	1
29547	C	66.94300	49.36980	78.37390	587.24687	-520.66731	421.28645	1
29548	H	67.87300	49.13980	77.81290	1542.98426	2357.81258	-1414.16151	1
29549	H	66.93800	48.50780	79.07490	1400.03810	711.37108	-2726.20084	1
29550	C	67.20200	50.71380	79.14890	-609.11670	384.00768	581.52964	1
29551	H	68.24400	50.65780	79.52990	-1761.03876	869.22056	-2477.11856	1
29552	H	66.39500	50.70680	79.91290	1648.09154	-1972.29562	1780.77709	1
29553	H	67.23000	51.56080	78.43090	2679.20498	-1431.16412	738.12134	1
29554	C	64.68400	47.94480	75.66090	-4.47276	-890.39056	77.07841	1
29555	O	64.12400	46.89680	75.93190	-386.48034	-521.45951	-444.19351	1
29556	N	64.12500	48.67480	74.69190	71.06841	145.52878	828.54755	1
29557	H	64.58500	49.51780	74.42290	1204.87276	2331.81292	-1748.33772	1
29558	C	62.87300	48.23880	73.93890	682.65756	593.53180	-100.94339	1
29559	H	62.32800	47.76380	74.74190	1608.70408	-717.09272	2590.47637	1
29560	C	62.19700	49.49980	73.38790	-843.63770	83.49633	381.37072	1
29561	H	62.95800	50.04680	72.79190	12.53410	2245.28363	2222.08826	1
29562	C	61.03600	49.08980	72.50190	-517.48125	-223.68730	-722.74656	1
29563	H	61.35600	48.76480	71.48890	-2545.55883	1873.57211	-280.80316	1

29564	H	60.40500	48.31080	72.98290	-2261.22495	-1775.77043	1283.75187	1
29565	H	60.31000	49.90180	72.28490	2295.02908	-1427.52812	-1564.35121	1
29566	C	61.82500	50.37880	74.60090	-608.12291	-642.80668	208.92363	1
29567	H	61.06500	51.09380	74.21890	1938.83000	-412.57060	2427.21487	1
29568	H	62.72800	50.86480	75.02890	1173.84945	-2475.05909	1503.92813	1
29569	H	61.21500	49.71080	75.24590	-2275.86113	2129.61154	-583.08871	1
29570	C	63.20100	47.23580	72.87290	398.65320	326.04880	749.19620	1
29571	O	62.38700	46.38080	72.49590	-512.46231	614.45072	-162.32727	1
29572	N	64.47400	47.13380	72.43890	-213.16995	690.80047	-473.47581	1
29573	H	65.23300	47.65180	72.82590	451.98819	-1141.71893	-2888.55572	1
29574	C	64.77200	46.31680	71.22390	-630.52424	232.96669	-644.66306	1
29575	H	64.08400	45.51580	70.99690	-2501.24040	1249.93230	-1494.77491	1
29576	C	64.96500	47.11680	69.95990	-668.00175	658.09326	55.62564	1
29577	H	65.19000	46.42980	69.11690	768.13137	-2369.07397	-1893.11762	1
29578	H	65.80000	47.84180	70.06290	-2017.38818	-1776.27298	-1643.59359	1
29579	N	62.80000	47.30780	68.67190	226.28293	-141.58457	-791.23272	1
29580	H	62.85700	46.39880	68.25890	-1794.65273	2294.88292	1255.60289	1
29581	C	63.74700	47.92880	69.43990	-698.84711	623.40693	78.22906	1
29582	C	61.90700	48.23880	68.29190	376.97620	-503.00922	632.31567	1
29583	H	61.02100	47.93880	67.73390	-707.40627	506.88706	-3031.01010	1
29584	N	62.23400	49.43580	68.75890	393.46663	-649.15653	-307.02506	1
29585	C	63.35500	49.21480	69.53490	-550.14866	716.92046	-252.67266	1
29586	H	63.91700	50.02480	69.98390	-1340.16791	1019.97910	2673.23123	1
29587	C	66.09300	45.60480	71.41390	727.55431	-184.90707	-482.78070	1
29588	O	67.00800	45.60980	70.60490	528.67711	-548.83896	24.48597	1
29589	N	66.26200	44.96680	72.58690	-422.18887	-324.11670	656.32044	1
29590	H	65.54000	44.88280	73.26990	-1670.45708	1025.70151	2479.09392	1
29591	C	67.55100	44.53680	72.97490	-464.56429	553.51374	-591.90628	1
29592	H	68.36100	45.24380	72.87890	2728.29858	-1433.62198	488.06698	1
29593	C	67.54100	44.11380	74.52790	665.11351	147.32855	-591.89725	1
29594	H	67.20500	45.01580	75.08290	1833.46719	-1050.60746	-2311.79038	1
29595	H	66.79700	43.31280	74.72290	2390.69056	612.73623	-1935.69336	1
29596	H	68.52800	43.74880	74.88590	-1402.31919	-894.98403	-2679.17864	1
29597	C	68.08100	43.25480	72.25790	-419.34462	117.26893	810.03220	1
29598	O	69.24900	42.90780	72.37290	615.23941	-447.11669	-66.98575	1
29599	N	67.23100	42.50780	71.53190	-17.64070	615.53019	591.83690	1
29600	H	66.32800	42.91980	71.44090	2890.75518	-457.64646	1087.61903	1
29601	C	67.54800	41.26580	70.93090	-358.15902	275.53679	803.75862	1
29602	H	68.32300	40.86780	71.56890	-2032.91833	1769.11326	-1673.31738	1
29603	C	66.43900	40.21380	70.95290	635.06003	531.00446	-369.53760	1
29604	H	66.01200	40.24680	71.97790	-1875.50752	1373.34505	-2153.77607	1
29605	O	66.96200	38.92080	70.87490	527.02303	99.53518	556.33722	1
29606	H	67.72100	38.72880	71.43090	-1600.10739	-1194.28707	2434.40270	1
29607	C	65.34400	40.37980	69.88590	725.98116	-17.71252	-519.93374	1
29608	H	64.40400	39.92280	70.26290	1692.15700	2088.26995	-1635.35071	1
29609	H	65.72800	39.97280	68.92590	-243.29724	-3049.84425	660.91254	1
29610	H	65.10900	41.45680	69.74290	1910.51114	2003.79376	-1490.18054	1
29611	C	68.04700	41.39180	69.50990	-702.42783	-581.51568	109.24285	1
29612	O	68.49600	40.41480	68.88190	268.45616	-327.39415	-652.08204	1
29613	N	67.97800	42.58880	68.90590	-122.37394	-210.39026	802.98671	1
29614	H	67.40400	43.31080	69.28390	1207.90456	1534.94607	2461.89759	1
29615	C	68.25700	42.84080	67.50690	-706.43442	489.10688	374.30481	1
29616	H	69.24300	42.47480	67.26390	1539.06241	-1915.60832	-1933.61835	1
29617	C	67.21300	42.10680	66.52190	731.90133	513.23244	105.52792	1
29618	H	67.50300	42.52180	65.53290	-2148.82595	383.96726	2289.05740	1
29619	H	67.39400	41.01280	66.44490	1678.78336	-116.72208	-2644.59873	1
29620	C	65.73100	42.38580	66.82990	-631.73612	-653.30083	-116.78060	1
29621	O	65.28300	43.17080	67.69590	676.36586	218.79586	301.87521	1
29622	N	64.85100	41.84280	65.95390	-496.60947	162.28026	683.81908	1
29623	H	65.23300	41.18080	65.30890	1871.33752	-1536.67222	-1971.75595	1
29624	H	63.87600	42.02380	66.07990	-1002.12328	-1760.86934	-2405.18452	1
29625	C	68.28700	44.37280	67.28890	579.54768	268.52599	631.27142	1

29626	O	67.32600	45.05080	66.84790	-307.12846	88.51277	-737.27454	1
29627	N	69.42800	45.01480	67.51390	-533.42642	455.56596	504.76870	1
29628	H	70.29900	44.54280	67.62790	3049.71477	112.37222	660.10064	1
29629	C	69.59800	46.39680	67.30590	-273.72489	-734.69227	-457.50595	1
29630	H	69.34300	46.64780	66.28690	2356.48873	544.13992	1983.71287	1
29631	C	68.81800	47.28080	68.35890	-773.36788	385.35006	-366.42072	1
29632	H	67.74200	47.08880	68.15690	-1157.65271	1179.81371	2690.14945	1
29633	H	68.95200	48.36380	68.15390	2599.98840	1615.42158	679.43721	1
29634	O	69.09100	46.87480	69.72790	61.60281	593.72252	-536.98787	1
29635	H	68.34100	46.30280	69.90690	-1015.77706	-1692.49893	2442.95832	1
29636	C	71.05900	46.81080	67.33990	-621.55580	-230.65392	-648.18942	1
29637	O	71.31200	47.99080	67.04890	-142.57377	-401.08519	653.98600	1
29638	N	72.08300	46.00080	67.59690	-258.60912	201.95991	-795.53263	1
29639	H	71.88000	45.04780	67.80590	-1964.90801	382.30492	2441.72884	1
29640	C	73.48600	46.44780	67.59790	-140.26433	822.73370	398.27858	1
29641	H	73.52400	47.26880	68.29890	-116.30935	570.18118	-3102.82192	1
29642	C	74.37500	45.29980	68.15590	326.19417	-680.25084	468.38670	1
29643	H	74.02300	44.33880	67.72490	2163.84090	1748.92591	-1458.60838	1
29644	H	74.17000	45.24680	69.24690	-484.56415	-661.19926	3029.76126	1
29645	C	75.92100	45.26480	67.94090	-711.54404	-174.87263	-576.73118	1
29646	H	76.30900	44.56380	68.70990	877.66942	2496.71360	1699.49766	1
29647	H	76.31100	46.28280	68.15790	2700.14948	930.70805	1272.49708	1
29648	C	76.47700	44.90180	66.52690	-718.68384	75.48813	578.14318	1
29649	O	77.48800	45.40880	66.06490	-607.76872	-389.88172	-357.94404	1
29650	N	75.84000	43.91380	65.89590	652.72093	-400.68386	-294.61459	1
29651	H	75.05300	43.46880	66.32490	1576.34272	2253.95854	1513.42188	1
29652	H	76.20200	43.57880	65.02690	1882.21450	-167.24706	-2504.42321	1
29653	C	74.06300	47.03080	66.32090	498.52752	-561.14870	-484.93286	1
29654	O	74.69700	48.06380	66.27790	221.34713	-332.85870	657.57196	1
29655	N	73.75600	46.55480	65.10790	-782.14070	159.11547	-351.02690	1
29656	H	73.25200	45.70380	64.98290	-509.23446	502.94546	3062.67198	1
29657	C	74.08400	47.23980	63.86290	-186.62791	-735.89511	484.23145	1
29658	H	75.12800	47.51180	63.92690	-1090.07629	-2918.22105	397.78926	1
29659	C	74.06800	46.20880	62.72890	-757.54866	-455.13379	267.81603	1
29660	H	73.13500	45.60880	62.79690	-2035.53110	-1584.11130	1810.57933	1
29661	H	74.85700	45.42680	62.72790	-443.16206	-514.52677	3064.79346	1
29662	C	74.06200	46.76480	61.27790	-803.95628	-421.79243	185.26739	1
29663	H	73.11700	47.30680	61.06290	1390.40288	2752.92717	-634.39532	1
29664	H	74.90400	47.46680	61.10090	-1673.91248	882.30307	-2544.57431	1
29665	C	74.25100	45.71380	60.15490	759.52852	-417.66615	-163.47816	1
29666	H	75.13100	45.04580	60.27290	-2369.33341	1048.77310	1821.00714	1
29667	H	73.41700	44.99080	60.02890	-304.91412	2918.37754	1172.20687	1
29668	N	74.37500	46.45680	58.85890	-570.68018	-469.81113	421.18117	1
29669	H	73.83000	47.27780	58.68890	411.18517	2691.77044	1585.59941	1
29670	C	74.66200	45.80580	57.73890	382.77277	617.22758	-554.26052	1
29671	N	75.21300	44.60980	57.67290	313.03825	-469.73695	591.70953	1
29672	H	75.14000	43.94180	58.41390	1036.61876	1716.34708	-2430.18600	1
29673	H	75.29600	44.15880	56.78390	-2772.64122	605.80544	-1434.24200	1
29674	N	74.43800	46.41980	56.59390	-683.00421	456.14816	-310.86550	1
29675	H	74.35200	47.41580	56.55990	-395.99661	-819.35373	-3019.49935	1
29676	H	74.81700	46.00380	55.76690	-2120.45504	-2337.52595	-19.98912	1
29677	C	73.45900	48.66280	63.65890	342.71824	-634.17633	517.25154	1
29678	O	74.22500	49.62080	63.25590	567.19180	-291.07702	-432.33047	1
29679	N	72.19600	48.93680	63.88290	-594.27707	573.20328	-283.47882	1
29680	C	71.15200	47.91380	63.64390	529.92875	330.26852	645.65378	1
29681	H	71.01200	47.26380	64.53490	-432.86052	-2492.02982	1849.53242	1
29682	H	71.30300	47.24080	62.77290	2288.38861	-2070.21231	431.71453	1
29683	C	71.58800	50.28980	63.86990	199.57404	-556.63007	667.72991	1
29684	H	71.84300	50.86080	62.98890	2419.74009	-1863.50427	622.00125	1
29685	C	70.07700	50.06480	63.96190	-463.70341	-555.82815	552.35887	1
29686	H	69.46100	50.84980	63.47390	-2728.94549	808.58495	1392.88859	1
29687	H	69.73700	49.93580	65.01190	-1639.43883	-394.98870	-2672.73840	1

29688	C	69.87000	48.68880	63.34890	-631.93455	-663.76713	16.54176	1
29689	H	69.82900	48.81780	62.24590	1976.09353	2207.58942	-1049.10531	1
29690	H	68.94600	48.19980	63.72390	-1205.74864	-2490.54757	1484.70112	1
29691	C	72.06400	51.10980	65.08690	395.78683	-600.08310	-533.32717	1
29692	O	72.36800	52.25980	64.91690	-333.22085	-672.72477	225.25080	1
29693	N	72.14200	50.58980	66.34490	-311.42711	-581.26428	516.10553	1
29694	H	71.85400	49.64680	66.48990	1341.27812	2608.39763	-1152.99536	1
29695	C	72.81900	51.31980	67.35990	336.16928	643.38829	548.76954	1
29696	H	72.31400	52.25080	67.56990	2482.03733	1413.04474	1289.85172	1
29697	C	72.89600	50.49980	68.67390	-278.11223	-467.63588	-736.64472	1
29698	H	73.60400	51.00680	69.36290	-2503.40464	1687.05494	958.62678	1
29699	H	73.30500	49.50780	68.38590	-1698.82538	2361.61575	1247.96685	1
29700	C	71.62900	50.31280	69.43890	-183.83590	-575.24672	-681.37666	1
29701	H	70.76200	49.92680	68.86190	-575.55450	3005.29427	-813.59676	1
29702	H	71.29200	51.26680	69.89990	461.61702	-1460.77149	-2742.27293	1
29703	C	71.72500	49.24180	70.58390	426.91109	-759.01238	-186.13744	1
29704	H	70.75000	48.93880	71.02290	1466.95438	-1555.41252	2279.04658	1
29705	H	72.23500	48.32680	70.21490	-1828.37912	1968.33492	1670.96689	1
29706	N	72.53600	49.96180	71.58390	-311.95104	801.51258	-96.51975	1
29707	H	72.73100	50.93480	71.46790	-1212.64101	2663.05254	-1214.95783	1
29708	C	73.24800	49.36280	72.44790	792.11054	-402.36640	12.54351	1
29709	N	73.02000	48.12780	72.87290	-806.20510	-145.32190	251.74889	1
29710	H	72.19900	47.67380	72.52690	-2532.84267	-411.68297	1836.63900	1
29711	H	73.73800	47.68480	73.40890	1826.38258	1776.42141	1833.34667	1
29712	N	74.05500	50.13280	73.16390	-29.14281	856.20099	52.61960	1
29713	H	74.03900	51.12880	73.07790	-1008.03837	-2622.47800	1393.87342	1
29714	H	74.58500	49.72780	73.90890	-1594.22518	1015.33874	2523.50076	1
29715	C	74.26400	51.75680	67.03390	469.63576	-74.22269	-771.24544	1
29716	O	74.70400	52.87880	67.34290	-118.15669	-767.67487	44.87440	1
29717	N	74.99000	50.84080	66.43790	369.51373	-402.16838	-629.82696	1
29718	H	74.53700	50.00780	66.12990	-2457.36411	1277.38753	-1548.94822	1
29719	C	76.32900	51.05180	65.91890	733.55505	438.55022	272.98377	1
29720	H	76.92000	51.30980	66.78590	2361.62865	988.65006	1797.96295	1
29721	C	76.94900	49.70280	65.47390	-150.13772	463.16745	-792.63510	1
29722	H	76.30500	49.24080	64.69590	-1485.75552	-763.36627	2665.94233	1
29723	H	76.96900	49.10280	66.40990	2328.69672	2051.93337	-471.55719	1
29724	C	78.38400	49.85180	64.90690	483.78691	442.23467	613.67626	1
29725	H	78.99800	50.42380	65.63490	1516.61402	2190.49923	-1679.95338	1
29726	H	78.48000	50.46080	63.98190	474.10293	1598.67728	-2681.90675	1
29727	C	79.08600	48.50880	64.76090	-489.48314	-567.02107	-539.33397	1
29728	H	80.13800	48.65880	64.43590	-1822.70781	2110.48558	-1515.21454	1
29729	H	79.13800	48.00180	65.74790	-1735.98716	2028.60095	1691.94511	1
29730	C	78.42400	47.54480	63.73590	-301.89539	-448.75926	725.28753	1
29731	H	77.43900	47.19580	64.11290	2037.83214	-887.55667	2188.00891	1
29732	H	78.43800	48.07180	62.75690	-607.26141	-1283.73654	2796.14025	1
29733	N	79.19100	46.31480	63.58490	643.14517	-36.40260	501.50132	1
29734	H	79.15700	45.54480	64.28290	-1480.86452	2746.43108	-564.14471	1
29735	H	78.84600	45.88880	62.70090	2775.86720	708.68404	-1260.50613	1
29736	H	80.20700	46.41180	63.38790	-1420.89386	179.61503	-2826.90106	1
29737	C	76.45600	52.09780	64.76190	-363.18204	392.56223	-765.47663	1
29738	O	77.33400	53.00380	64.73790	458.65112	287.33432	-573.14363	1
29739	N	75.49900	52.07180	63.80890	451.48526	177.42827	-687.40687	1
29740	H	74.82500	51.33980	63.87890	-1367.15007	-1814.66724	-2187.21074	1
29741	C	75.37200	53.05880	62.72290	482.36877	-630.53717	-408.65361	1
29742	H	76.24900	53.07880	62.09390	1972.40452	-1781.47850	1631.03955	1
29743	C	74.08200	52.69580	61.93290	442.86034	-621.14159	-465.09569	1
29744	H	73.19500	52.54980	62.58490	2968.25882	-683.14379	669.99170	1
29745	H	74.18000	51.73280	61.38690	-2668.58208	-1363.51666	997.20390	1
29746	C	73.59900	53.60380	60.75090	721.83525	-133.26470	494.98694	1
29747	H	73.51200	54.61580	61.20090	-2283.46529	2015.60436	881.21091	1
29748	C	74.75200	53.70080	59.70190	367.63506	832.56869	-95.94297	1
29749	H	75.73100	53.99880	60.13390	949.14581	-2217.01392	-2001.83255	1

29750	H	74.40100	54.35980	58.87990	-2833.07999	-596.20793	-1289.58252	1
29751	H	74.77600	52.72380	59.17190	435.04214	-2952.25405	932.33557	1
29752	C	72.26900	52.99980	60.24790	120.66809	-596.22051	-666.93037	1
29753	H	72.31900	51.91280	60.01990	-2703.60663	732.58603	-1494.18110	1
29754	H	71.53100	53.17380	61.05890	2786.50945	732.04649	-1223.81321	1
29755	H	71.90400	53.53280	59.34390	-607.59474	1830.24676	-2509.54587	1
29756	C	75.26700	54.48680	63.29190	841.81818	-196.25397	-208.69804	1
29757	O	75.99400	55.39780	62.81990	-745.45686	-51.31241	-319.88395	1
29758	N	74.42500	54.77980	64.32690	34.52346	676.48878	-528.59308	1
29759	H	73.71000	54.13580	64.58490	1459.87010	2738.46161	-540.09202	1
29760	C	74.40000	55.99780	65.09690	114.58077	903.21777	144.08943	1
29761	H	74.15100	56.75380	64.36690	1795.46629	-1644.83157	1953.37289	1
29762	C	73.31000	55.86980	66.17990	127.31832	817.78242	-413.20864	1
29763	H	73.30000	56.73880	66.87090	-1898.79583	573.02636	2453.38100	1
29764	H	73.61800	54.94780	66.71790	-144.45411	1137.10557	2929.10056	1
29765	C	71.87600	55.65080	65.62390	-313.10467	-443.68883	-737.70481	1
29766	H	71.83700	54.60480	65.25090	832.41854	-36.56366	-3033.87889	1
29767	C	70.97400	55.48080	66.86590	-282.02625	292.08281	-834.02334	1
29768	H	71.23100	54.55980	67.43290	-55.64683	1355.00355	-2852.35123	1
29769	H	71.08600	56.36480	67.52890	671.16866	-2286.40938	2024.75947	1
29770	H	69.94100	55.32880	66.48690	768.96241	-2482.93822	1735.85434	1
29771	C	71.25800	56.61480	64.56090	486.22862	576.35809	-515.59325	1
29772	H	70.17700	56.37880	64.46190	-1767.50921	-1844.54850	1835.05229	1
29773	H	71.83700	56.72880	63.61990	1414.38720	2814.80854	10.88353	1
29774	H	71.32500	57.64680	64.96790	-622.50290	-2172.07149	-2185.07896	1
29775	C	75.73500	56.27280	65.77590	429.05365	704.37917	-399.54564	1
29776	O	76.34600	57.33580	65.63190	78.17463	-723.89738	-273.98663	1
29777	N	76.31200	55.24680	66.49890	453.88427	709.26817	53.86020	1
29778	H	75.88100	54.35180	66.58390	-2148.77026	2183.34108	804.20953	1
29779	C	77.48200	55.40080	67.33590	-208.42471	697.50872	-581.97539	1
29780	H	77.32600	56.29280	67.92390	-2267.15827	1537.86877	-1596.57283	1
29781	C	77.62100	54.17580	68.29490	637.33299	-238.48474	570.46506	1
29782	H	78.49700	54.34580	68.95590	-1374.11278	2569.72205	1223.31663	1
29783	H	76.75900	54.12480	68.99390	-205.30539	-686.61047	-3071.10177	1
29784	H	77.70900	53.20180	67.76690	743.82328	-1514.55992	2632.10920	1
29785	C	78.78300	55.65680	66.64290	-524.42585	530.18152	545.04863	1
29786	O	79.62000	56.37780	67.15490	-539.59922	-543.94477	197.42139	1
29787	N	78.96700	55.15180	65.41590	-191.09168	795.63336	-276.24272	1
29788	H	78.26300	54.58880	64.98890	-2851.76599	308.32957	-1352.01178	1
29789	C	80.24300	55.01480	64.81890	-764.03569	-307.77898	-433.11206	1
29790	H	80.93500	55.54480	65.45490	-1304.76890	1418.36472	2491.95929	1
29791	C	80.74100	53.60680	64.68090	347.64743	-778.46887	-277.20648	1
29792	H	81.54200	53.50280	63.91790	1344.54311	2841.39313	-158.03815	1
29793	H	79.93900	52.99380	64.21490	-1253.26172	-435.76906	-2872.17778	1
29794	C	81.19200	53.07180	66.00590	-461.14121	442.68196	660.01151	1
29795	H	80.21400	52.97080	66.52290	801.29749	-2065.33064	2203.35796	1
29796	H	81.98500	53.67880	66.49090	2404.95835	1976.82249	-401.08802	1
29797	C	81.80000	51.67080	65.81990	-216.88792	653.20898	-630.52146	1
29798	O	82.54700	51.38680	64.86090	467.75225	522.29643	335.45347	1
29799	O	81.46400	50.77080	66.62690	565.02086	109.02146	506.64633	1
29800	C	80.24800	55.64180	63.46990	-415.56508	-287.72738	754.21692	1
29801	O	81.28400	56.18180	63.05390	163.45510	-752.14790	-88.82587	1
29802	N	79.10300	55.73680	62.73990	-21.21825	632.81864	-583.60703	1
29803	H	78.21300	55.39680	63.03490	-3013.62999	-310.50730	909.31905	1
29804	C	79.08500	56.37380	61.44790	433.82684	-539.34013	553.10950	1
29805	H	80.07800	56.57180	61.07090	2057.78257	-145.94245	2342.75525	1
29806	C	78.41800	55.43180	60.43790	571.34098	-249.93928	-649.17488	1
29807	H	77.80000	55.86380	59.62190	-1225.63371	1929.95916	-2196.69015	1
29808	H	77.61800	54.90880	61.00490	-2363.61121	2093.49897	-320.23712	1
29809	C	79.39200	54.30580	59.96390	499.10178	562.78431	-515.34531	1
29810	H	80.20100	54.78780	59.37390	1607.37996	624.26687	2607.23921	1
29811	H	79.81400	53.79280	60.85490	3057.92791	-617.87408	-23.34365	1

29812	C	78.69400	53.25980	59.05890	509.48602	-541.14404	-498.62082	1
29813	H	78.18300	53.69880	58.17490	-2922.69958	-1215.03088	-33.65169	1
29814	H	77.89200	52.86580	59.71890	549.23746	-3055.35805	-400.40692	1
29815	C	79.52300	52.08780	58.64990	93.33772	-204.89371	-888.74206	1
29816	H	78.88900	51.18480	58.52290	1523.94530	-124.17991	2722.88827	1
29817	H	80.17100	51.87080	59.52690	-1861.89217	88.30939	-2565.66026	1
29818	N	80.41500	52.29680	57.45590	-368.03579	-226.44064	722.65073	1
29819	H	81.01600	53.14280	57.39090	2050.53027	1722.58877	1617.37162	1
29820	H	80.99800	51.45480	57.27390	2009.21329	-1667.40749	-1723.71791	1
29821	H	79.79000	52.30380	56.62490	-164.67336	-2220.28084	2200.79580	1
29822	C	78.36900	57.66680	61.44790	-458.52390	507.92811	-639.88576	1
29823	O	78.89200	58.71780	61.08490	-109.81548	-599.46288	480.44712	1
29824	N	77.09500	57.58980	61.86190	585.27683	540.66970	-265.64489	1
29825	H	76.77100	56.72180	62.22990	1436.17534	-1983.69580	-1954.16475	1
29826	C	76.09900	58.66480	61.66090	111.35294	-770.67174	436.43447	1
29827	H	76.35500	59.15680	60.73390	-2997.67933	-979.34372	234.74259	1
29828	C	74.63500	58.10880	61.42090	-257.98420	701.20741	-559.46836	1
29829	H	74.40700	57.32080	62.17090	-2614.91633	300.77749	-1766.70875	1
29830	C	73.63900	59.25180	61.53490	390.77225	82.45531	803.12076	1
29831	H	73.66300	59.64980	62.57190	1103.73768	1045.63878	-2758.71296	1
29832	H	72.61900	58.85480	61.34290	-2464.68180	-1670.48787	1037.58116	1
29833	H	73.85800	60.07080	60.81690	1033.93615	-1516.44893	2530.14592	1
29834	C	74.54200	57.54180	59.97590	-346.17131	400.37581	752.64770	1
29835	H	75.40900	56.88280	59.75790	1196.67336	-2089.39260	1987.41206	1
29836	H	73.71200	56.81880	59.81990	1991.22041	1381.42151	1985.10810	1
29837	H	74.61300	58.32480	59.19190	277.73328	-2501.21054	1857.21890	1
29838	C	76.21100	59.84480	62.65990	-33.23072	20.49669	-920.64385	1
29839	O	75.93300	60.98580	62.30390	555.87201	226.86979	-504.64127	1
29840	N	76.85000	59.71980	63.88290	-415.13800	473.20345	-596.84476	1
29841	H	76.85700	58.81880	64.30890	-1765.71622	-2601.85453	-116.91871	1
29842	C	77.20900	60.88380	64.76190	663.59528	-352.83305	471.63169	1
29843	H	76.28000	61.42980	64.83790	-1987.66060	1650.55200	1819.18011	1
29844	C	77.73400	60.39280	66.08790	-546.34206	-94.95929	-745.41438	1
29845	H	77.00500	59.71580	66.58190	2055.83324	1556.84236	1783.25150	1
29846	C	79.03700	59.53180	65.95890	-177.81357	-547.46969	-712.66147	1
29847	H	79.91700	60.21080	65.96790	3063.42207	-2.07587	621.12846	1
29848	H	79.30200	58.94780	65.05190	-1139.20218	-2540.03413	-1470.37454	1
29849	H	79.18400	58.75480	66.73890	-2417.45821	598.36163	-1960.28240	1
29850	C	77.96200	61.63780	66.98490	220.49921	-715.48726	484.40501	1
29851	H	78.82900	62.29580	66.75890	2513.53494	1767.99113	-652.80066	1
29852	H	78.00300	61.31880	68.04790	-1582.89057	1847.97400	2009.17368	1
29853	H	77.05900	62.28480	66.98290	-1212.05072	2435.27605	-1622.97925	1
29854	C	78.17500	61.78680	63.99590	572.31497	309.87981	-637.39535	1
29855	O	78.09900	62.98780	64.12390	-698.55700	414.42223	-12.29448	1
29856	N	79.04000	61.27880	63.15690	441.64972	235.26770	-681.59896	1
29857	H	79.21600	60.30180	63.07090	-371.81184	1965.08064	2430.84884	1
29858	C	79.83300	62.16880	62.23990	-763.42303	-439.30775	262.72285	1
29859	H	80.38500	62.91080	62.79690	-586.92214	2269.42859	2105.10646	1
29860	C	80.87800	61.35180	61.53590	226.70471	888.74311	-46.73912	1
29861	H	81.46900	62.00780	60.86190	1647.05193	-2650.69948	153.21541	1
29862	H	80.48200	60.49880	60.94490	3010.60956	332.40926	763.48274	1
29863	C	81.78800	60.76180	62.55890	-562.79992	463.87893	-589.34038	1
29864	C	81.47900	59.48980	63.13990	589.81396	91.79874	-685.00101	1
29865	H	80.54500	58.99280	62.92390	2073.13163	-2295.69014	-445.14454	1
29866	C	82.33100	58.99680	64.14690	-648.00206	-274.53922	583.35206	1
29867	H	82.11600	58.00880	64.52490	1268.55757	-2488.11130	-1423.61344	1
29868	C	83.50600	59.67180	64.52090	577.69141	569.21156	-417.12450	1
29869	O	84.34300	59.10380	65.48790	765.60059	-5.83404	-100.42061	1
29870	H	85.16400	59.59980	65.50190	1970.30362	2349.99992	-696.91631	1
29871	C	82.96400	61.42180	62.94590	-763.68705	-216.68672	-489.24367	1
29872	H	83.22800	62.37680	62.51590	-1621.30581	-1942.84420	-1888.71825	1
29873	C	83.79600	60.81880	63.85490	-666.20929	653.41798	-26.23819	1

29874	H	84.68400	61.36680	64.13590	-1096.68094	1771.56723	2359.35172	1
29875	C	79.07200	63.01480	61.18490	735.49586	-491.49769	65.63105	1
29876	O	79.35300	64.19780	61.05590	285.18429	545.43288	485.55080	1
29877	N	78.11400	62.42880	60.51990	-351.64314	765.97113	-201.15841	1
29878	H	77.89300	61.46280	60.63090	-1822.22015	-2405.18132	-908.56702	1
29879	C	77.45200	63.00280	59.37490	-192.71139	900.60106	112.55971	1
29880	H	77.88600	63.93180	59.03590	1723.75386	-279.97630	-2611.09447	1
29881	C	77.51400	62.02580	58.15990	473.41740	437.06405	-646.56364	1
29882	H	78.58700	61.74980	58.07590	-2010.63254	1607.06392	1835.21782	1
29883	C	76.64800	60.74380	58.20490	-861.45420	72.74156	345.19755	1
29884	H	76.89000	60.04880	57.37290	1925.83833	-920.11511	-2294.90365	1
29885	H	75.57900	61.03780	58.26890	-1418.54269	2701.92608	844.14314	1
29886	H	76.88300	60.24480	59.16990	-878.65220	697.51559	2939.92129	1
29887	C	77.07000	62.83080	56.90790	-594.15422	-596.05529	356.74141	1
29888	H	77.53500	63.83980	56.88090	453.66373	-670.16756	3024.11880	1
29889	H	77.24600	62.12980	56.06390	-2213.37536	-1797.60064	1341.66881	1
29890	H	75.98500	63.07180	56.90790	-1353.94056	-1403.88912	2464.63617	1
29891	C	75.96700	63.43180	59.71690	-293.51150	-578.19325	-646.41353	1
29892	O	75.23100	63.95280	58.88690	-105.12726	424.82490	-677.51275	1
29893	N	75.55600	63.14580	60.96990	-171.14636	839.53238	84.10231	1
29894	H	76.07500	62.48980	61.51290	483.68026	2429.59711	1942.67180	1
29895	C	74.24300	63.52480	61.53090	-543.96125	376.24909	-660.28795	1
29896	H	73.64800	62.66780	61.80990	-1302.80220	2685.48711	1051.40769	1
29897	H	73.74100	64.17580	60.82990	-2184.42489	-655.18881	-2190.19523	1
29898	C	74.39400	64.47380	62.76890	648.56060	-579.36666	-190.33287	1
29899	O	73.38900	65.08080	63.16490	195.10019	507.73342	572.01960	1
29900	N	75.62000	64.65580	63.34290	389.36652	-514.15298	508.86598	1
29901	H	76.40600	64.05980	63.19790	-1584.18586	-711.28807	2622.08093	1
29902	C	75.80700	65.65780	64.37690	231.23815	574.06568	666.67305	1
29903	H	74.96800	66.32780	64.49790	-151.93751	2869.72340	-1321.55872	1
29904	C	76.01200	64.93380	65.67590	261.87085	-356.87160	776.56130	1
29905	H	76.89500	64.26080	65.65490	2076.57215	-2290.35292	-465.36475	1
29906	C	76.30800	65.94080	66.83790	644.24336	-139.76307	-619.18954	1
29907	H	77.32300	66.35880	66.66890	2588.79155	1431.11390	-1060.70847	1
29908	H	76.23100	65.35680	67.77990	1827.70459	1289.12398	2199.16484	1
29909	H	75.48500	66.68680	66.80890	2541.73960	-1814.73792	-134.85568	1
29910	C	74.73100	64.15080	66.04990	-277.66086	604.39471	-652.06502	1
29911	H	73.85200	64.82480	66.13390	-1576.37658	-2575.54295	-876.88015	1
29912	H	74.86500	63.63880	67.02690	-1599.58447	904.44955	-2576.74932	1
29913	H	74.49800	63.28680	65.39090	-1495.46225	-1549.37550	-2303.10196	1
29914	C	76.98200	66.54980	64.00090	-328.55588	-650.56289	532.74843	1
29915	O	76.81300	67.75280	63.82890	476.27161	-554.62996	231.34555	1
29916	N	78.17500	65.95380	63.88490	651.94454	335.51572	-410.51963	1
29917	H	78.34800	64.98480	64.04090	-1970.06585	-1889.14951	1561.29330	1
29918	C	79.38000	66.79380	63.80390	258.11152	282.03506	-837.17940	1
29919	H	79.33300	67.52180	64.60090	419.18585	-1553.02487	-2704.78844	1
29920	C	80.72500	65.95580	63.88190	766.44774	-396.60390	-235.35583	1
29921	H	81.57500	66.47980	63.39390	934.94302	2557.22429	1572.13033	1
29922	H	80.62700	65.05980	63.23190	-953.91417	-1349.52370	-2689.22773	1
29923	C	81.07600	65.46380	65.23690	739.77648	-490.41253	-95.24035	1
29924	C	81.17800	64.13780	65.68490	-809.81521	-339.90189	-293.88712	1
29925	H	81.15400	63.23580	65.09090	391.62755	1632.61012	-2677.21789	1
29926	N	81.54500	64.11680	67.03990	-644.25002	260.72046	-518.29767	1
29927	H	81.89000	63.41080	67.61890	-815.61175	1863.78110	-2426.49013	1
29928	C	81.67300	65.44380	67.41590	784.44636	-387.80033	-192.33382	1
29929	C	81.36600	66.28480	66.35090	-277.27973	-591.59123	619.81206	1
29930	C	81.43800	67.69780	66.49390	434.84020	-613.65533	-500.20146	1
29931	H	81.35400	68.36680	65.64990	2121.98480	1838.02869	1400.00875	1
29932	C	81.95200	68.19480	67.67890	781.54167	-391.25005	178.39887	1
29933	H	82.20600	69.23880	67.78590	-1113.60822	2905.98861	542.38047	1
29934	C	81.95100	65.96580	68.65390	-491.16223	775.73592	127.45049	1
29935	H	82.12500	65.34080	69.51690	2138.10913	785.12273	2147.76691	1

29936	C	82.16800	67.36880	68.71590	98.50983	-680.63564	-595.99151	1
29937	H	82.68500	67.67280	69.61390	-1264.43500	-1408.84150	2500.35865	1
29938	C	79.54100	67.60780	62.56990	-679.76081	-386.40412	-494.72139	1
29939	O	79.68900	68.83180	62.62190	-89.87941	695.46232	378.49413	1
29940	N	79.43900	66.98780	61.39490	215.37280	-463.44457	-667.61625	1
29941	H	79.52900	65.99580	61.36090	-1677.66921	-131.28844	2658.72555	1
29942	C	79.40100	67.72880	60.09790	645.42909	-574.79053	200.60068	1
29943	H	80.27400	68.36380	60.06790	797.90010	613.12597	-2989.51420	1
29944	C	79.57800	66.71580	58.97690	-109.96400	142.23864	887.19364	1
29945	H	79.06400	65.76680	59.23990	1499.86836	1992.59875	1904.10575	1
29946	C	79.02300	67.18080	57.59490	-587.43531	599.26844	397.85399	1
29947	H	79.08700	66.33780	56.87390	-767.44093	-1555.87647	2612.74870	1
29948	H	77.97200	67.53780	57.64990	2907.33541	1097.53405	-393.60650	1
29949	H	79.57700	68.09680	57.29790	2022.77549	-2072.41047	-1183.15945	1
29950	C	81.08100	66.50980	58.92390	367.87403	707.06640	432.22919	1
29951	H	81.56100	66.51280	59.92590	2702.00885	-1222.04349	971.36788	1
29952	H	81.53800	67.31980	58.31590	1778.72814	2413.22667	932.89374	1
29953	C	81.48100	65.22680	58.17990	533.03895	-303.21584	-663.88390	1
29954	H	82.58100	65.23080	58.01990	-570.67765	-2322.63801	-2050.00629	1
29955	H	81.14600	64.38880	58.82690	-1084.21193	1857.62025	2303.56107	1
29956	H	81.07500	65.34680	57.15190	-2548.97133	-1833.33395	-341.63066	1
29957	C	78.20300	68.68480	59.97390	-188.05390	522.15087	727.36989	1
29958	O	78.39300	69.81780	59.50690	-749.80419	-150.26458	240.33880	1
29959	N	76.94300	68.38580	60.25590	363.41952	-436.96493	593.84810	1
29960	C	76.40600	67.04980	60.23790	82.07405	53.35219	-914.10816	1
29961	H	76.84500	66.50280	61.09990	-54.39298	-2351.25864	-2083.93235	1
29962	H	76.61900	66.55080	59.26890	-2235.81047	1845.46957	-1287.36046	1
29963	C	75.89100	69.36780	60.47890	-522.09636	-369.05291	-664.94251	1
29964	H	75.63800	69.83980	59.54090	2391.51668	1732.96257	-1073.05229	1
29965	C	74.79500	68.58480	61.07990	304.35295	-408.47049	732.96642	1
29966	H	74.84900	68.53780	62.18890	-1058.29241	-1887.37103	-2287.83745	1
29967	H	73.81200	69.09380	60.98690	2223.88125	-2133.31577	-514.33489	1
29968	C	74.91000	67.23780	60.38990	-344.70845	-641.92381	-550.87328	1
29969	H	74.48000	66.36180	60.92190	2385.81493	212.39416	2010.96923	1
29970	H	74.36300	67.34880	59.42990	-76.38756	860.57589	3022.28659	1
29971	C	76.27700	70.60180	61.32290	685.69598	-32.88575	-587.43544	1
29972	O	75.93900	71.65980	60.85690	-740.91714	-188.08774	-251.40051	1
29973	N	76.98300	70.49280	62.53090	425.16778	364.70537	618.71903	1
29974	H	77.22900	69.59880	62.89790	-1015.26444	-2113.98651	2082.56042	1
29975	C	77.34300	71.60280	63.34590	36.19724	720.88806	-581.98740	1
29976	H	76.43300	72.10680	63.63490	2882.94814	-1158.62587	-362.12852	1
29977	C	78.07100	71.11780	64.56590	-268.08664	672.00053	-586.81119	1
29978	H	77.40400	70.42680	65.12390	-1426.04120	-2301.28879	-1606.30218	1
29979	H	78.32800	71.98480	65.21090	-2723.94744	380.61775	1545.77142	1
29980	H	79.06500	70.67980	64.33290	-3082.43821	149.96009	-697.48455	1
29981	C	78.26200	72.58380	62.57290	666.80156	460.07104	397.17663	1
29982	O	77.99600	73.79480	62.52490	-493.49587	563.38721	293.62022	1
29983	N	79.28600	72.04380	61.88190	-206.43529	-618.73808	-537.89278	1
29984	H	79.45000	71.06180	61.82190	1697.33518	1961.21505	-1788.93987	1
29985	C	80.16600	72.83480	60.97290	-498.10898	-355.59770	670.36384	1
29986	H	80.56600	73.62780	61.58790	-14.00103	3153.54062	-181.22975	1
29987	C	81.26100	71.99780	60.26490	-659.70240	-589.05082	229.00397	1
29988	H	80.87300	71.21680	59.57690	1235.67288	-2865.74911	-223.59785	1
29989	H	81.86300	72.79880	59.78490	1334.48573	-2398.90033	-1515.67612	1
29990	C	82.21600	71.17680	61.14290	19.99461	710.16300	572.04390	1
29991	H	81.67600	70.33280	61.62390	-1352.92363	-1067.95755	-2648.24927	1
29992	C	83.30900	70.67280	60.22790	-665.69108	-282.10696	557.80668	1
29993	H	82.82200	70.02180	59.46990	-353.18708	1922.60909	2463.47941	1
29994	H	83.81700	71.51980	59.71990	-1112.51872	2161.76419	2004.69475	1
29995	H	84.03400	70.09680	60.84190	2151.58025	-2221.64256	-470.77553	1
29996	C	82.83200	72.00880	62.34890	-750.38940	-18.61901	-552.66480	1
29997	H	81.97800	72.18080	63.03890	1602.91117	2653.12862	535.31648	1

29998	H	83.61500	71.40980	62.85990	1018.94721	1229.63154	-2722.92607	1
29999	H	83.28400	72.93580	61.93590	888.09318	2730.44202	1284.85778	1
30000	C	79.39800	73.56380	59.85490	-429.99027	824.13171	-57.98303	1
30001	O	79.60700	74.74080	59.58190	-282.06662	699.25515	274.88930	1
30002	N	78.44400	72.86480	59.19490	612.64292	468.95767	-337.42468	1
30003	H	78.25100	71.91980	59.44990	-2246.33320	1251.05939	1834.05951	1
30004	C	77.51900	73.42580	58.26290	448.32714	-588.39576	492.39152	1
30005	H	78.15500	73.93980	57.55690	1318.78923	-2709.54319	-844.74825	1
30006	C	76.60000	72.37380	57.56490	290.86854	444.66058	-750.16063	1
30007	H	75.90000	72.97980	56.94990	323.15996	-2231.91234	2168.12513	1
30008	H	76.05600	71.96080	58.44090	1065.98456	942.81287	-2811.78736	1
30009	C	77.41200	71.39580	56.68990	846.40717	266.22435	120.18107	1
30010	H	78.23700	70.92380	57.26490	-1890.21724	-1579.91039	1955.42085	1
30011	C	76.51500	70.32580	56.03890	-600.43183	-511.29687	460.14933	1
30012	H	75.79800	70.79480	55.33190	1927.78776	-2436.22691	300.69450	1
30013	H	77.06300	69.52180	55.50390	914.23042	-2822.80664	979.38593	1
30014	H	76.02800	69.82180	56.90090	-2224.60498	1011.91571	-2019.56893	1
30015	C	78.08700	72.20080	55.55590	-569.16026	-202.71366	685.80191	1
30016	H	78.93000	72.84180	55.89090	2426.53511	-877.61648	-1776.57320	1
30017	H	77.35600	72.90380	55.10290	-39.92693	-3066.81927	-649.16940	1
30018	H	78.47800	71.55980	54.73690	-1993.58597	-1437.25591	1966.04063	1
30019	C	76.65800	74.51080	58.81890	214.58987	575.99155	-688.00716	1
30020	O	76.44500	75.53780	58.13990	696.63971	-26.41188	-343.40018	1
30021	N	76.13800	74.39180	60.04090	600.73281	300.44987	-507.76731	1
30022	H	76.10800	73.55980	60.58990	2148.98618	-1839.66138	-1339.94471	1
30023	C	75.18900	75.41980	60.53390	685.23654	-510.85609	245.61488	1
30024	H	74.52600	75.63580	59.70990	926.43261	-2929.61772	577.18154	1
30025	C	74.32700	74.98880	61.72290	-465.07341	-328.96637	-722.13693	1
30026	H	73.68700	75.85480	61.99690	2620.26036	203.07263	1701.91824	1
30027	H	75.08200	74.73680	62.49790	-2851.09544	1136.09092	763.92785	1
30028	C	73.43400	73.79580	61.37990	-416.29149	381.79212	725.89496	1
30029	H	73.87200	73.05280	60.67990	-2498.73701	-1097.89566	1574.22312	1
30030	C	73.20600	72.96180	62.64590	509.07181	388.54635	-652.01916	1
30031	H	72.47500	72.15780	62.41390	-151.17279	1464.81775	-2795.06980	1
30032	H	72.89900	73.58880	63.51090	-234.34462	-1185.94391	2893.31351	1
30033	H	74.09900	72.35780	62.91390	1549.31401	1595.34742	-2232.08385	1
30034	C	72.04600	74.18280	60.80190	-289.91124	431.50176	758.14329	1
30035	H	71.38500	73.30880	60.62390	733.30032	-2790.51320	1203.31607	1
30036	H	71.56400	75.00680	61.36990	1611.36028	-1957.53265	-1837.87055	1
30037	H	72.15400	74.59180	59.77490	-2174.11647	-581.48986	-2216.54248	1
30038	C	75.85100	76.71480	60.91390	406.93213	-374.86015	-716.77074	1
30039	O	75.24100	77.76980	61.06290	-550.89367	161.80549	552.85568	1
30040	N	77.17700	76.61080	61.06990	420.20103	439.77911	-593.30061	1
30041	H	77.61500	75.74080	60.85690	3061.10143	-160.10851	625.01887	1
30042	C	78.06900	77.62580	61.56690	-399.63185	636.43980	-552.06244	1
30043	H	77.44900	78.34180	62.08490	1205.51732	2266.92002	1816.42519	1
30044	C	79.05700	77.17280	62.62790	-223.46438	-664.02958	563.97874	1
30045	H	79.78300	77.96780	62.90290	-2060.16441	803.38635	2243.79976	1
30046	O	79.81600	75.99880	62.30490	-551.78980	499.64314	-322.86248	1
30047	H	79.18000	75.28680	62.20490	1711.35581	-1693.71569	1991.42416	1
30048	C	78.13500	76.76780	63.83490	231.13246	-847.57813	167.42441	1
30049	H	77.36500	77.55080	64.00490	-1799.58688	-1420.07931	-2165.74323	1
30050	H	78.74600	76.71880	64.76190	-1231.20952	2039.55887	2064.73338	1
30051	H	77.51500	75.84680	63.79690	-480.28011	-679.61210	3023.97608	1
30052	C	78.80100	78.28280	60.43990	-680.64961	469.55628	-433.59445	1
30053	O	79.82000	78.91780	60.65690	-566.67439	569.88849	77.27419	1
30054	N	78.35900	78.17880	59.20190	-177.93915	-561.51985	587.18398	1
30055	H	77.57900	77.59780	58.98190	-383.56238	-1888.52383	-2488.41196	1
30056	C	78.86300	79.05080	58.16390	-30.03666	-434.94655	-804.26209	1
30057	H	79.93700	78.96980	58.24790	-2008.64668	-1597.47417	1815.69993	1
30058	C	78.55500	78.55580	56.73090	638.81518	-516.45001	-357.56385	1
30059	H	77.45400	78.54380	56.58590	-2232.66330	2241.28042	-172.55210	1

30060	C	79.23400	79.47680	55.69190	-176.93589	515.14449	733.76019	1
30061	H	79.23300	79.06580	54.66090	2860.85790	-1254.05216	52.09138	1
30062	H	78.67300	80.41380	55.48890	3115.50773	-42.34284	-294.94769	1
30063	H	80.26600	79.78080	55.97290	-383.35573	-1144.25102	-2913.79084	1
30064	C	79.06900	77.10780	56.54390	-412.07130	633.86047	-549.00554	1
30065	H	79.00500	76.45980	57.44390	-2516.86790	-1538.12978	1106.12574	1
30066	H	80.15200	77.14780	56.29690	682.63287	2275.05019	-2081.56448	1
30067	C	78.26600	76.33080	55.51690	-584.80899	-620.53972	-340.81147	1
30068	H	78.23500	76.94280	54.59090	-1820.11218	-2231.88142	-1280.42444	1
30069	H	77.16900	76.27180	55.68190	2399.97448	-1950.29159	428.35159	1
30070	H	78.74700	75.33680	55.39290	647.92010	-2135.92674	2188.88098	1
30071	C	78.55300	80.52180	58.35990	626.23156	-0.16840	-657.67627	1
30072	O	79.45400	81.34280	58.28290	414.97386	-378.57390	-544.94789	1
30073	N	77.30800	80.94280	58.79090	-716.70673	123.64681	446.96591	1
30074	C	76.06600	80.31780	58.47990	-473.52457	458.11001	-659.41161	1
30075	H	75.80500	79.49080	59.17390	1819.34360	2559.02579	227.94337	1
30076	H	76.09400	79.92480	57.44090	-2305.13421	1694.39037	1346.31879	1
30077	C	77.11200	82.34380	59.28390	671.47978	601.54467	117.05608	1
30078	H	77.25900	83.06080	58.48990	-2817.81509	-1118.18058	-879.01050	1
30079	C	75.62100	82.35380	59.68890	251.42593	823.55163	-333.20298	1
30080	H	75.54600	82.00980	60.74290	-1983.94338	2018.37929	-1420.76919	1
30081	H	75.08500	83.32580	59.65190	-1988.82522	261.12119	2428.67845	1
30082	C	75.00600	81.34580	58.64290	-744.27117	525.60171	-201.96549	1
30083	H	74.62200	81.75380	57.68290	12.16783	2692.38142	1644.06835	1
30084	H	74.09500	80.94680	59.13790	-1456.99917	-2472.36246	-1284.42710	1
30085	C	78.03700	82.78180	60.40490	-301.39839	-851.56357	-36.29490	1
30086	O	78.48700	83.90380	60.44290	58.72214	-674.51236	-391.81650	1
30087	N	78.30300	81.91980	61.40090	186.00309	755.44739	339.46141	1
30088	H	77.87300	81.02280	61.32790	-2912.58550	1103.17175	541.08261	1
30089	C	79.25100	82.16380	62.47790	-734.87077	429.89488	-376.95550	1
30090	H	78.89200	83.09180	62.89790	1616.86741	-2310.89359	-1369.63435	1
30091	C	79.28600	81.04580	63.50590	807.89779	355.39066	195.09301	1
30092	H	80.16800	81.03780	64.18090	-2682.63331	1126.10342	-1243.98824	1
30093	H	79.41000	80.13580	62.87990	-1633.26636	-1169.78156	2413.17665	1
30094	C	78.00000	80.97680	64.30490	471.09444	649.94014	-448.85138	1
30095	O	77.75200	81.96580	65.02190	-557.61244	576.76530	69.79401	1
30096	O	77.25500	79.98480	64.24790	460.28990	-359.93667	502.60882	1
30097	C	80.65900	82.48880	61.91190	-618.49939	-448.68931	490.46686	1
30098	O	81.35100	83.42380	62.34390	414.57460	-528.34168	376.44723	1
30099	N	81.09300	81.65880	60.95190	209.30851	240.52797	770.16629	1
30100	H	80.60900	80.81980	60.71590	864.57071	-192.40818	-3025.31509	1
30101	C	82.35100	81.84880	60.18090	-79.32094	-897.03487	32.81394	1
30102	H	83.14500	81.81080	60.91190	947.27305	-2222.35034	-2009.84774	1
30103	C	82.61200	80.57680	59.36790	641.66352	-399.76908	-494.00064	1
30104	H	81.68500	80.38480	58.78690	2122.79395	267.71193	-2305.83297	1
30105	H	82.65500	79.66680	60.00390	1796.85245	2269.99472	1218.30681	1
30106	C	83.86900	80.51280	58.43890	576.89851	-536.54043	-439.11338	1
30107	C	85.11900	81.10280	58.74990	444.03478	-624.97935	-480.41478	1
30108	H	85.29600	81.67880	59.64590	-1983.13677	-1693.35468	1751.76602	1
30109	C	86.16200	81.10780	57.83790	-592.73130	-695.87528	-23.11409	1
30110	H	87.06200	81.63480	58.11890	902.21451	2219.42874	-2058.18197	1
30111	C	85.98200	80.43580	56.65890	-899.71832	218.02858	74.46682	1
30112	H	86.69700	80.46980	55.84990	-1082.16911	-974.93980	-2806.94528	1
30113	C	83.79600	79.72480	57.31990	446.60675	632.95892	-492.99713	1
30114	H	82.86100	79.25980	57.04390	-904.85741	1712.85020	-2505.40639	1
30115	C	84.80600	79.76980	56.36290	514.89261	-477.19103	-571.50106	1
30116	H	84.81800	79.17080	55.46490	-2259.62899	-1129.43474	-1904.13324	1
30117	C	82.49700	83.11280	59.39990	-18.11284	-662.65810	-626.50793	1
30118	O	83.51000	83.80280	59.50090	276.07494	-596.36093	400.84923	1
30119	N	81.49500	83.40680	58.56490	-497.92656	-621.31895	-290.43427	1
30120	H	80.75700	82.74780	58.43890	-2108.01639	-1994.70424	1208.55370	1
30121	C	81.46900	84.64280	57.71890	437.45055	-772.65044	99.51707	1

30122	H	82.41100	84.77380	57.20590	-1832.39997	-1519.00794	-2073.91340	1
30123	C	80.38000	84.70980	56.67890	576.74069	-249.99754	-653.43866	1
30124	H	79.41800	84.79380	57.22890	-1948.12818	-1001.82929	-2275.04352	1
30125	C	80.47683	85.97837	55.70362	-703.79114	595.67061	-288.69444	1
30126	H	79.61928	86.04323	54.97975	2341.07209	1220.05751	438.43773	1
30127	H	81.42431	86.03348	55.13243	1883.75914	2133.50799	1233.36194	1
30128	H	80.39979	86.90340	56.34521	-2454.08342	-3456.59586	-333.74109	1
30129	C	80.27800	83.41680	55.77490	55.42290	-717.97129	530.54759	1
30130	H	80.08400	82.53880	56.42690	1865.57872	2015.29104	-1542.77076	1
30131	H	81.26700	83.29280	55.28390	570.51330	2105.07963	2262.85741	1
30132	C	79.15000	83.46480	54.79990	504.94686	-363.76020	-656.48909	1
30133	H	79.31000	82.70080	54.00990	-874.79052	1970.66570	2298.33230	1
30134	H	79.14200	84.43280	54.25390	1788.83255	-561.75902	-2521.87228	1
30135	H	78.13300	83.27280	55.20590	1482.78418	-2740.10251	-275.13322	1
30136	C	81.42059	85.89459	58.74064	-514.18691	-340.64829	-1074.78351	1
30137	O	82.07638	86.90052	58.47108	656.82591	29.13312	-475.42463	1
30138	N	80.54554	85.81155	59.73531	-465.34940	-23.37629	-521.34176	1
30139	H	79.86570	85.05386	59.77324	-1937.03742	353.32026	2080.41318	1
30140	C	80.19030	86.94752	60.49885	98.55395	-220.11172	-678.59585	1
30141	H	80.74984	87.81433	60.08673	1165.94902	899.73661	920.82934	1
30142	C	78.61023	87.06498	60.49199	-938.54261	-440.17168	377.79823	1
30143	H	78.12344	86.24121	60.93168	107.27140	-1028.99871	821.99070	1
30144	H	78.26642	87.94752	61.12483	-1464.89936	-436.47475	-564.69195	1
30145	C	77.80727	87.22341	59.14869	54.05274	-378.71793	-146.77966	1
30146	C	78.41250	88.21657	58.36071	244.18555	398.27660	694.37925	1
30147	H	79.21035	88.86033	58.74675	-868.62913	762.47366	-313.10527	1
30148	C	77.73214	88.53103	57.15959	-176.09438	327.24821	1013.11527	1
30149	H	78.20060	89.39229	56.61115	4253.39456	-572.30744	472.84910	1
30150	C	76.50690	87.87764	56.84739	438.61791	-120.01391	553.55460	1
30151	H	75.95184	87.98888	55.92824	-900.36536	3824.51079	562.72588	1
30152	C	76.65774	86.48660	58.78912	782.08020	251.24793	478.27003	1
30153	H	76.41370	85.55919	59.43838	-1351.53618	-242.74789	-834.04315	1
30154	C	75.94003	86.82724	57.58901	-375.07905	-249.94955	458.80266	1
30155	H	75.00959	86.28261	57.30608	713.46414	-564.17265	-1308.34626	1
30156	C	80.64013	86.85941	62.09582	53.00488	178.01059	-220.99039	1
30157	O	79.84784	87.01716	62.98349	-15.99988	-147.61668	437.75314	1
30158	N	81.97457	86.76707	62.13932	123.20123	-157.85537	437.06348	1
30159	H	82.51071	86.70754	61.26513	-569.95393	351.98862	282.58630	1
30160	C	82.55216	86.90633	63.43283	-153.64106	880.38772	-676.93311	1
30161	H	81.75070	87.27297	64.10051	-459.30868	1044.97309	537.86467	1
30162	C	83.24003	85.50266	63.78869	499.54079	-866.93705	637.94127	1
30163	H	84.03624	85.63599	64.49984	582.13883	952.25808	1643.75037	1
30164	H	83.68000	84.87680	62.92990	-2807.67331	-1162.79618	821.78714	1
30165	H	82.44800	84.78880	64.16490	731.47546	1469.88670	-2699.40099	1
30166	C	83.81528	87.86092	63.14953	92.54969	-541.73297	414.69824	1
30167	O	84.63158	87.73085	62.21433	-112.60947	-509.29203	-281.17496	1
30168	N	83.84015	88.72605	64.15243	382.98188	566.91091	171.32197	1
30169	H	83.12239	88.60129	64.84533	171.28083	2474.97533	-3821.88207	1
30170	C	84.36588	90.04642	63.96926	226.58211	-379.38364	-9.69986	1
30171	H	85.25602	90.01436	63.25130	2637.12229	2623.28535	-3101.64622	1
30172	C	83.37562	90.95392	63.12810	305.67440	255.98792	-1162.13303	1
30173	H	83.36985	90.48975	62.12758	2476.76574	-853.99312	-1172.46234	1
30174	H	83.84609	91.95297	63.08972	1028.14277	1025.10284	672.54916	1
30175	C	81.86411	90.80387	63.58933	-12.04988	-377.63287	-332.65587	1
30176	O	81.13556	89.83748	63.34793	-180.70843	-402.86238	1170.82642	1
30177	N	81.57755	91.88567	64.29951	-524.33051	-316.30682	118.12987	1
30178	H	82.26296	92.71168	64.56355	-744.98755	1188.22892	-298.73397	1
30179	H	80.64220	92.13391	64.72880	380.67419	2067.64519	-1755.15952	1
30180	C	84.74700	90.60508	65.42512	-745.39905	-79.19080	289.92033	1
30181	O	84.25178	90.15738	66.50859	268.80317	811.94653	115.04554	1
30182	N	85.41486	91.74982	65.35465	267.44027	510.79061	-208.80849	1
30183	H	85.69738	91.77410	64.33483	-702.70020	-421.06228	2537.69064	1

30184	C	85.30871	92.78819	66.42263	73.68057	778.58470	119.94354	1
30185	H	85.37999	92.21315	67.40094	2769.16653	-210.38552	-437.10021	1
30186	C	86.44274	93.74571	66.21085	157.55446	-597.64538	264.58455	1
30187	H	87.41526	93.20915	66.28526	-519.10966	3542.92382	1497.07954	1
30188	C	86.44136	94.41292	64.84726	-98.51070	-73.78093	733.97991	1
30189	H	85.60744	95.14338	64.66169	-437.05115	1477.86999	-293.60710	1
30190	H	86.29294	93.62609	64.04697	1620.67050	587.69437	-1015.17060	1
30191	H	87.40066	94.95318	64.57078	-42.62374	-620.49757	1731.93113	1
30192	C	86.54008	94.78485	67.29763	-612.23252	340.44081	1331.38905	1
30193	H	86.54234	94.46378	68.39056	-920.09496	1192.21540	677.94611	1
30194	H	87.38975	95.57425	67.15823	-54.86380	1893.86724	4529.80341	1
30195	H	85.61506	95.39914	67.28407	-797.26851	-390.35185	2726.61436	1
30196	C	83.81611	93.43934	66.30190	-55.52113	-477.01001	144.70479	1
30197	O	83.20934	93.82288	65.26507	-795.38846	355.51303	-42.97888	1
30198	N	83.38018	93.49465	67.52969	-1020.40667	36.30082	757.33321	1
30199	H	84.01571	93.06881	68.22832	3846.94032	-1094.37517	2021.92498	1
30200	C	82.73384	94.66642	68.07260	233.85361	-3.88793	166.38336	1
30201	H	82.43331	95.29535	67.19452	-1819.26227	-1182.01000	-1474.91639	1
30202	C	81.53968	94.24804	69.04532	-237.25321	920.55485	-138.31514	1
30203	H	81.71425	93.35476	69.67511	3011.82694	-4051.82870	357.30786	1
30204	H	80.73234	93.75845	68.38895	1409.32497	-674.48264	-1625.35075	1
30205	O	80.89262	95.34230	69.65549	830.34426	69.02248	85.83901	1
30206	H	81.59597	95.76503	70.17465	-1904.89237	883.03791	-2191.99193	1
30207	C	83.78379	95.24820	69.14104	-735.55082	183.59647	-98.73376	1
30208	O	84.53795	94.63500	69.86552	532.91260	725.99886	153.82513	1
30209	N	83.91692	96.47926	68.74047	-72.60095	37.99988	-767.98180	1
30210	H	83.19855	96.92874	68.13270	2230.34747	2258.05141	2541.15291	1
30211	C	84.57894	97.39950	69.62811	1171.56960	-691.18588	-148.18285	1
30212	H	85.54219	96.98443	70.00537	-31.49419	-2030.97488	1185.79145	1
30213	C	84.67177	98.89863	68.98977	242.77304	157.76868	-20.82341	1
30214	H	84.81390	99.70409	69.73309	-3160.94654	-2643.41459	-64.08104	1
30215	H	83.83683	99.24224	68.28179	-180.19457	791.93143	-747.39929	1
30216	C	85.97519	98.75210	68.17252	704.20667	207.28352	-551.56756	1
30217	H	86.45778	99.82745	68.03814	2124.12683	397.15477	-2281.46638	1
30218	H	86.75786	98.21867	68.72081	-1673.42691	1656.84148	2595.06140	1
30219	C	85.78243	98.01149	66.70373	453.67097	682.94736	62.68246	1
30220	O	84.66609	98.23935	66.08475	454.49637	-328.68308	-56.94637	1
30221	O	86.72586	97.46533	66.15970	-646.27954	303.29008	-573.46006	1
30222	C	83.45242	97.58823	70.78956	618.84715	115.61295	613.25040	1
30223	O	82.25436	97.57902	70.50249	-924.59786	769.13473	16.39390	1
30224	N	84.01831	97.70280	71.98147	420.76195	-276.25440	290.90358	1
30225	H	85.00721	97.55689	72.02532	1766.12698	804.01076	-4530.64389	1
30226	C	83.33862	97.09466	73.11195	212.67835	-378.02357	995.13434	1
30227	H	82.31343	97.27797	72.70933	-865.66433	2226.11845	2002.28887	1
30228	C	83.75520	95.58636	73.14053	-797.33519	-367.20507	215.68386	1
30229	H	83.18094	94.98421	73.86242	500.65973	4852.11033	-904.38909	1
30230	H	84.82778	95.51275	73.44238	-365.44102	-2141.88859	-837.29252	1
30231	H	83.67884	95.05215	72.14343	-2046.81911	-938.41403	-701.45519	1
30232	C	83.81285	97.94904	74.44285	-614.52294	-73.87793	-224.36432	1
30233	O	84.41239	97.39602	75.36448	-285.96958	-367.60405	-89.87654	1
30234	N	83.27223	99.18057	74.37931	690.59934	-834.21082	-540.89012	1
30235	H	83.00499	99.21480	73.35291	1129.05192	414.44320	245.97407	1
30236	C	84.05913	100.21763	74.97781	-50.04160	-271.59019	205.31356	1
30237	H	83.48217	101.09870	74.59632	-2119.36191	5.65664	2229.56297	1
30238	C	84.15852	100.19070	76.55476	-532.79041	576.66351	549.07713	1
30239	H	84.33829	99.10350	76.80884	-360.18677	1474.23949	-456.85509	1
30240	H	85.09392	100.69517	76.89064	1053.49071	1184.36146	3143.72736	1
30241	C	82.92786	100.67231	77.31255	-16.13978	345.80554	447.13643	1
30242	O	82.15203	101.54320	76.99357	-258.99089	394.45491	193.80587	1
30243	O	82.95473	100.13952	78.60342	328.44727	540.25844	1002.06257	1
30244	C	85.57080	100.33024	74.44560	569.97634	926.53021	-333.30281	1
30245	O	86.51886	100.53630	75.25072	-653.60451	-90.62342	1378.90835	1

30246	N	85.68786	100.08781	73.15053	-45.39022	1014.44972	312.61559	1
30247	H	84.72701	99.85496	72.78120	-3587.40958	-2711.78095	-360.12356	1
30248	C	86.67191	100.80185	72.40277	767.15485	-422.90994	783.58241	1
30249	H	86.26285	100.67756	71.36296	-1030.80786	328.24959	-2633.01068	1
30250	C	86.90259	102.29453	72.78168	-143.74359	359.72436	148.52605	1
30251	H	87.89580	102.57605	72.44234	-801.88309	310.85844	-474.09557	1
30252	H	86.78483	102.48961	73.87143	781.18796	210.88148	82.70113	1
30253	C	85.82146	103.28096	71.96966	461.06397	-197.32860	-662.36013	1
30254	O	85.70222	103.07465	70.77320	-373.40144	-557.92033	37.77295	1
30255	O	85.32838	104.23791	72.61684	805.03428	-150.12960	307.09052	1
30256	C	88.15405	100.04066	72.73931	-140.74083	671.05006	102.29808	1
30257	O	89.20692	100.59150	72.99647	1333.91816	-288.96087	46.61890	1
30258	N	87.93897	98.75828	72.63058	225.37036	-30.16267	655.24008	1
30259	H	86.97219	98.67962	72.20285	-2144.02957	-440.40252	-2705.69115	1
30260	C	88.74158	97.57314	72.72636	890.97265	-630.41464	-699.38849	1
30261	H	89.78902	97.84487	72.40154	-629.30657	-2540.67675	399.43886	1
30262	C	88.65641	97.11041	74.21844	128.90217	-64.84743	-758.59751	1
30263	H	88.89938	96.02268	74.27711	1090.32432	-86.28821	-1354.84444	1
30264	H	89.44539	97.63100	74.83392	1346.90677	1558.45444	1325.95381	1
30265	C	87.19510	97.35947	74.79905	-196.31169	342.61028	-118.70056	1
30266	H	86.56075	96.84413	74.07838	1228.18088	701.78807	545.36249	1
30267	H	86.94586	98.46429	74.76374	-453.94878	-151.28055	-1324.78526	1
30268	C	87.12015	96.87453	76.33875	-489.65916	-312.29805	-292.15086	1
30269	H	86.11652	97.18007	76.65892	-3303.34895	-2726.09163	-515.30427	1
30270	H	87.89205	97.41130	76.91733	1979.20104	-413.27556	-130.46082	1
30271	N	87.32566	95.50866	76.41517	648.22809	258.56909	-147.33141	1
30272	H	88.23770	95.13463	76.66303	-531.40252	625.74272	-1905.30322	1
30273	C	86.55688	94.55816	76.02567	0.00430	69.54331	-234.69833	1
30274	N	87.09592	93.24249	76.04834	159.39855	-390.34963	208.13587	1
30275	H	87.96099	93.10759	76.57664	-3411.59888	1900.56538	-2594.64166	1
30276	H	86.65120	92.32339	75.97418	1747.67366	-3981.68104	698.23661	1
30277	N	85.24256	94.83610	75.67520	424.09658	-151.95183	-214.51192	1
30278	H	84.77835	95.79118	75.63663	-3684.06714	-4201.72154	-603.73567	1
30279	H	84.55573	94.13283	75.54791	1188.89703	-3554.81605	-1097.04706	1
30280	C	87.71199	96.55865	71.90123	-585.42648	422.32098	18.79562	1
30281	O	86.50499	96.71662	71.67560	-1417.18628	972.36171	653.73584	1
30282	N	88.48151	95.56203	71.61639	-350.47356	694.10384	-251.97022	1
30283	H	89.47796	95.51563	71.96204	726.03082	1907.89984	-469.79565	1
30284	C	87.92032	94.50415	70.82242	51.19309	-24.48687	306.25645	1
30285	H	87.04836	94.83972	70.31714	47.27682	-2487.59697	-2400.15924	1
30286	C	89.22808	94.11408	69.92656	-367.16356	-465.21973	-221.41672	1
30287	H	90.08048	93.86368	70.56904	3448.06250	-2623.43417	1729.39774	1
30288	H	89.65433	95.01758	69.48200	-2056.54111	-76.57194	41.91124	1
30289	C	88.87129	93.01626	68.93510	387.95123	705.38382	380.97483	1
30290	C	87.94390	91.96725	69.30351	190.12946	-785.25578	255.58734	1
30291	H	87.57912	92.06220	70.38900	4229.32779	-2960.12350	-1519.40610	1
30292	C	87.64810	90.92654	68.46118	261.25880	-881.75671	-480.13420	1
30293	H	87.02570	90.15997	68.97138	-429.64587	-448.14870	-2243.21418	1
30294	C	88.12365	90.74754	67.11301	1345.69405	-813.54708	-102.99921	1
30295	O	87.70762	89.76756	66.30187	316.05343	16.82633	113.41299	1
30296	H	86.68460	89.42797	66.91378	-541.27315	-3430.31145	4298.94579	1
30297	C	89.58772	92.85216	67.69319	35.65618	32.99318	-367.43615	1
30298	H	90.24756	93.64329	67.37987	-625.00183	2516.53930	924.26750	1
30299	C	89.14911	91.79393	66.88299	-7.10129	138.33613	14.59496	1
30300	H	89.55955	91.45430	65.95013	-576.02908	971.58659	789.51241	1
30301	C	87.38905	93.43862	71.86420	-597.90210	-901.25416	-577.62565	1
30302	O	88.09719	92.92500	72.68931	-687.66136	-217.30835	-1185.24454	1
30303	N	86.01665	93.29518	71.67930	-313.79176	184.07639	752.21597	1
30304	H	85.54655	93.65986	70.85402	-2171.19258	-288.63814	289.16691	1
30305	C	85.50061	92.04344	72.13699	1385.87397	-15.38912	-500.21827	1
30306	H	86.30443	91.70902	72.90379	2021.33643	-630.51575	1138.67940	1
30307	C	84.14315	92.43371	72.84638	619.82400	15.56190	686.53669	1

30308	H	84.11633	93.46684	73.20113	-1549.93260	-223.88269	-1964.74517	1
30309	C	82.97489	92.54241	71.79812	574.72916	333.75339	-628.97379	1
30310	H	83.36377	93.04086	70.84586	1633.31257	-2125.86724	239.89891	1
30311	H	82.67746	91.51695	71.46413	4220.99352	885.50828	1083.36576	1
30312	H	82.07516	93.04283	72.14673	811.76503	-3483.40276	466.99273	1
30313	C	83.74383	91.48443	74.00573	298.16131	157.56659	-93.67994	1
30314	H	82.85979	91.88257	74.59995	-657.90864	3953.75975	-885.05250	1
30315	H	84.54520	91.60518	74.75670	1469.96151	2363.57298	996.32605	1
30316	C	83.42685	90.00848	73.60048	-294.80864	-822.94993	250.71187	1
30317	H	84.18288	89.65843	72.88530	4835.89470	-1960.02263	-2483.69559	1
30318	H	83.31628	89.33029	74.48299	1615.50503	6154.84860	-1447.43823	1
30319	H	82.51550	89.98856	72.93222	-2681.75316	619.45331	-1351.58345	1
30320	C	85.28900	91.05959	70.84734	196.25888	247.95397	527.39060	1
30321	O	84.87741	91.55543	69.81426	291.10696	-415.31239	-406.88262	1
30322	N	85.51885	89.76003	71.03358	-88.68282	-371.08810	683.38889	1
30323	H	85.85958	89.21469	71.84392	-933.97232	-598.61417	1913.06016	1
30324	C	84.97954	88.93327	69.93838	-443.60967	-143.67415	24.85504	1
30325	H	85.42860	89.35334	69.04459	-374.91694	-143.87599	-1666.60235	1
30326	C	85.51462	87.51042	70.25342	-131.16960	-752.65825	428.23582	1
30327	H	85.88655	87.47589	71.34312	952.19972	2510.96459	-1174.17059	1
30328	H	84.68721	86.78861	70.20322	-198.72154	1769.06977	-3881.59733	1
30329	S	86.85300	87.24335	69.03811	572.96822	-477.25246	248.95255	1
30330	C	83.34648	88.94516	69.99750	-69.29720	-54.13213	-444.09007	1
30331	O	82.73012	88.74771	71.01631	-362.86021	-303.11046	-465.08192	1
30332	N	82.87870	89.29972	68.80721	429.15052	1394.12498	-250.54940	1
30333	H	83.52911	89.37045	67.97613	-698.22156	-581.15427	86.74328	1
30334	C	81.46815	89.44363	68.50769	807.45754	1278.25277	-364.23095	1
30335	H	80.82447	89.16831	69.43425	3722.30954	-21.28077	530.04130	1
30336	C	81.50716	90.96035	68.20581	-251.94074	436.76373	578.40836	1
30337	H	82.33679	91.12875	67.39746	71.71854	-98.59837	2088.23342	1
30338	H	81.85701	91.48636	69.13797	-1399.09949	852.06812	528.67426	1
30339	C	80.16123	91.67290	67.56129	171.24363	341.17953	-530.17606	1
30340	O	79.27940	91.89452	68.36478	-268.12860	-339.30711	-4.72740	1
30341	O	80.10987	91.89093	66.31924	-73.21932	35.08541	-508.19800	1
30342	C	81.06442	88.76613	67.04841	-804.19678	309.63534	-558.41072	1
30343	O	81.83862	88.46353	66.19851	1385.30507	-203.94595	57.96185	1
30344	N	79.69121	88.75596	66.87189	-183.72066	-301.91170	-384.91634	1
30345	H	79.17570	89.00414	67.72680	2152.64265	356.47470	-4033.51455	1
30346	C	79.21442	88.76380	65.54315	-649.87953	392.03780	150.03627	1
30347	H	80.09346	88.79864	64.89808	-2071.55816	257.16324	10.65568	1
30348	C	78.40176	87.42217	65.25262	-731.60608	892.93887	-882.70538	1
30349	H	78.02309	87.43731	64.23204	1427.37221	1798.21918	-895.69218	1
30350	H	77.57605	87.40577	66.02977	-1826.93178	-484.30571	-554.01790	1
30351	C	79.12705	86.01602	65.29912	58.40184	14.68499	521.51957	1
30352	H	80.19170	86.24149	65.12218	450.70271	558.73194	270.40834	1
30353	H	78.81269	85.29824	64.40474	2237.81410	-1404.50400	-620.31268	1
30354	C	78.82711	85.46873	66.72363	-35.70388	392.67116	900.49952	1
30355	H	79.37436	85.95212	67.58108	823.79734	1406.56444	1033.04459	1
30356	H	77.86388	85.76031	67.01201	-1926.80480	-632.07130	-51.79034	1
30357	N	78.71300	83.93980	66.64390	131.07907	644.82924	531.94161	1
30358	H	78.51800	83.39480	65.82790	1536.82760	1724.27943	-2149.42011	1
30359	C	78.40500	83.36480	67.75690	-668.19313	389.35659	-513.16330	1
30360	N	78.10900	83.97080	68.86490	777.66031	319.07458	-66.34553	1
30361	H	78.26600	84.95480	68.95690	-1723.90401	1651.35989	-2074.25040	1
30362	H	77.74400	83.35480	69.56290	-1359.64793	1948.29748	-2088.08756	1
30363	N	78.05200	82.10080	67.70790	-573.85900	541.21727	-346.70435	1
30364	H	78.04200	81.66580	66.80690	-1277.87858	2596.79312	1260.20199	1
30365	H	77.44800	81.87880	68.47390	-1859.95249	1836.07853	-1782.46082	1
30366	C	78.12383	90.03695	65.47186	272.77306	132.64390	702.29637	1
30367	O	77.31964	90.30691	66.33009	371.38480	269.06276	-755.34579	1
30368	N	78.20061	90.29753	64.16525	-100.53996	212.53917	349.50678	1
30369	H	79.09886	89.92582	63.85709	-3424.85991	2010.05828	249.82724	1

30370	C	77.33951	91.07412	63.35627	483.70698	148.54106	690.89781	1
30371	H	76.41204	91.18682	63.90951	-184.70728	-1679.96693	962.85785	1
30372	C	78.00964	92.50005	63.22066	-768.23780	837.85982	52.50038	1
30373	H	78.64815	92.65774	64.08627	1757.06791	-537.45871	-323.09082	1
30374	H	78.57971	92.64758	62.28230	1464.31967	-2920.25581	2541.15739	1
30375	C	76.89889	93.59121	63.16773	354.09057	-39.22979	-1005.41057	1
30376	C	76.47129	94.25751	64.34687	-362.46203	35.91224	-311.28738	1
30377	H	76.67785	93.89107	65.41013	-198.78444	-1244.17353	1790.23957	1
30378	C	75.58355	95.34240	64.16722	-518.47051	476.58586	-135.40313	1
30379	H	75.10254	95.86461	65.07891	-269.26495	34.78924	1925.73448	1
30380	C	75.35916	95.93319	62.91270	49.82272	-62.85638	-578.57098	1
30381	H	74.84202	96.91163	62.76603	-2279.31115	-2419.52334	2615.73023	1
30382	C	76.68262	94.10087	61.85259	233.25997	-315.40626	-83.12488	1
30383	H	77.04205	93.56255	60.95090	-1040.57395	-1002.87310	247.62766	1
30384	C	75.90133	95.28087	61.81181	802.50113	197.31549	-203.05392	1
30385	H	75.71963	95.79958	60.85634	278.20930	-326.78012	1381.94065	1
30386	C	77.00179	90.51287	61.79475	-481.75213	71.49283	-647.99754	1
30387	O	77.82635	90.18738	60.95066	653.14193	173.55545	-188.57204	1
30388	N	75.71591	90.71395	61.56931	-40.31913	-194.94136	323.99754	1
30389	H	75.12050	91.10876	62.32082	3088.09160	-2763.26340	-2765.36512	1
30390	C	75.06846	89.91038	60.56128	-159.47435	-240.09769	642.31766	1
30391	H	75.93743	89.27622	60.19512	2331.41681	754.70932	-474.56491	1
30392	C	73.78303	89.26971	61.28025	-236.37034	208.42012	239.32390	1
30393	H	73.09797	88.72572	60.58923	-2195.92112	2250.61869	768.26510	1
30394	H	73.03254	89.98994	61.78674	411.18843	1632.25099	1369.45714	1
30395	C	74.40472	88.33972	62.34069	-48.81680	26.45901	1159.92790	1
30396	C	74.63225	86.94339	62.13089	-418.89623	-545.52092	-624.96104	1
30397	H	74.53894	86.56096	61.06375	87.97756	2746.44045	-245.57840	1
30398	C	74.99213	86.06903	63.13369	520.96507	-350.81085	1058.02947	1
30399	H	75.08561	85.04976	62.96150	-747.98739	-1288.90998	-215.78277	1
30400	C	75.17357	86.54658	64.46203	-216.28543	-166.10557	-170.62484	1
30401	O	75.59473	85.62333	65.46114	768.28100	-658.64502	-364.13818	1
30402	H	75.54600	84.77580	64.99090	2.73547	-1160.05418	2911.22341	1
30403	C	74.66310	88.80738	63.62669	-216.88524	519.20853	-625.06643	1
30404	H	74.53289	89.92178	63.79289	-452.41101	1757.61260	949.16367	1
30405	C	75.01948	87.93577	64.69080	300.54865	-54.78962	-10.58659	1
30406	H	75.22733	88.28940	65.78166	1244.65561	903.43238	3771.50992	1
30407	C	74.65188	90.99008	59.44877	-964.09938	184.67953	1301.47773	1
30408	O	74.96368	92.13373	59.61429	-12.85589	-408.16926	36.02575	1
30409	N	73.82118	90.43504	58.50346	758.67273	233.06147	-87.28040	1
30410	C	74.00465	89.02160	58.22035	-229.82152	-372.68909	-96.43630	1
30411	H	75.08465	88.79674	58.21650	-692.17292	-2431.64971	-4353.02671	1
30412	H	73.47133	88.45851	59.03139	420.36888	1695.80998	2627.08065	1
30413	C	73.23181	91.18155	57.44180	-1290.78319	-246.97199	912.31853	1
30414	H	73.90159	92.05037	57.22721	1969.62882	-1577.40778	-797.27482	1
30415	C	73.06595	90.18006	56.21347	315.97490	-8.53362	393.81665	1
30416	H	72.10498	90.24979	55.75401	-2044.66241	205.63720	1648.60875	1
30417	H	73.75246	90.30007	55.42363	250.15247	194.73430	224.39988	1
30418	C	73.27550	88.77527	56.81784	-151.13798	-77.23034	-569.67884	1
30419	H	72.31310	88.21688	56.86442	1801.97900	337.64873	-842.37538	1
30420	H	73.93667	88.21547	56.10126	1576.13120	1178.79669	26.90772	1
30421	C	71.74711	91.82622	57.80127	-781.22953	-113.72034	189.02232	1
30422	O	71.27528	92.56576	56.93927	-204.49936	126.87129	-207.82032	1
30423	N	71.40213	91.58189	59.02957	-203.93111	-365.06867	-401.16394	1
30424	H	72.12059	91.04402	59.46834	977.70379	-520.79416	-1436.23121	1
30425	C	70.16603	92.14951	59.60142	627.60338	285.70790	532.67175	1
30426	H	70.44051	93.23296	59.62433	1369.23280	1166.02451	-1707.61792	1
30427	C	68.98160	91.97786	58.61304	695.99051	-335.41280	645.11988	1
30428	H	69.33708	92.47232	57.64583	1325.41429	2183.83391	-363.94136	1
30429	H	68.85783	90.91150	58.32931	1682.26146	-18.70764	-1246.45737	1
30430	C	67.58972	92.68643	58.88147	-807.46977	831.64266	134.47166	1
30431	O	67.32170	93.42211	59.79619	-663.10368	-266.85087	804.86681	1

30432	N	66.83233	92.50310	57.76861	-96.17016	-244.00984	-483.04887	1
30433	H	67.04389	91.67826	57.16950	1741.55410	-494.57070	-887.45851	1
30434	H	65.77522	92.74767	57.90727	-1397.03093	1694.03984	-1114.93438	1
30435	C	70.05996	91.47641	61.00443	966.44926	579.21657	1329.40184	1
30436	O	70.67037	90.48523	61.41794	258.26805	-317.25049	-85.89824	1
30437	N	69.03723	92.08171	61.64042	169.97077	-62.59030	-325.23486	1
30438	H	68.56411	92.90662	61.23453	-824.66778	-1221.07696	-294.59481	1
30439	C	68.63646	91.42352	62.86453	-40.46531	315.11968	-82.68223	1
30440	H	69.49448	90.65446	63.09095	281.87536	642.48100	-3034.20804	1
30441	C	68.60309	92.53991	63.94911	305.60554	120.88744	-223.26283	1
30442	H	68.63675	93.55383	63.50554	2002.67384	-1271.80389	653.23948	1
30443	H	67.75238	92.53684	64.65716	681.54013	315.84832	2600.06363	1
30444	C	70.06352	92.37356	64.77502	1009.79617	-221.89824	680.48286	1
30445	O	71.07112	92.86482	64.33582	170.65007	-243.73971	-23.49670	1
30446	O	69.99399	91.75195	65.84337	-274.85295	414.78624	63.42477	1
30447	C	67.11675	90.81542	62.75024	441.98042	200.56510	-585.81022	1
30448	O	66.61012	90.34171	63.73683	-117.43608	296.76653	160.50648	1
30449	N	66.58777	90.95971	61.49847	-365.78962	-376.12804	-53.68624	1
30450	H	67.15645	91.42363	60.82986	379.04734	359.06706	1024.26128	1
30451	C	65.74809	89.91972	60.99323	-950.10465	-297.08321	16.24047	1
30452	H	65.25965	89.50892	61.86367	2479.36898	3452.98167	4.05636	1
30453	C	64.80677	90.59415	59.85227	274.69367	370.49204	89.32658	1
30454	H	64.68581	91.68111	60.05770	30.91077	-2668.33473	2222.70823	1
30455	H	65.36930	90.50862	58.91181	-3048.84217	-2001.13742	-85.35277	1
30456	C	63.45124	89.96298	59.74678	-332.39468	348.89767	-983.81391	1
30457	H	63.66691	88.85460	59.57369	260.01759	-1571.57224	-674.26283	1
30458	C	62.65053	90.01329	61.03052	145.23052	-348.40296	-276.89220	1
30459	H	62.51525	91.04038	61.44631	-2241.50128	-2009.10954	-1444.02548	1
30460	H	63.16679	89.42797	61.84739	2463.44628	-230.03327	2719.85813	1
30461	H	61.57762	89.68662	60.87481	2227.18983	2058.26152	3273.15366	1
30462	C	62.59632	90.40787	58.56386	533.86995	-243.18750	876.45367	1
30463	H	62.18518	89.61298	57.94186	-2108.70762	-1537.55910	263.78508	1
30464	H	61.71740	90.88402	59.08810	-2655.09516	-1468.70712	75.39894	1
30465	H	63.07579	91.13817	57.90218	-752.03917	2006.38447	137.82888	1
30466	C	66.68801	88.75347	60.38391	280.46525	-565.75100	861.43566	1
30467	O	66.08139	87.75863	60.00888	-57.20047	218.66044	-616.79259	1
30468	N	67.98889	88.96805	60.26023	-990.69257	-82.84231	135.69706	1
30469	H	68.46692	89.85402	60.45107	1624.25726	-1730.80904	-445.42970	1
30470	C	68.76061	87.92337	59.76644	299.00506	572.40290	-79.34437	1
30471	H	67.96269	87.27673	59.23695	2870.05027	-2253.87842	-1162.42543	1
30472	C	69.95356	88.48398	58.83458	-31.92092	281.23575	-597.81469	1
30473	H	70.91582	88.03180	59.16470	-1654.88344	-1263.55298	-2932.22082	1
30474	H	70.04747	89.62694	58.94755	-25.92705	907.57112	1156.42810	1
30475	C	69.78364	88.15097	57.36455	691.56615	-216.54935	735.53168	1
30476	C	69.53603	89.00937	56.25942	-352.22028	-980.00286	110.79769	1
30477	H	69.47018	90.12579	56.14522	2825.29431	1774.15770	996.12649	1
30478	N	69.38015	88.31169	55.13687	-463.27348	-521.70571	232.20814	1
30479	H	69.19937	88.85800	54.24073	-3796.58039	-1447.13146	530.26322	1
30480	C	69.46853	86.96353	55.39930	21.38250	-825.39006	-387.05234	1
30481	C	69.72681	86.79486	56.85377	-294.09557	275.52774	258.99487	1
30482	C	69.85326	85.50164	57.43480	1104.16052	-100.55312	175.93375	1
30483	H	69.89024	85.35587	58.55405	-2054.86933	594.32101	-1083.33156	1
30484	C	69.68000	84.43180	56.55090	-264.05665	536.71245	702.45555	1
30485	H	69.73600	83.43380	56.95890	1494.77344	480.45994	2717.07189	1
30486	C	69.38005	85.81075	54.52786	-222.40167	-957.56036	-492.37930	1
30487	H	69.30457	85.93970	53.42264	1720.27688	-450.40851	-1678.53370	1
30488	C	69.46400	84.55980	55.13790	-741.78443	-500.22876	189.05846	1
30489	H	69.43900	83.61780	54.60990	-1253.76470	2898.34254	248.53410	1
30490	C	69.45913	87.20572	61.01354	-207.50965	-1380.29753	-640.55232	1
30491	O	69.51017	85.97497	60.86759	284.30404	-169.11655	769.75645	1
30492	N	69.98828	87.93254	62.00923	-769.79026	-457.93906	421.55579	1
30493	H	69.84598	88.96037	62.03931	-88.56550	112.49659	-4935.56296	1

30494	C	70.40994	87.22823	63.12434	-664.03232	1028.00984	-578.34455	1
30495	H	70.77781	86.28808	62.68505	1034.43856	4242.85049	-206.07179	1
30496	C	71.66926	87.74951	63.91508	-513.63420	629.27629	-120.08702	1
30497	H	72.48777	87.84736	63.14651	-1499.20868	1594.06362	608.66501	1
30498	C	71.32951	89.17537	64.47648	31.20621	-179.35170	171.83421	1
30499	H	72.25492	89.59833	65.04068	1198.75426	1381.53612	-1396.63097	1
30500	H	70.43643	89.03872	65.17818	2399.13818	1922.19012	-499.94306	1
30501	H	70.96241	89.92302	63.72358	-3978.93620	-2503.37028	1805.80199	1
30502	C	72.13145	86.69806	64.97343	-388.23797	-504.16893	-392.25451	1
30503	H	71.72374	85.63016	64.90487	-2097.74344	-2374.17237	2874.88869	1
30504	H	73.24130	86.70909	64.94301	-3463.18789	-1076.57518	1056.04299	1
30505	H	71.89099	86.93062	66.04394	-387.65126	2664.03812	1618.31372	1
30506	C	69.19896	87.18595	64.30541	-143.60581	-554.88626	-423.89308	1
30507	O	69.55304	86.93165	65.43642	399.03647	292.55939	661.09378	1
30508	N	68.00591	87.49230	63.85625	-364.89084	620.22533	-131.25815	1
30509	H	67.94591	87.71204	62.87635	99.23339	-288.77039	-1599.43783	1
30510	C	66.88932	86.74278	64.37415	312.12900	130.96618	40.01779	1
30511	H	67.27332	86.71844	65.41006	1500.12764	-3561.51007	-13.39094	1
30512	C	65.53846	87.54356	64.19256	351.10597	-31.59207	1076.80707	1
30513	H	65.76531	88.64600	64.06616	-974.57516	-2774.95832	533.23266	1
30514	C	64.84327	87.10543	62.83495	-936.83633	-934.69760	162.06682	1
30515	H	65.44813	87.37725	61.92677	-1251.61681	-654.28164	4447.53157	1
30516	H	64.66107	86.04110	62.78069	2372.10597	1111.52223	-510.09842	1
30517	H	63.82928	87.56324	62.76920	-1029.54496	523.96428	-397.61235	1
30518	C	64.78405	87.59294	65.57530	154.10226	-260.43810	874.77060	1
30519	H	63.71226	87.78991	65.40316	519.33962	980.79216	-680.93995	1
30520	H	64.93701	86.65745	66.11423	1043.75644	-967.74860	274.42558	1
30521	H	65.23802	88.37895	66.27067	-2831.42741	468.78313	-624.20898	1
30522	C	66.79822	85.33010	63.56005	302.30528	1527.35249	580.84159	1
30523	O	66.19800	84.42780	64.14390	-492.44435	610.36568	197.27762	1
30524	N	67.13750	85.40193	62.27642	915.47631	65.14025	-394.28044	1
30525	H	67.79969	86.06775	61.95761	-1479.40913	-387.42340	-1196.87262	1
30526	C	67.17300	83.92780	61.67790	673.99000	339.07482	505.58797	1
30527	H	66.24200	83.39480	61.79890	1637.78249	2274.46796	1442.15621	1
30528	C	67.57000	83.97580	60.15290	592.42603	-395.00489	540.99551	1
30529	H	68.48300	84.59580	60.02690	2092.10852	2035.03564	-1184.53209	1
30530	C	67.61400	82.57980	59.52390	-557.58336	470.70911	571.97627	1
30531	H	66.79600	81.88480	59.80990	1848.57723	-1426.41165	-2086.37818	1
30532	H	68.52000	82.02080	59.84090	2850.80815	1317.67516	-33.88827	1
30533	H	67.66500	82.68580	58.41990	-2626.29637	-1720.97531	-235.63591	1
30534	C	66.50700	84.79580	59.46790	821.61765	367.06690	-116.41441	1
30535	H	66.63300	84.77480	58.36390	-2520.29162	-454.24019	-1843.43086	1
30536	H	66.38145	85.86428	59.69765	193.22165	1987.29409	-902.99702	1
30537	H	65.54000	84.29880	59.69790	-1710.91123	-2176.94706	-1483.12435	1
30538	C	68.20200	83.10680	62.39890	538.94756	606.28795	-428.41971	1
30539	O	68.02100	81.91380	62.76490	253.25544	-628.46677	-372.54079	1
30540	N	69.35700	83.66280	62.70190	600.38797	-436.45326	-369.07951	1
30541	H	69.64500	84.55180	62.35490	-1794.86027	-999.87435	-2387.73904	1
30542	C	70.38900	83.01780	63.55090	-427.83772	410.03103	704.43456	1
30543	H	70.48900	81.98180	63.26390	-1083.02382	2683.35732	-1283.15729	1
30544	C	71.76000	83.63580	63.31290	-495.20999	722.96993	304.98175	1
30545	H	72.58800	82.97480	63.64590	-2649.42222	1686.72747	370.57397	1
30546	H	71.82400	84.63980	63.78390	-808.93805	3056.01955	116.86859	1
30547	C	72.03300	83.72280	61.79390	-227.00176	-506.56625	710.59408	1
30548	C	71.81600	82.59080	60.95990	267.14002	-702.32467	-492.91195	1
30549	H	71.47000	81.69580	61.45590	-2329.23019	1925.53899	935.42704	1
30550	C	72.08100	82.67680	59.54890	593.03564	114.63114	668.05646	1
30551	H	71.79200	81.91980	58.83390	-2143.26637	1683.43720	-1612.91881	1
30552	C	72.48800	83.89180	59.02390	182.47455	869.41193	-257.89654	1
30553	H	72.66000	83.92580	57.95890	-2552.22180	1511.09657	1098.31838	1
30554	C	72.42300	84.92880	61.19290	-61.90843	141.92661	-907.19770	1
30555	H	72.46324	85.82922	61.91847	-109.70341	1659.83123	-2818.08329	1

30556	C	72.70509	85.04124	59.80621	216.41624	-340.22511	-11.64643	1
30557	H	73.09769	85.97979	59.30009	2029.06782	-1269.48167	-2036.14259	1
30558	C	70.05300	82.90880	64.99590	-713.56785	583.89438	114.10551	1
30559	O	70.29400	81.84380	65.59190	572.26267	-241.81029	-471.38361	1
30560	N	69.42700	83.89580	65.60790	-679.10760	-211.87727	-463.74875	1
30561	H	69.17200	84.72080	65.10890	-2607.33203	1232.31820	1288.52598	1
30562	C	68.97800	83.85380	67.00790	-792.04331	-163.04844	426.54666	1
30563	H	69.89000	83.70380	67.56490	338.32501	-2261.60473	-2146.47669	1
30564	C	68.27752	85.22580	67.46525	-223.14274	-867.54878	-599.46261	1
30565	H	67.36151	85.33434	66.88752	-189.76783	-724.76364	-394.71734	1
30566	H	68.93627	86.05814	67.07592	-481.10032	-1101.99763	2200.70138	1
30567	C	67.92033	85.33979	68.96555	-506.89171	-428.81704	-485.48277	1
30568	H	67.37700	84.47980	69.36990	-258.18711	472.42267	-3105.09644	1
30569	H	67.36839	86.29201	69.16471	-1030.08063	-936.13509	-816.60280	1
30570	C	69.47388	85.51463	69.54677	428.78155	-112.13439	657.74661	1
30571	O	69.92846	86.63348	69.49432	-435.57565	-154.34032	87.65603	1
30572	N	70.01700	84.39780	70.10590	424.94057	-458.23436	-553.69339	1
30573	H	69.81800	83.47480	69.77790	1624.93034	1478.09238	-2262.02886	1
30574	H	70.95200	84.61280	70.38790	-1623.66137	-2619.50514	575.53971	1
30575	C	68.01400	82.64180	67.17590	-690.56906	-58.37452	-603.33232	1
30576	O	68.15500	81.79780	68.04290	495.25050	307.59384	531.39090	1
30577	N	67.09000	82.50080	66.23490	-551.26637	117.07815	-641.64494	1
30578	H	67.03700	83.21580	65.54290	-1836.68293	1544.80651	2053.67871	1
30579	C	66.19800	81.42780	66.04390	-659.05272	648.76514	106.35915	1
30580	H	65.61500	81.36480	66.95090	-759.07284	3009.27619	621.22164	1
30581	C	65.20800	81.57280	64.87290	365.77335	-407.87410	-713.95590	1
30582	H	64.70000	82.55680	64.95890	702.59464	-2260.52341	-2049.30353	1
30583	H	65.78400	81.60080	63.92390	-2792.50528	1471.96502	-220.39016	1
30584	C	64.14300	80.54880	64.85190	186.72927	-860.20148	141.88081	1
30585	C	64.10100	79.51580	63.85590	-301.99217	-524.21995	672.59496	1
30586	H	64.80100	79.56380	63.03490	2735.01437	349.88863	1495.61877	1
30587	C	63.15900	78.47080	63.93090	604.37807	340.71240	589.78955	1
30588	H	63.17600	77.65880	63.21990	2072.62860	1612.47560	-1734.14706	1
30589	C	62.29400	78.35380	65.04990	322.46218	-787.22155	264.21671	1
30590	H	61.65200	77.48780	65.10490	-1207.32924	-2688.13750	1068.08265	1
30591	C	63.23200	80.41480	65.92290	644.99046	-188.81829	599.40506	1
30592	H	63.26300	81.05080	66.79490	-1817.03816	957.23624	2398.31328	1
30593	C	62.34100	79.34080	66.02690	-648.59883	647.33273	-172.27072	1
30594	H	61.57100	79.40480	66.78190	-2438.29176	840.29230	1825.86096	1
30595	C	66.93500	80.04880	65.78090	184.49588	-775.16845	-408.69721	1
30596	O	66.63200	79.06580	66.49690	41.75594	697.74998	-399.59236	1
30597	N	67.94200	79.96780	64.95690	-158.51082	-808.17185	97.55133	1
30598	H	68.28900	80.79880	64.52890	630.70526	-2932.43359	884.70279	1
30599	C	68.76200	78.73780	64.76490	-295.35007	429.86184	758.38786	1
30600	H	68.18600	77.88280	64.44390	880.81267	-314.48301	-3001.48202	1
30601	C	69.92700	79.06480	63.73590	-32.32694	752.99786	-540.99053	1
30602	H	70.79800	79.64880	64.10390	708.34100	-270.41057	-3053.89730	1
30603	H	69.47600	79.59580	62.87090	-1779.00708	2493.88179	796.48507	1
30604	C	70.63800	77.74080	63.25190	-581.00318	-679.78086	-162.66025	1
30605	H	69.81100	77.09780	62.88090	1455.98444	2656.25683	-881.02809	1
30606	H	71.15600	77.18480	64.06190	1317.54525	2338.90148	1647.58224	1
30607	C	71.61500	77.98280	62.06390	-187.16058	691.62235	-592.14249	1
30608	O	71.30400	77.62580	60.88590	238.42231	763.76149	-8.15666	1
30609	N	72.76000	78.65180	62.30290	-770.15590	263.30576	274.02545	1
30610	H	73.02500	78.74080	63.26290	-88.78522	1777.25102	2598.96441	1
30611	H	73.53400	78.74680	61.67590	-1143.70746	2038.50799	-2134.02893	1
30612	C	69.42700	78.31480	66.03490	-562.37980	-295.34901	652.19828	1
30613	O	69.49300	77.10380	66.30090	595.95210	169.03563	477.14480	1
30614	N	69.91900	79.24580	66.90290	434.17175	-368.95251	-609.91323	1
30615	H	69.86900	80.20080	66.61990	2585.58646	51.91199	-1781.75251	1
30616	C	70.55000	78.86580	68.12590	-793.63088	-36.76784	457.83326	1
30617	H	71.32000	78.13480	67.92590	-472.05197	-2683.71299	1543.71471	1

30618	C	71.25000	80.09480	68.80590	188.58765	905.68009	9.41202	1
30619	H	71.58700	79.73080	69.79990	2738.28833	318.92789	-1509.80319	1
30620	H	70.61000	80.97980	69.01290	-3105.66214	-531.12796	-67.01369	1
30621	N	73.40700	81.20880	68.59690	-217.30226	636.79724	524.57484	1
30622	H	73.43300	81.28880	69.59390	-2048.22215	1025.92511	2164.12062	1
30623	C	72.35200	80.62980	68.01290	-256.97260	579.28512	-677.68715	1
30624	C	74.26900	81.55580	67.58590	-164.07542	-884.16347	-11.43727	1
30625	H	75.19500	82.08080	67.81790	965.22958	-206.48339	2976.05171	1
30626	N	73.76200	81.31280	66.40590	153.79916	-137.54876	807.53836	1
30627	C	72.56300	80.67780	66.66290	675.08876	315.52198	-527.56345	1
30628	H	72.02400	80.25780	65.82290	1188.92313	-2011.06934	-2092.00092	1
30629	C	69.64000	78.25780	69.17190	-756.21148	371.74839	379.10027	1
30630	O	70.02400	77.39280	69.98090	-543.11126	-563.69417	42.44631	1
30631	N	68.39300	78.68480	69.17490	36.61568	-826.28463	3.22973	1
30632	H	68.03400	79.38880	68.56790	-2092.56994	1374.71599	-1929.80324	1
30633	C	67.34400	78.10680	69.99190	-494.96092	376.12794	680.13333	1
30634	H	67.88300	77.80780	70.87890	1815.54409	-2231.72876	-1234.33586	1
30635	C	66.26800	79.14380	70.38190	346.51131	-737.53416	-370.23094	1
30636	H	65.65100	79.44880	69.50990	-1693.46606	2226.10685	1475.78441	1
30637	C	65.27500	78.49980	71.45990	810.72844	387.76770	157.73250	1
30638	H	65.85400	78.09680	72.31790	-711.63206	2376.11147	1957.89064	1
30639	H	64.71300	77.63880	71.03790	-1930.46762	1078.39568	-2254.25834	1
30640	H	64.49100	79.19980	71.82090	959.14126	2029.79364	2217.17585	1
30641	C	66.88300	80.46080	70.88990	571.44088	-621.48315	296.07201	1
30642	H	67.63100	80.93980	70.22190	1954.01545	-570.00332	-2391.51651	1
30643	H	67.49200	80.42380	71.81890	-2317.83917	1830.33541	1123.19926	1
30644	C	65.83800	81.51180	71.27090	-835.56219	-327.31760	-159.00859	1
30645	H	65.02200	81.53180	70.51890	1139.75108	807.56767	-2822.19098	1
30646	H	65.46700	81.24480	72.28390	424.04720	-2147.75968	-2242.56322	1
30647	H	66.38100	82.47880	71.20490	-2337.24520	-1855.13292	-979.98171	1
30648	C	66.76900	76.84280	69.45490	-349.61673	627.61306	-588.00599	1
30649	O	66.63400	75.81380	70.12590	92.49403	-605.50489	472.59048	1
30650	N	66.31500	76.98580	68.18590	148.78392	845.99184	30.68418	1
30651	H	66.41500	77.87280	67.74190	-2626.69389	-307.79790	-1718.26782	1
30652	C	65.74200	75.94280	67.37790	140.44380	-204.86423	-872.61889	1
30653	H	64.79300	75.72480	67.84490	321.78134	2463.08027	1951.04066	1
30654	C	65.55500	76.47180	65.99690	504.61687	762.56996	99.61377	1
30655	H	65.01800	77.43680	65.87590	-2320.89090	-1631.67257	1356.73428	1
30656	H	66.57200	76.68280	65.60290	-2390.90100	1342.72615	1573.77022	1
30657	C	64.89500	75.49180	64.95890	686.10479	-69.09125	577.99709	1
30658	H	65.50600	74.59380	64.72490	1863.50208	-2481.31601	357.47443	1
30659	H	64.58300	76.09980	64.08290	-1226.85721	2916.94721	153.26655	1
30660	S	63.30800	74.83580	65.62490	403.46294	-298.59669	192.95926	1
30661	C	62.41500	74.52080	64.05090	-737.05317	553.64367	152.25393	1
30662	H	61.57500	73.84080	64.30990	1880.39484	-1380.23631	-2084.42317	1
30663	H	63.09600	74.03980	63.31690	1004.83392	2227.15568	1995.95125	1
30664	H	62.01300	75.46580	63.62590	-1996.07904	1169.65526	2156.40707	1
30665	C	66.62700	74.71180	67.33690	562.75922	-534.85942	-445.30181	1
30666	O	66.22400	73.62780	67.63590	476.97064	-590.57880	119.50248	1
30667	N	67.94400	74.80680	67.04190	400.98860	234.52860	700.51255	1
30668	H	68.38100	75.69680	66.93390	-1578.30725	1051.19360	2521.33784	1
30669	C	68.78100	73.65580	66.86890	-609.26956	99.55536	680.79836	1
30670	H	68.16600	72.78480	66.69290	1484.26199	742.94449	2666.93534	1
30671	C	69.72500	73.87980	65.70990	-188.72651	-805.18569	-358.95445	1
30672	H	70.51200	74.64080	65.89490	2158.68153	2271.73856	-312.42347	1
30673	C	70.49500	72.60180	65.37190	364.67678	67.95846	-832.65516	1
30674	H	71.16400	72.77680	64.50290	-1844.76242	-1911.19832	1678.54785	1
30675	H	71.16100	72.19280	66.16290	-1708.11421	-1020.56916	-2444.99682	1
30676	H	69.76400	71.82480	65.06090	1325.66898	2685.67917	-992.52900	1
30677	C	69.01400	74.34080	64.41390	-827.78357	-193.36743	-356.90262	1
30678	H	68.75000	75.40280	64.60590	-2520.34952	1891.99469	305.78678	1
30679	H	69.68600	74.31480	63.52990	-1959.81687	-2273.90474	-935.95316	1

30680	H	68.06000	73.80680	64.21390	2313.66276	2133.10329	36.97650	1
30681	C	69.60800	73.28180	68.10590	720.78022	-341.72329	404.19885	1
30682	O	69.97600	72.13480	68.30190	-10.74072	-534.76989	-570.27685	1
30683	N	69.88600	74.25980	68.99390	352.25858	-715.55768	209.28108	1
30684	H	69.62600	75.21180	68.84890	1744.85302	-2592.31232	-117.15991	1
30685	C	70.53000	73.95480	70.25190	887.63030	-87.28784	-127.03251	1
30686	H	70.92300	74.92080	70.53490	-46.19118	-2554.99814	-1818.47011	1
30687	H	71.34000	73.25280	70.12490	2696.70304	1517.45125	554.71855	1
30688	C	69.62700	73.38380	71.24690	-464.74455	579.56534	549.80490	1
30689	O	70.00600	72.62580	72.09890	-195.76408	-672.32869	335.02515	1
30690	N	68.35400	73.82580	71.22490	301.63168	621.04630	497.27166	1
30691	H	67.99000	74.44980	70.53890	1516.39301	646.90223	-2681.12018	1
30692	C	67.42000	73.44580	72.28490	479.96277	-645.88991	-393.90197	1
30693	H	67.91200	72.76780	72.96590	-211.46650	-159.78558	-3137.65442	1
30694	C	66.91300	74.68680	73.11490	276.40498	654.69946	584.34543	1
30695	H	66.12200	75.16780	72.50090	628.05619	1558.92830	-2669.60959	1
30696	H	67.73000	75.39380	73.37290	-1160.30113	-992.89992	-2750.46508	1
30697	C	66.30000	74.35180	74.45690	522.22120	615.82667	-441.26894	1
30698	H	65.60900	73.48980	74.34190	-1412.05910	1911.22258	2081.76912	1
30699	C	67.30900	73.99080	75.58390	-363.00005	208.76840	-819.62331	1
30700	H	67.94500	74.88180	75.77790	-2892.47435	-556.10341	1110.01852	1
30701	H	67.87700	73.11080	75.21290	1547.59030	1923.98497	1957.43618	1
30702	H	66.84500	73.70680	76.55190	1694.31130	-1740.87626	1976.81944	1
30703	C	65.46100	75.57580	74.92890	-563.17971	-691.55791	134.23530	1
30704	H	66.10500	76.45080	75.16190	2758.77214	979.51463	1151.37945	1
30705	H	64.93300	75.42080	75.89390	-653.41384	-1885.19217	-2421.12644	1
30706	H	64.70300	75.83080	74.15790	-733.04858	980.86238	-2906.57753	1
30707	C	66.18200	72.68480	71.76890	-561.13542	162.73244	-713.30887	1
30708	O	65.92800	71.57280	72.17990	650.91178	-70.30873	421.83483	1
30709	N	65.43300	73.25880	70.81490	340.88281	-77.96707	763.19628	1
30710	H	65.71600	74.14280	70.44990	-1165.76940	2436.97797	1644.45587	1
30711	C	64.18200	72.72380	70.30190	-377.62431	-571.74461	589.79375	1
30712	H	63.58800	72.69080	71.20390	-2355.01336	1362.79820	-1610.09640	1
30713	C	63.33000	73.64380	69.47090	-892.16986	-129.48362	-180.30267	1
30714	H	63.72500	73.82480	68.44790	-1274.52996	-2844.61613	-323.69594	1
30715	C	61.92300	73.14780	69.18390	-174.08252	908.75434	-116.20613	1
30716	H	61.36800	72.94880	70.12590	1858.21621	2292.55596	1114.41975	1
30717	H	61.30500	73.85280	68.58890	-2074.12018	1118.16088	-2104.72100	1
30718	H	61.96700	72.21880	68.57590	2151.61877	-1212.49705	-1922.69999	1
30719	C	63.22400	75.10980	70.05690	-720.61195	-183.13061	534.34469	1
30720	H	62.72800	74.93580	71.03590	-1732.01498	-2201.79664	-1413.20543	1
30721	H	64.20300	75.58080	70.29190	65.10655	-2973.37469	-971.25621	1
30722	C	62.38800	76.05980	69.16990	-911.86758	-70.70296	-98.76861	1
30723	H	62.69600	75.86280	68.12090	-2205.69281	-1300.68114	-1826.67637	1
30724	H	62.61200	77.12580	69.38790	-2968.23410	962.55096	503.60411	1
30725	H	61.29600	75.86780	69.23290	605.62058	248.14055	-3075.39437	1
30726	C	64.17900	71.32780	69.69790	604.27505	-482.29497	448.43263	1
30727	O	63.61300	70.39280	70.22690	661.33949	429.07881	-48.76916	1
30728	N	64.84000	71.21580	68.46890	18.58213	-672.17557	-486.00985	1
30729	H	65.25800	71.95580	67.94690	2822.01630	-1107.45393	771.83503	1
30730	C	64.86800	69.95580	67.69390	585.53266	-646.42249	175.30282	1
30731	H	63.81200	69.72680	67.68790	-2278.96705	-1187.41021	1819.31780	1
30732	C	65.36600	70.19380	66.22890	-489.94767	767.95685	205.23288	1
30733	H	66.39600	70.60980	66.18990	1933.85882	-2059.66206	1335.36587	1
30734	H	65.22500	69.21180	65.72890	-1117.97957	-1686.53474	2401.97084	1
30735	C	64.53200	71.18780	65.44590	631.43424	-507.19592	-372.58484	1
30736	H	64.74800	72.23680	65.73890	1020.77602	-414.33692	-2940.47471	1
30737	C	64.82900	71.16480	63.94490	-208.80936	513.67914	739.65020	1
30738	H	64.37600	72.06480	63.47790	1015.10307	-2811.67117	-909.95927	1
30739	H	64.51100	70.21780	63.45690	-1804.16034	1890.52620	-1788.63665	1
30740	H	65.92000	71.13280	63.73590	-2335.21213	447.86168	2079.67061	1
30741	C	63.01800	70.99680	65.50990	322.88446	482.14121	-709.17138	1

30742	H	62.67500	69.94880	65.36790	-2184.73479	-2080.72404	884.00897	1
30743	H	62.52000	71.27080	66.46390	1273.45540	-1953.94195	2085.81858	1
30744	H	62.58300	71.55980	64.65590	918.31808	2327.69667	-1922.63132	1
30745	C	65.59900	68.81180	68.33190	-500.72265	423.71478	-656.77664	1
30746	O	65.01500	67.77580	68.08990	37.76457	771.03326	-233.61701	1
30747	N	66.67700	68.82680	69.08290	703.42772	-399.19134	158.93818	1
30748	C	67.51000	69.99280	69.37990	-326.00354	-681.83265	491.75406	1
30749	H	67.00000	70.92280	69.70990	-1129.66113	2957.64321	43.83143	1
30750	H	68.07300	70.27080	68.46290	331.29334	2923.30487	-1157.40782	1
30751	C	67.20100	67.63480	69.73590	-547.42624	726.89988	202.30085	1
30752	H	67.07000	66.78880	69.07690	-871.30119	3041.00528	136.78571	1
30753	C	68.66500	68.04580	70.17490	468.82507	407.76838	664.68585	1
30754	H	69.12400	67.49880	71.02590	-2153.12083	-1987.14317	1136.51609	1
30755	H	69.38400	67.82280	69.35690	659.66763	2157.02922	2200.99531	1
30756	C	68.55100	69.51580	70.42490	-707.90153	-390.34414	-429.28302	1
30757	H	69.49600	70.06980	70.24090	-974.20664	2625.15733	1467.23493	1
30758	H	68.18300	69.79180	71.43690	-2272.38068	-1910.50686	-1037.80597	1
30759	C	66.39300	67.26680	71.00390	-466.02299	756.97790	278.19088	1
30760	O	66.32900	66.10480	71.31490	-150.09125	656.96208	440.20231	1
30761	N	65.84600	68.26680	71.68190	513.76504	662.17368	-148.03819	1
30762	H	65.99600	69.19580	71.35290	2319.16459	701.46555	-2001.76025	1
30763	C	64.95700	68.17180	72.79490	389.06432	-659.82578	459.49809	1
30764	H	64.63100	69.17880	73.00590	2046.39916	1138.12788	2100.02295	1
30765	H	65.55800	67.86280	73.63690	1723.18623	112.59404	-2625.40216	1
30766	C	63.76000	67.32980	72.57190	-21.30539	-820.60442	-357.34307	1
30767	O	63.42600	66.47880	73.44190	-448.00605	-198.62453	-621.12956	1
30768	N	63.06200	67.53680	71.42990	754.52286	179.22616	315.50583	1
30769	H	63.28600	68.31780	70.85290	-1873.63713	1388.10766	2134.61436	1
30770	C	61.89500	66.79280	71.11990	121.60613	-564.35091	688.46362	1
30771	H	61.24900	66.80980	71.98490	-1375.33907	-2702.90060	-791.12605	1
30772	C	61.08100	67.31480	69.93990	580.28294	-668.69814	-74.57125	1
30773	H	60.31700	66.55780	69.66190	1181.02093	2597.85034	-1349.38890	1
30774	C	60.20100	68.50380	70.43690	-74.34757	-688.26364	572.93428	1
30775	H	59.64400	68.05180	71.28490	1652.67390	1204.08622	2395.21850	1
30776	H	59.37700	68.71880	69.72290	-678.24249	3074.99816	-349.42670	1
30777	H	60.89200	69.32080	70.73390	1484.98373	-1883.48888	-2007.58191	1
30778	C	61.97000	67.64580	68.73790	-17.63365	839.75422	-397.06512	1
30779	H	62.59600	68.53580	68.96190	-18.25479	-217.61598	3137.58847	1
30780	H	62.67200	66.81080	68.52690	1497.72601	-429.24012	2722.69511	1
30781	C	61.18200	67.81180	67.43490	-843.04135	-300.31320	-204.79352	1
30782	H	61.83300	68.03080	66.56190	2971.80351	-718.11003	-657.84784	1
30783	H	60.42100	68.61980	67.48290	1457.39240	635.13065	2713.73669	1
30784	H	60.54100	66.91780	67.27590	1954.50529	-2293.78268	818.11783	1
30785	C	62.10100	65.27780	70.85890	529.32498	-392.42834	606.99488	1
30786	O	61.32600	64.41780	71.31790	-103.49480	-176.76743	-758.52511	1
30787	N	63.17400	64.90480	70.18990	-131.21398	393.78872	747.00106	1
30788	H	63.73500	65.66780	69.88090	720.76343	-2805.12670	-1177.69592	1
30789	C	63.66700	63.56780	70.06490	-604.32106	657.94367	-273.66119	1
30790	H	62.88200	62.91180	69.71890	1853.31171	2206.14022	-1274.34533	1
30791	C	64.85000	63.46980	69.11790	58.16240	-729.56064	515.51707	1
30792	H	65.76400	63.92480	69.55590	-75.50654	-1112.56511	-2937.35210	1
30793	C	65.11100	61.98380	68.79790	572.41423	-550.71958	-403.90924	1
30794	H	65.53400	61.39180	69.63790	2113.93278	1705.10685	1584.53752	1
30795	H	65.93800	61.98080	68.05590	852.91629	-2706.60128	1309.72868	1
30796	H	64.16200	61.56580	68.39990	-1399.91182	-1769.22361	-2189.11027	1
30797	C	64.66600	64.18280	67.82090	-527.62217	763.94529	113.75255	1
30798	H	64.71900	65.29080	67.87690	1572.86085	-170.50609	-2710.55012	1
30799	H	65.40800	63.84580	67.06590	1784.40842	-1917.68335	1703.97710	1
30800	H	63.66800	64.06080	67.34590	1331.82042	2050.82597	-1988.41479	1
30801	C	64.06000	63.02280	71.47490	-15.39063	770.45807	-516.31567	1
30802	O	63.68600	61.86980	71.71690	700.85197	-75.11305	-322.85731	1
30803	N	64.69800	63.81880	72.35490	538.52708	-380.33646	498.83185	1

30804	H	64.92200	64.75380	72.09190	1052.81417	2449.48702	-1689.76298	1
30805	C	64.99500	63.39580	73.70990	72.16217	873.43714	-305.36442	1
30806	H	65.58600	62.49180	73.72390	-1390.99786	-2156.36147	-1810.51360	1
30807	C	65.90700	64.41680	74.47290	-559.89923	-706.10638	79.97550	1
30808	H	65.40800	65.40280	74.35890	-809.72560	-2986.15997	485.00071	1
30809	C	65.96600	64.10380	75.97690	111.25084	485.60913	770.96179	1
30810	H	64.99500	64.04380	76.51390	1054.72471	1376.05910	-2631.92931	1
30811	H	66.52400	63.15380	76.11390	717.70981	-2491.03669	1751.61793	1
30812	H	66.62700	64.80880	76.52590	-2167.45642	233.26511	2276.89402	1
30813	C	67.28900	64.30380	73.77390	737.87078	-440.44737	-248.74013	1
30814	H	67.15200	64.24880	72.67190	-432.53565	-1891.73011	-2468.20154	1
30815	H	67.80800	63.36280	74.05590	1280.28223	-2496.60691	-1385.89842	1
30816	C	68.16400	65.49680	74.02690	-405.49306	479.81434	-682.57555	1
30817	H	67.70100	66.33980	73.47090	2075.48538	1753.50326	-1593.23277	1
30818	H	68.23500	65.67980	75.11990	2812.53809	-532.24153	1272.94427	1
30819	H	69.22100	65.29580	73.74790	1914.83276	-1469.56736	1991.10527	1
30820	C	63.73700	63.05580	74.48490	481.77398	-480.94537	-582.49075	1
30821	O	63.59500	61.94380	75.01890	-744.08672	109.22593	280.74989	1
30822	N	62.71100	63.97680	74.42690	-399.72526	-482.07131	-557.51434	1
30823	H	62.97700	64.85880	74.04390	1939.71577	-1133.31430	-2182.86401	1
30824	C	61.40000	63.89880	75.00690	-76.72985	706.91388	596.24820	1
30825	H	61.51400	63.67880	76.05790	-1961.60824	1557.32720	-1929.16780	1
30826	C	60.66100	65.21180	74.74190	512.00698	746.02020	-173.45174	1
30827	H	60.92700	65.60280	73.73690	-1885.87036	1791.62483	-1799.56234	1
30828	H	59.56300	65.07380	74.83190	-3117.88741	323.17157	-386.78908	1
30829	C	61.13800	66.33980	75.75290	-535.91476	-278.53441	683.60118	1
30830	H	62.24600	66.39680	75.69090	-1305.83172	1094.76639	-2656.62772	1
30831	C	60.60400	67.72780	75.32790	550.41532	591.14253	-436.06795	1
30832	H	60.92600	68.06380	74.31990	2167.11284	908.66900	2091.62142	1
30833	H	59.49500	67.79180	75.33190	-1727.08826	-2167.17815	-1468.36182	1
30834	H	60.93400	68.51280	76.04190	930.61724	2106.78920	-2157.11517	1
30835	C	60.79400	66.15080	77.20290	784.88557	-200.07839	-390.40527	1
30836	H	61.31900	65.24480	77.57390	-589.93803	1188.02658	-2861.49478	1
30837	H	60.95400	67.10180	77.75390	-2962.49464	525.89187	956.37925	1
30838	H	59.72800	65.90580	77.39990	1744.23696	252.61727	2604.39967	1
30839	C	60.68300	62.63780	74.55090	-434.63344	700.08040	436.89505	1
30840	O	60.15800	61.87580	75.38690	496.18579	617.22203	-92.55770	1
30841	N	60.66600	62.35580	73.27790	-585.23687	409.24186	484.31097	1
30842	H	61.20100	62.96480	72.69590	1737.03890	-1994.72742	-1665.92880	1
30843	C	60.10100	61.11180	72.65490	132.46947	319.14598	-847.08476	1
30844	H	59.04500	61.08180	72.87990	765.06247	-2109.83791	2182.92142	1
30845	C	60.12500	61.11180	71.07890	-96.26446	660.77907	645.28365	1
30846	H	59.92400	60.10280	70.65790	2225.42823	-2078.12381	690.75152	1
30847	H	61.15700	61.42380	70.81190	1720.04467	-2467.70070	-836.94633	1
30848	O	59.30200	62.05380	70.45490	-369.12544	-28.23802	706.37639	1
30849	H	58.40200	61.85880	70.72590	-986.67934	3005.77609	-203.10707	1
30850	C	60.70300	59.78680	73.11590	582.37163	-611.91733	278.85775	1
30851	O	59.91400	58.83680	73.29290	-351.72463	9.25293	715.66016	1
30852	N	62.04400	59.67780	73.24190	201.29654	-335.96422	-734.61808	1
30853	H	62.55400	60.48180	72.94690	-1127.21398	-2264.61561	-1855.66175	1
30854	C	62.74300	58.45280	73.65390	-426.81143	-230.29933	773.92629	1
30855	H	62.41300	57.69680	72.95690	-632.91877	2917.92837	-1054.48916	1
30856	C	64.26900	58.73380	73.87290	-742.79817	277.74158	481.31952	1
30857	H	64.76100	57.78280	74.17290	887.52915	949.33308	-2868.12459	1
30858	H	64.35500	59.49580	74.67690	-1465.48843	-2603.71982	955.17750	1
30859	S	64.98900	59.21680	72.26490	-208.83841	-58.38274	515.87020	1
30860	H	64.69800	60.50780	72.31790	-695.52101	-1434.84002	2704.82262	1
30861	C	62.19100	57.92080	74.99590	103.42838	758.48111	-520.23781	1
30862	O	61.86400	56.75380	75.16990	168.89964	612.25997	488.75061	1
30863	N	62.14600	58.80680	76.01990	33.31321	823.91979	-249.93436	1
30864	H	62.48500	59.73680	75.89890	-686.98342	-2308.68185	-2006.19680	1
30865	C	61.69700	58.38880	77.38590	-752.64618	-460.14440	-228.95245	1

30866	H	62.07100	57.41880	77.67990	-2657.82022	1536.57437	770.99000	1
30867	C	62.30100	59.29480	78.44190	746.91613	487.32327	-195.04774	1
30868	H	61.96400	58.85080	79.40290	2395.99048	1340.19347	-1536.75719	1
30869	H	61.85500	60.29480	78.25690	2772.60517	1121.02599	969.69131	1
30870	C	63.83700	59.35180	78.28390	-813.81509	159.20311	407.33001	1
30871	C	64.38900	60.56680	77.83490	559.42456	553.86760	-469.60196	1
30872	H	63.80300	61.43580	77.57490	890.96830	2325.75849	1938.74793	1
30873	C	65.78200	60.60780	77.65190	-48.35528	-580.05727	-689.76408	1
30874	H	66.16600	61.51380	77.20790	-915.39167	1370.66368	2689.95312	1
30875	C	66.60500	59.53580	77.92290	-827.99765	0.13943	-406.82523	1
30876	O	67.97300	59.58680	77.66090	-664.43109	-374.99303	204.67685	1
30877	H	68.15200	60.22280	76.96390	1748.89852	-2560.45003	-403.06642	1
30878	C	64.61200	58.27280	78.57190	-396.67729	455.02756	699.80138	1
30879	H	64.11800	57.43480	79.04090	2249.50471	-978.40411	1947.22459	1
30880	C	66.01500	58.33080	78.34490	-487.79341	-350.92177	682.28092	1
30881	H	66.62900	57.44280	78.37690	947.30203	-2895.56222	-706.70402	1
30882	C	60.22600	58.36380	77.44290	29.03212	854.17430	-363.71295	1
30883	O	59.63100	57.65280	78.25890	-333.93653	546.19622	-490.59072	1
30884	N	59.50100	59.13780	76.59090	176.85199	-543.20888	-597.75768	1
30885	H	59.91300	59.78880	75.95890	-2215.58354	1711.44935	1478.72252	1
30886	C	58.09000	58.99580	76.38390	-913.61978	-75.39378	100.23420	1
30887	H	57.66200	59.15280	77.36290	1901.84599	-2176.32686	1191.06659	1
30888	C	57.49900	60.00280	75.39790	-16.22754	-795.35896	409.90528	1
30889	H	57.89000	60.99280	75.71490	-1944.52583	-1875.58259	-1598.82305	1
30890	H	57.90100	59.81880	74.37790	717.69775	-2999.89537	493.05135	1
30891	S	55.72300	60.08580	75.22290	-21.01888	-276.84887	475.86486	1
30892	H	55.62900	59.09380	74.34990	-2351.13678	1934.85832	883.72810	1
30893	C	57.68600	57.57480	75.97290	-738.74424	232.84104	-506.32010	1
30894	O	56.79800	56.98380	76.56690	-688.17774	-350.31199	-167.91005	1
30895	N	58.36000	56.95880	75.04090	-1.62307	-794.57545	-216.59174	1
30896	H	58.91300	57.53180	74.44090	-741.83034	2465.55836	1843.42837	1
30897	C	58.10400	55.59180	74.61790	-605.56273	151.25925	684.94131	1
30898	H	57.05600	55.50580	74.37190	1965.11030	-2419.96231	-135.80952	1
30899	C	58.88400	55.19280	73.32890	610.63450	-563.47435	-311.25408	1
30900	H	59.96700	55.39580	73.47690	-2108.56647	1806.18823	-1523.57896	1
30901	C	58.75700	53.70380	73.07890	-721.32627	128.92453	570.52693	1
30902	H	59.12800	53.48880	72.05390	2465.01097	1424.99052	-1325.97805	1
30903	H	59.29400	53.04680	73.79590	2767.53524	-1375.51341	-446.41290	1
30904	H	57.68400	53.41180	73.07590	2803.15802	1416.28076	25.25229	1
30905	C	58.35700	55.95380	72.10590	609.17489	-43.96426	-657.76143	1
30906	H	57.42400	55.51380	71.69390	1366.81363	2846.02567	-58.24651	1
30907	H	58.03500	56.99480	72.32590	2376.47824	2063.94638	44.54225	1
30908	C	59.39500	56.11680	70.97890	680.28328	-507.34529	-257.09103	1
30909	H	59.93700	55.16780	70.78090	1892.52141	-1404.41330	2056.35259	1
30910	H	59.03200	56.60880	70.05190	1903.63385	198.54913	2487.64517	1
30911	H	60.04100	56.97780	71.25290	2509.92970	1599.72988	1012.05594	1
30912	C	58.48800	54.59080	75.69290	-687.21356	56.02023	-611.70156	1
30913	O	57.74000	53.60180	75.90990	-493.04920	-379.77298	-480.92468	1
30914	N	59.64700	54.78980	76.37390	-608.43491	-498.83541	-297.97709	1
30915	H	59.99800	55.71780	76.27190	-2814.89252	-1140.73472	840.32655	1
30916	C	60.34200	53.84080	77.29690	-479.48418	-612.35989	-462.22100	1
30917	H	60.57700	52.90980	76.80290	2090.39055	-1379.20371	-1872.87302	1
30918	C	61.81500	54.30380	77.78890	550.69135	-459.74731	533.71509	1
30919	H	61.72400	55.38780	78.01790	-193.07907	2680.88306	-1666.93834	1
30920	C	62.20200	53.43880	79.01190	-748.31374	514.39371	211.29130	1
30921	H	62.13300	52.35980	78.75490	1731.49041	1938.27941	1780.65390	1
30922	H	63.25500	53.63080	79.30990	-2467.32649	-1844.69493	-632.98060	1
30923	H	61.54700	53.49980	79.90690	-3086.12462	529.50231	-432.18616	1
30924	C	62.82100	54.15980	76.66190	-549.41646	411.58805	-624.94434	1
30925	H	62.32800	54.42880	75.70290	2520.79210	-1797.62098	-413.94054	1
30926	H	63.23200	53.13380	76.55490	623.62536	-2977.69496	-717.48735	1
30927	C	64.08400	54.91880	76.90390	-194.21635	870.78060	266.85098	1

30928	H	63.83200	55.97580	77.13390	-2175.74993	-219.52744	-2273.16245	1
30929	H	64.72100	54.56480	77.74290	-694.92398	-2919.08916	-900.06891	1
30930	H	64.80100	54.81880	76.06190	-116.86504	-362.46141	-3122.91644	1
30931	C	59.39500	53.38480	78.45890	352.44959	-751.75450	321.83837	1
30932	O	59.23700	52.19880	78.85690	-144.15323	-562.04800	-515.28783	1
30933	N	58.74100	54.39080	79.02790	-592.23801	-477.58716	360.74100	1
30934	H	58.82900	55.33080	78.70690	-2477.19196	1970.21137	139.18783	1
30935	C	57.95400	54.24980	80.20890	541.46549	-518.14109	488.29708	1
30936	H	58.55600	53.66780	80.89190	-1947.49405	1702.03589	1824.85720	1
30937	C	57.67700	55.58980	80.88790	-555.44147	545.12727	-506.08187	1
30938	H	57.07200	55.33580	81.78590	2306.47559	-1866.37110	-981.65834	1
30939	C	58.98100	56.16480	81.44990	624.87760	601.54259	303.06871	1
30940	H	58.79600	57.04280	82.10490	2065.68679	-1583.31870	1741.03283	1
30941	H	59.55900	55.40180	82.01390	-3037.34163	750.02766	-444.23323	1
30942	H	59.56000	56.60080	80.60790	482.00735	-2994.03053	758.50602	1
30943	C	56.89100	56.57580	80.03690	-746.14461	-46.86438	-530.94229	1
30944	H	57.59600	57.08480	79.34490	-2022.07043	2132.62497	1183.61021	1
30945	H	56.23000	55.99780	79.35490	-1766.58538	1831.90277	1885.33344	1
30946	C	56.10400	57.58680	80.84990	604.99269	95.80931	673.65824	1
30947	H	55.43400	57.04080	81.54790	2501.21476	1908.00410	194.15721	1
30948	H	55.39900	58.12580	80.18290	-22.47001	82.98538	-3140.74664	1
30949	H	56.80600	58.30380	81.32690	2069.79088	-1714.24354	1605.58928	1
30950	C	56.78400	53.35880	80.02290	-755.48431	532.50475	-126.59841	1
30951	O	56.23600	52.76380	80.96890	576.83295	546.11965	47.30556	1
30952	N	56.27700	53.27880	78.79190	0.49060	609.87910	609.02717	1
30953	H	56.73500	53.86180	78.12490	933.06809	-1957.80656	2259.22396	1
30954	C	55.13000	52.49880	78.47790	-309.21123	813.40574	-337.49412	1
30955	H	54.47900	52.42980	79.33690	830.65555	1723.38438	2513.58278	1
30956	C	54.26500	53.22480	77.40490	740.29574	533.19302	-35.71430	1
30957	H	53.70300	54.02080	77.93790	-1922.66158	-2463.52536	274.47655	1
30958	H	53.51500	52.55080	76.93890	-2526.08321	-1556.25907	1053.20377	1
30959	O	55.06400	53.77880	76.36790	-414.71341	657.37456	-238.63184	1
30960	H	55.77900	53.17280	76.16290	112.18282	3145.45457	355.52403	1
30961	C	55.34500	51.08080	78.13790	715.52039	-424.81487	320.41029	1
30962	O	54.38400	50.33480	77.74290	428.25850	-629.85248	-44.33796	1
30963	N	56.56600	50.60580	78.30390	-121.95796	-744.76291	342.04035	1
30964	H	57.18900	51.23380	78.76590	-217.41241	1815.58534	-2572.62864	1
30965	C	56.93000	49.22180	78.07690	634.76279	-618.80876	6.16695	1
30966	H	56.17700	48.60980	78.54990	-1698.37715	-1987.08651	1744.73170	1
30967	C	56.90500	48.80080	76.58590	534.31140	524.23153	528.22933	1
30968	H	55.84500	48.89880	76.26890	-1929.64774	2489.33389	387.47459	1
30969	H	57.16400	47.73180	76.43290	1229.55171	2708.99317	1061.51016	1
30970	C	57.61500	49.74880	75.55590	-541.21863	677.70438	355.84544	1
30971	H	58.66700	49.92380	75.86590	37.59936	-3076.98169	-546.91306	1
30972	H	57.07500	50.71580	75.64090	798.02883	1751.04824	-2495.12843	1
30973	C	57.50000	49.15880	74.14190	-237.58920	515.38811	736.93104	1
30974	H	58.09000	49.79580	73.44890	-2588.99014	-1791.29619	62.36509	1
30975	H	58.01800	48.17680	74.12790	2240.26478	464.16927	-2142.52494	1
30976	C	56.08000	49.16180	73.63190	552.32837	-652.44390	232.34148	1
30977	H	55.39300	48.50380	74.20690	1454.85906	-1709.82666	-2170.67806	1
30978	H	55.70700	50.20880	73.64390	2296.67120	156.27329	-2122.89403	1
30979	N	56.00100	48.71280	72.26790	-383.72817	-321.19687	-675.72201	1
30980	H	56.26500	49.45680	71.59090	146.00795	-2597.07021	1740.03483	1
30981	H	55.01000	48.47780	72.05990	1466.45972	2127.17862	1810.05488	1
30982	H	56.61600	47.89280	72.09290	2536.38108	-639.74582	-1707.85180	1
30983	C	58.25800	48.62980	78.70690	515.95747	565.87688	504.90381	1
30984	O	58.67000	47.50480	78.41790	-499.09320	-530.61399	295.77110	1
30985	N	58.87400	49.39780	79.67090	-23.09482	-819.85822	85.45525	1
30986	H	58.55300	50.33080	79.81490	2283.70561	2071.85288	-640.26008	1
30987	C	60.05300	49.01480	80.43090	-751.61360	72.18142	534.12327	1
30988	H	60.85900	48.83280	79.73490	-224.19283	1465.40529	2787.08287	1
30989	C	60.48400	50.11080	81.40890	-603.80262	438.73431	-551.88028	1

30990	H	60.55300	51.07380	80.85790	-1994.04452	-881.40462	2272.58399	1
30991	H	59.62900	50.22680	82.10890	-1619.54170	-1647.89954	-2127.20591	1
30992	C	61.81200	49.86180	82.09690	-28.13460	74.04818	910.29652	1
30993	H	61.77700	48.88480	82.62590	475.91534	2640.41413	1669.93191	1
30994	C	62.94700	50.01980	81.06690	692.57137	-557.96632	-43.80452	1
30995	H	62.97300	51.01480	80.57190	-2317.94410	1847.44380	1112.29872	1
30996	H	62.94200	49.14980	80.37590	-391.68039	-348.41990	-3102.19523	1
30997	H	63.86500	49.83680	81.66490	2793.47900	1350.33698	-502.08545	1
30998	C	61.98100	50.95380	83.20990	-540.08003	-508.30406	-522.77272	1
30999	H	61.11500	50.89480	83.90290	-2610.44973	8.23323	1772.13809	1
31000	H	62.95000	50.78680	83.72690	-2867.76862	-1145.44631	-616.87489	1
31001	H	62.00600	51.98380	82.79390	-1988.89504	-1075.20882	2188.36283	1
31002	C	59.83400	47.69080	81.19690	15.90635	609.99751	-692.88628	1
31003	O	60.73700	46.80980	81.21890	-409.14284	-135.73948	666.67260	1
31004	N	58.64700	47.46780	81.86090	177.38988	-773.14988	-214.47660	1
31005	H	57.93700	48.16280	81.93990	-2355.68506	-2073.23886	162.14257	1
31006	C	58.32400	46.20480	82.43990	-710.79079	601.17235	-84.03016	1
31007	H	59.16000	45.72380	82.92390	-148.72064	-1199.94326	2898.72804	1
31008	C	57.25300	46.40580	83.55490	426.58912	-346.24550	713.14027	1
31009	H	56.46500	47.09480	83.18390	-2995.94711	-772.77005	-601.70701	1
31010	H	56.84700	45.42880	83.89290	-1541.04820	2412.08574	-1354.57311	1
31011	O	57.79400	47.05480	84.72390	-69.72626	-251.14759	-736.39945	1
31012	H	58.33600	46.39680	85.16390	-3079.12643	-84.73276	692.44711	1
31013	C	57.74300	45.15880	81.47690	-774.93089	388.77484	-339.73110	1
31014	O	57.44700	44.02980	81.86390	644.47641	-34.51336	-428.68608	1
31015	N	57.64000	45.44880	80.18090	-42.68253	-179.44283	-816.79560	1
31016	H	57.87600	46.33480	79.79090	-2420.53053	1989.08740	488.89822	1
31017	C	57.07300	44.51080	79.22090	207.52345	550.66338	-704.46919	1
31018	H	56.64100	43.64980	79.70890	-2210.29765	2090.61521	898.28024	1
31019	C	55.93600	45.12680	78.34290	-535.27016	-123.92693	739.58546	1
31020	H	56.29600	45.99180	77.74590	2168.29481	121.94524	2265.43372	1
31021	H	55.54800	44.49680	77.51490	1231.24263	-580.98695	-2820.04590	1
31022	N	53.71900	46.31980	78.70290	-466.28967	558.05998	-466.26954	1
31023	H	53.67500	46.71180	77.78490	2129.10604	714.59885	-2189.23068	1
31024	C	54.76900	45.59380	79.19390	731.96112	342.18212	417.00950	1
31025	C	52.84700	46.50780	79.73890	-668.69046	384.59491	528.56259	1
31026	H	51.89400	47.02380	79.61890	806.93058	-2981.28162	-437.47675	1
31027	N	53.29900	45.96080	80.86590	-535.53131	-341.54874	561.30769	1
31028	C	54.52600	45.35480	80.48390	136.15571	195.78019	887.20699	1
31029	H	55.14700	44.83680	81.20490	-1948.34274	1936.71448	1582.92011	1
31030	C	58.04800	44.00880	78.19490	720.23953	280.72267	471.95797	1
31031	O	57.88200	42.94680	77.55890	242.95660	-481.60112	553.44672	1
31032	N	59.14200	44.76280	78.02990	-245.94003	-747.14216	-265.43977	1
31033	H	59.21600	45.65280	78.47390	2706.66704	-1511.34020	-371.76729	1
31034	C	60.37000	44.45780	77.32690	458.20704	-614.74365	451.45146	1
31035	H	60.06600	43.86780	76.47490	1908.60101	-1427.81867	-2021.23111	1
31036	C	61.19700	45.73880	76.87590	-770.20175	-9.78285	513.82284	1
31037	H	62.10800	45.47580	76.29590	-220.68398	-2867.71865	1234.42780	1
31038	H	61.43300	46.19080	77.86290	-2234.11583	880.10954	-2058.29987	1
31039	O	60.39300	46.65880	76.10090	282.23104	677.56138	319.10140	1
31040	H	59.93500	47.30180	76.64590	-947.86037	1941.76740	2311.67270	1
31041	C	61.25600	43.57680	78.15690	-195.84746	-141.59167	880.00059	1
31042	O	61.74400	44.02380	79.23190	652.71382	428.46412	92.19366	1
31043	O	61.55900	42.43480	77.70390	589.59443	-477.71161	-87.57705	1
31044	N	68.09800	39.69880	83.86190	556.67163	366.21965	509.10069	1
31045	H	68.31400	38.85080	84.42290	895.17183	2185.30874	2084.85965	1
31046	H	68.24600	39.59180	82.83790	1760.35254	-2225.34715	1306.83644	1
31047	H	67.12500	40.02180	84.03590	1006.67596	1028.81658	-2801.88675	1
31048	C	68.95200	40.75780	84.30590	763.33933	162.61783	448.40240	1
31049	H	68.94300	40.82480	85.38390	1932.61191	241.96193	2456.94237	1
31050	C	70.47100	40.56280	83.91090	-126.17098	628.65798	659.70982	1
31051	H	70.98000	41.53880	84.06090	2017.22036	2414.33199	-132.34205	1

31052	H	70.47900	40.45980	82.80490	215.39335	-2484.62161	-1901.80963	1
31053	C	71.15500	39.33080	84.51890	-141.37774	-740.32587	488.53310	1
31054	H	72.17500	39.10180	84.14190	2802.21383	-1301.42045	472.14880	1
31055	H	70.62200	38.43880	84.12690	2571.49253	193.37365	-1787.81205	1
31056	C	71.32300	39.38980	86.03290	449.54245	696.53167	-396.65910	1
31057	H	70.30800	39.45380	86.48090	126.86194	-540.83380	-3099.10321	1
31058	H	71.82700	40.34380	86.29990	-1208.05498	1321.91630	2593.62779	1
31059	C	71.99000	38.13380	86.56490	178.78461	-842.32884	238.04532	1
31060	H	71.54000	37.18180	86.20890	2208.89330	-2096.89628	697.51694	1
31061	H	73.02200	38.05280	86.16090	-2237.26693	-1813.99119	1262.63210	1
31062	N	72.01700	38.08680	88.06190	-244.28613	327.09421	742.43432	1
31063	H	72.40100	38.94980	88.49690	-1231.27725	2202.20654	-1911.17941	1
31064	H	71.06600	37.95380	88.46190	-1448.58804	-1984.78686	-1965.11353	1
31065	H	72.60700	37.30680	88.41590	2872.43571	1150.35882	-538.77606	1
31066	C	68.42100	42.10180	83.76190	-842.92262	-82.77771	362.53647	1
31067	O	67.82500	42.17680	82.71690	-537.06743	-560.77362	-136.47941	1
31068	N	68.61900	43.27580	84.43490	-660.07961	557.08595	-42.09834	1
31069	H	69.20800	43.27780	85.23890	2256.58630	2063.93003	739.68554	1
31070	C	67.99400	44.54780	83.99690	229.38844	257.48278	-849.32872	1
31071	H	68.34000	44.71780	82.98890	846.14580	-1407.67360	-2674.74101	1
31072	H	66.91700	44.46680	83.96490	-784.60878	-589.04457	-2992.54816	1
31073	C	68.37200	45.68480	84.92590	172.85123	-305.20879	828.91015	1
31074	O	68.20000	46.83880	84.64490	-694.36213	-351.95288	143.63503	1
31075	N	68.83800	45.43480	86.17690	-162.89885	609.28063	-585.51629	1
31076	H	69.14100	44.52880	86.46290	2025.98455	2026.24857	1301.36155	1
31077	C	69.04600	46.53980	87.06590	-553.68093	-329.18332	-650.29371	1
31078	H	68.12300	47.09580	87.14390	56.55391	-2786.22240	1424.40912	1
31079	C	69.42500	45.95680	88.48290	-281.37010	-694.00705	-508.76321	1
31080	H	69.61000	46.79780	89.18490	-418.46299	2779.84386	-1450.21936	1
31081	H	70.26400	45.23680	88.37490	2370.01287	943.18860	1831.40516	1
31082	N	68.12900	45.25980	90.58990	452.49721	327.12393	-639.37394	1
31083	H	68.44200	46.05880	91.10290	-337.71670	2979.23366	999.79552	1
31084	C	68.28000	45.18480	89.23290	510.37201	345.39026	-677.25295	1
31085	C	67.11100	44.45380	90.92790	636.05522	-321.48304	546.11704	1
31086	H	66.88800	44.18780	91.96090	1802.00731	2582.22470	-203.57760	1
31087	N	66.50500	43.97780	89.88790	-550.07167	482.83324	-453.50251	1
31088	C	67.24500	44.40280	88.80090	224.05025	648.54922	610.73191	1
31089	H	67.06100	44.12980	87.76890	2189.76115	787.93230	-2115.68559	1
31090	C	70.13100	47.50080	86.71590	163.55806	455.04756	-785.08633	1
31091	O	69.95600	48.68880	86.84090	213.05959	-611.68010	420.13683	1
31092	N	71.22300	46.97380	86.14590	194.11938	824.98621	115.10375	1
31093	H	71.30800	45.98380	86.05590	1384.63772	-1020.62824	2616.49843	1
31094	C	72.34500	47.79380	85.73390	650.37805	642.84011	-4.47069	1
31095	H	72.45100	48.61880	86.42290	-1555.17184	590.67923	-2685.88919	1
31096	C	73.65200	47.05680	85.70090	-436.54061	62.13583	797.24156	1
31097	H	73.55600	46.00080	85.36790	3027.85821	644.58745	-521.00603	1
31098	H	74.35000	47.50180	84.95990	-1983.78634	1051.91974	-2228.16821	1
31099	C	74.30700	47.04680	87.09390	470.69595	165.52581	751.85170	1
31100	H	74.48500	48.04780	87.54190	2361.54860	2043.05959	-407.39991	1
31101	H	75.34400	46.64680	87.06490	1457.21044	-1246.14561	2473.03163	1
31102	C	73.53900	46.29480	88.22990	49.32915	879.82028	272.21654	1
31103	O	73.14300	46.94180	89.21590	692.09349	-322.78549	-146.39691	1
31104	N	73.26100	44.98580	88.05190	-515.83006	173.32056	-664.32669	1
31105	H	73.59700	44.45680	87.27190	3134.20625	22.45956	-93.20885	1
31106	H	72.71800	44.56680	88.77890	2883.70278	228.73979	-1223.78486	1
31107	C	72.00600	48.49580	84.37690	-663.09841	191.81373	-618.80391	1
31108	O	72.38900	49.64980	84.14890	340.26526	185.37572	-693.20236	1
31109	N	71.16500	47.88080	83.49290	-314.40587	-751.26247	-190.01472	1
31110	H	70.90700	46.92780	83.63290	352.27328	-1749.25878	2573.34893	1
31111	C	70.59400	48.62080	82.36290	-874.82338	-273.94450	-67.64943	1
31112	H	71.41900	49.01280	81.78590	1023.46754	2223.51516	-1992.93363	1
31113	C	69.70100	47.63480	81.51590	-177.83518	-328.43521	-833.21643	1

31114	H	69.09700	47.05380	82.24590	645.42583	-2130.02202	2199.78193	1
31115	H	69.01800	48.11480	80.78390	2971.53365	-648.81186	733.94420	1
31116	C	70.56200	46.67680	80.62690	269.29461	226.94576	834.80666	1
31117	H	71.33500	46.24680	81.29890	-1930.82533	837.63585	-2361.41853	1
31118	H	71.11300	47.16180	79.79190	-959.31920	-430.95299	2961.64434	1
31119	C	69.74500	45.52780	80.02090	509.17130	-375.99930	629.78403	1
31120	H	69.31500	44.92580	80.84990	-1244.38950	1860.39312	2227.69923	1
31121	H	70.38800	44.89380	79.37490	999.82863	-764.71331	-2879.22058	1
31122	C	68.59400	45.99380	79.11190	-678.99821	3.52169	-629.71583	1
31123	H	67.85700	46.48980	79.77890	2238.19884	-480.61906	-2142.67656	1
31124	H	68.97400	46.63180	78.28490	900.80687	-2504.10773	1640.55170	1
31125	N	68.02900	44.78280	78.47990	-663.10998	428.12842	349.63284	1
31126	H	67.98800	44.08980	79.25490	440.34977	-1674.61512	2609.41266	1
31127	H	67.10500	44.86980	78.00990	1916.04341	1377.10870	2073.26748	1
31128	H	68.67200	44.54580	77.69790	400.61558	2964.74622	1010.59861	1
31129	C	69.71700	49.79980	82.79390	-629.23298	-309.00560	581.99408	1
31130	O	69.79800	50.86580	82.22390	528.65569	490.47385	-331.18599	1
31131	N	68.85600	49.66080	83.84290	583.56021	448.66919	-419.18798	1
31132	H	68.79800	48.77280	84.29290	-989.51927	2679.27111	-1363.69145	1
31133	C	68.00000	50.77580	84.28590	704.96814	-539.84464	99.56972	1
31134	H	67.57400	51.25780	83.41790	2418.42483	1136.62707	1652.90750	1
31135	C	66.81200	50.11480	85.12790	-342.01999	-288.03486	789.58305	1
31136	H	67.22400	49.50880	85.96190	-148.89448	1667.84609	-2677.67129	1
31137	H	66.27300	50.96480	85.59790	-1704.05461	936.64692	2483.32881	1
31138	C	65.87200	49.30880	84.17590	384.68052	668.93575	-502.67452	1
31139	H	66.45800	48.61780	83.53290	-1821.47345	392.99549	2542.94447	1
31140	H	65.40700	50.13980	83.60490	-2349.09870	-424.11206	-2060.26427	1
31141	C	64.58100	48.69080	84.76490	215.77696	692.42183	568.40652	1
31142	H	63.91200	48.26980	83.98490	-2077.99900	-2127.83892	-1012.48630	1
31143	H	64.00700	49.44380	85.34690	2902.64384	1202.49532	105.52401	1
31144	N	64.98200	47.51680	85.61290	-675.53305	262.15055	-460.93892	1
31145	H	64.97100	46.61780	85.17490	-2248.26796	386.11751	2179.41412	1
31146	C	64.91300	47.44980	86.91190	506.13405	637.97408	-426.44777	1
31147	N	65.22000	46.31280	87.50190	280.41503	-617.77050	-476.47275	1
31148	H	65.23700	45.48880	86.93590	-2941.60853	4.84867	1141.13906	1
31149	H	64.79200	46.14780	88.39090	-229.03081	1149.34317	2925.44569	1
31150	N	64.55700	48.39180	87.74590	357.84799	750.32047	201.71925	1
31151	H	64.32200	49.30080	87.40390	1708.81816	-1447.64407	2189.71459	1
31152	H	64.48300	48.15980	88.71590	888.58109	624.40720	2952.36322	1
31153	C	68.76300	51.77380	85.17190	-294.69297	647.16149	-597.18960	1
31154	O	68.31700	52.89480	85.38790	446.48457	-452.95932	-447.15507	1
31155	N	69.99200	51.44480	85.66490	-5.77924	-323.06581	768.25466	1
31156	H	70.22400	50.48180	85.78290	-2470.56616	961.39478	-1721.51370	1
31157	C	71.03900	52.33780	86.14090	-589.76630	522.86037	479.53416	1
31158	H	70.60600	52.99280	86.88290	-1998.14161	-1227.07992	-2101.29000	1
31159	C	72.06500	51.49980	86.96290	565.80011	-539.92791	434.64915	1
31160	H	72.56500	50.79680	86.26290	-1941.68531	2244.02759	-1098.26154	1
31161	H	71.46100	50.99980	87.75090	552.56969	3098.85065	-276.16611	1
31162	C	73.17300	52.34480	87.63990	52.73969	715.95054	-586.19432	1
31163	H	73.64300	52.97080	86.85090	1248.08932	-169.49906	2871.41421	1
31164	H	74.04000	51.75980	88.01390	312.63103	2028.39593	2387.48535	1
31165	C	72.66500	53.24480	88.79790	-484.35671	577.97277	527.14860	1
31166	H	72.29600	54.16380	88.29490	-1905.76300	-2161.58153	1240.31119	1
31167	H	71.81600	52.78380	89.34490	-617.95893	2494.70927	-1842.79743	1
31168	C	73.72900	53.65480	89.76990	774.02313	-140.39501	439.93054	1
31169	H	74.54200	54.24280	89.29390	-2187.92445	-1057.14035	1989.20389	1
31170	H	74.15700	52.71680	90.18490	-264.03075	198.11877	3122.28289	1
31171	N	73.08500	54.51480	90.80690	-316.97508	-433.39767	636.96758	1
31172	H	72.42900	53.95380	91.38690	1686.68658	-1849.55302	-1894.76515	1
31173	H	72.53100	55.23180	90.29690	240.75732	3114.11079	472.22632	1
31174	H	73.73600	55.06480	91.40390	2151.45467	-2095.39632	889.62861	1
31175	C	71.68500	53.15880	85.00390	615.01496	-410.56175	-517.44722	1

31176	O	71.94000	54.39380	85.13790	202.17436	-49.31663	752.20715	1
31177	N	72.06400	52.55680	83.85790	-522.43009	-546.37329	361.03592	1
31178	H	72.02800	51.56080	83.83890	-1350.25557	-2216.35419	-1774.10089	1
31179	C	72.45900	53.18580	82.59290	262.12152	732.21746	485.50978	1
31180	H	73.31700	53.82280	82.75190	-2576.32580	755.05617	-1669.47840	1
31181	C	72.73700	52.17980	81.49090	-536.80232	-443.49466	581.09221	1
31182	H	73.16400	52.69180	80.60190	-881.60524	-2290.82899	-1963.61818	1
31183	H	73.43100	51.39180	81.85490	1341.53252	512.25996	-2803.66961	1
31184	H	71.81100	51.66480	81.15690	-253.27386	2462.99779	-1967.58432	1
31185	C	71.42300	54.10280	82.09390	-700.25861	-570.89941	103.98633	1
31186	O	71.72400	55.20980	81.62890	-562.97916	-231.76152	500.99676	1
31187	N	70.15100	53.68580	82.18190	-352.68543	474.28207	-625.64016	1
31188	H	69.93300	52.74080	82.41190	-2063.67853	-895.50155	2197.96673	1
31189	C	69.05200	54.61880	81.81290	-672.10052	393.21910	496.75288	1
31190	H	69.27300	54.93580	80.80490	2232.47940	946.57785	-2004.45183	1
31191	C	67.72000	53.76380	81.88590	628.64670	-535.18516	340.71760	1
31192	H	67.86000	52.87180	81.23890	-2075.07843	-2272.32401	629.28007	1
31193	H	67.52600	53.54180	82.95690	-1569.62450	-2689.31946	375.81058	1
31194	C	66.42000	54.44080	81.37090	419.58400	-29.28561	-805.26116	1
31195	H	66.26400	55.30580	82.05090	-691.79970	-566.27326	3012.93387	1
31196	C	66.51600	54.88780	79.91790	-184.54132	-417.89353	779.80760	1
31197	H	67.34800	55.61980	79.84090	-814.88562	-2357.47667	-1904.60422	1
31198	H	66.83700	54.05780	79.25390	1886.73324	2086.65311	-1420.22214	1
31199	H	65.61300	55.35880	79.47290	-1678.91463	-61.67137	2664.71667	1
31200	C	65.08700	53.64980	81.60090	-742.14644	318.84243	-455.44473	1
31201	H	64.19400	54.26480	81.35690	-2522.25175	1590.17292	1056.43768	1
31202	H	65.13500	52.68680	81.04990	-607.28557	-3056.17934	-310.41973	1
31203	H	65.04700	53.31080	82.65790	-2832.94231	-1335.12140	315.61021	1
31204	C	68.94000	55.86580	82.65390	-79.67120	-812.70483	369.55721	1
31205	O	68.94800	56.97480	82.06590	-455.94571	153.34897	632.28730	1
31206	N	68.95500	55.70480	84.03490	271.22631	-538.99241	567.18269	1
31207	H	68.90000	54.78480	84.41390	1037.61234	-516.24397	2914.77017	1
31208	C	69.01700	56.76980	84.97390	-541.85235	-418.20557	593.44855	1
31209	H	68.18000	57.41880	84.76190	-1653.11815	-1783.11988	-1991.50329	1
31210	C	68.98700	56.10080	86.37390	379.28148	785.84931	-303.65322	1
31211	H	67.97000	55.65380	86.34790	1882.22155	1426.23710	2080.05729	1
31212	H	69.84200	55.41280	86.55090	-1626.02358	831.21259	2566.33370	1
31213	C	69.01600	57.12980	87.55390	-629.05109	600.86167	312.43931	1
31214	H	68.64300	58.10980	87.18590	2084.91923	-1148.81152	-2046.64011	1
31215	H	70.04000	57.51080	87.75690	2150.11927	1410.69219	-1823.19035	1
31216	C	68.28500	56.64680	88.80690	-61.47567	-633.75874	-640.93873	1
31217	H	67.27800	56.32580	88.46590	-521.63500	-2460.63378	-1872.71996	1
31218	H	68.78000	55.77180	89.27990	-2713.15118	-114.62270	1591.59365	1
31219	C	68.18300	57.76180	89.88990	-305.02751	-704.40393	466.99425	1
31220	H	67.70500	58.60680	89.34890	-1414.74807	-1830.26332	2117.35498	1
31221	H	69.18300	58.07080	90.26390	2502.05510	-5.68622	1898.57766	1
31222	N	67.28600	57.24180	90.94090	-430.69230	-708.69100	-67.40659	1
31223	H	67.23400	57.85680	91.77790	-2219.73120	420.72136	-2198.05609	1
31224	H	66.34800	56.94180	90.60490	2021.39414	1909.25538	-1491.31008	1
31225	H	67.76700	56.37380	91.25190	2448.03777	-648.22734	1853.32923	1
31226	C	70.26400	57.65280	84.87290	236.26941	-459.35204	-744.57218	1
31227	O	70.14300	58.87780	84.98790	-356.80421	658.18359	-301.17114	1
31228	N	71.49100	57.15780	84.71690	518.07174	-562.02414	316.28834	1
31229	H	71.63100	56.17080	84.69590	185.23901	-1732.06224	-2615.47172	1
31230	C	72.71900	57.94580	84.52690	-337.34373	636.18588	572.81505	1
31231	H	72.79500	58.56780	85.40690	-1959.22187	2436.90067	-470.96786	1
31232	C	74.01800	57.10780	84.51390	-96.45379	870.78664	291.20709	1
31233	H	74.13900	56.57280	83.54790	1089.23736	-2271.00981	-1871.22637	1
31234	O	74.08600	56.29880	85.65490	-374.34694	-680.42335	74.43406	1
31235	H	73.52300	55.52680	85.55590	2448.24224	-854.16385	-1771.97509	1
31236	C	75.19200	58.07780	84.76890	13.39147	-896.06069	-70.82601	1
31237	H	75.21200	58.81580	83.93790	3111.80458	80.38320	-415.49933	1

31238	H	76.17100	57.55180	84.75690	2074.72611	-2314.16537	-394.14497	1
31239	H	75.14700	58.74180	85.65790	1237.08262	335.96853	-2880.31869	1
31240	C	72.59200	58.81480	83.22690	-338.08954	275.95471	-815.19353	1
31241	O	73.01500	59.98280	83.18890	-347.74758	-6.19117	-718.99275	1
31242	N	72.00200	58.27580	82.17390	259.77809	-459.44296	-651.00326	1
31243	H	71.78800	57.30480	82.23390	1705.69965	760.40282	-2536.40645	1
31244	C	71.67800	58.96180	80.92490	188.68936	-834.86403	-270.80221	1
31245	H	72.62500	59.27280	80.50790	155.20179	885.36507	3012.19707	1
31246	C	71.09500	58.12480	79.80190	-418.02311	-492.26086	-643.99885	1
31247	H	70.05700	57.80880	80.03990	-2615.96805	1057.25520	1417.37407	1
31248	O	71.89200	56.91180	79.71290	470.17444	472.14661	421.97851	1
31249	H	71.56000	56.30780	80.38190	-2288.67753	2143.44290	-427.89738	1
31250	C	71.17200	58.81080	78.46790	498.53515	35.91374	750.44180	1
31251	H	72.19700	59.09080	78.14290	1921.20142	935.64225	2299.66621	1
31252	H	70.51100	59.70180	78.53390	-418.22345	3076.71981	595.53554	1
31253	H	70.87600	58.20880	77.58290	625.70431	-1557.49038	-2654.62009	1
31254	C	70.83300	60.20580	81.08790	-918.33694	-20.49983	-53.56739	1
31255	O	71.24500	61.35880	80.80990	289.99198	-461.03849	549.36864	1
31256	N	69.70300	59.95480	81.76090	-234.26752	-399.91886	694.51236	1
31257	H	69.43500	59.01180	81.94290	-1323.88823	1585.85610	2383.56843	1
31258	C	68.79200	60.93480	82.26090	-463.43249	53.53286	-792.70592	1
31259	H	68.27700	61.41580	81.44290	-293.87437	1180.78567	2905.04607	1
31260	C	67.64800	60.18880	82.90290	563.08666	-666.29384	-202.98375	1
31261	H	68.05500	59.43180	83.60690	-1283.32056	2190.87023	1878.19507	1
31262	C	66.77000	61.10180	83.78390	320.24140	676.91186	-540.32976	1
31263	H	65.86900	60.56480	84.14890	2402.78114	659.90066	1916.64597	1
31264	H	66.36600	61.97780	83.23390	-1851.08608	2383.57328	-948.17905	1
31265	H	67.30500	61.44380	84.69590	-2713.25963	1618.64866	-17.34642	1
31266	C	66.87700	59.43380	81.79990	-560.51401	-563.11311	-438.83203	1
31267	H	65.98800	58.91880	82.22390	1813.71671	-2547.17633	48.64213	1
31268	H	67.56900	58.76680	81.24290	2697.23106	-1081.20019	-1173.54125	1
31269	H	66.48400	60.21480	81.11490	1602.34292	1.08580	-2704.94085	1
31270	C	69.33700	61.96280	83.14390	165.54098	765.31861	-494.35453	1
31271	O	69.12900	63.14880	82.91090	-223.49717	-630.31979	394.28326	1
31272	N	70.16800	61.60980	84.15190	633.84292	-164.26829	515.82374	1
31273	H	70.42600	60.68180	84.41090	568.38691	-1705.33365	2565.43209	1
31274	C	70.81100	62.52780	85.05990	760.73321	-73.60586	481.92853	1
31275	H	70.02500	63.10980	85.51790	-1694.56892	-1770.06366	-1967.71547	1
31276	C	71.57800	61.78180	86.15290	-651.18020	82.27751	633.50332	1
31277	H	72.12500	60.95180	85.65690	-2587.80426	1116.34809	-1425.45941	1
31278	C	72.63700	62.69880	86.91090	506.23517	469.27269	-610.24865	1
31279	H	73.14200	62.11380	87.70790	-1400.77029	-1319.08048	2476.71590	1
31280	H	72.14800	63.58180	87.37590	-38.61135	3132.54546	-424.52869	1
31281	H	73.44600	62.89480	86.17490	-1424.41073	-1969.17962	-1993.81563	1
31282	C	70.63500	61.17080	87.20590	549.30268	549.19340	484.78542	1
31283	H	69.64800	60.89180	86.77890	-1582.48943	155.82697	2713.60032	1
31284	H	70.45800	61.96580	87.96190	2865.09470	911.61742	926.31428	1
31285	C	71.26700	59.95680	87.91890	81.32966	-796.16304	-413.50580	1
31286	H	70.48700	59.54080	88.59190	-1874.30310	-1661.04469	-1899.78510	1
31287	H	71.59500	59.21580	87.15890	-1929.51089	-1964.88361	1502.38913	1
31288	H	72.13800	60.22880	88.55390	-2476.99964	-62.19251	1936.54988	1
31289	C	71.66200	63.52580	84.35490	433.09815	648.54612	-493.60999	1
31290	O	71.52800	64.71780	84.59990	-447.67249	-334.56918	546.56167	1
31291	N	72.44000	63.06280	83.35390	-630.22673	571.62328	-118.03636	1
31292	H	72.41000	62.08380	83.16990	380.04774	-120.74287	3113.06198	1
31293	C	73.23300	63.90780	82.52590	359.32087	-412.12577	711.62401	1
31294	H	73.88400	64.42880	83.21190	545.60071	1406.32718	2759.72780	1
31295	C	74.22100	63.07780	81.65290	-152.98946	822.80860	-402.19529	1
31296	H	73.76600	62.28180	81.02690	-2513.12318	2.41667	1895.62745	1
31297	H	74.79000	62.50380	82.41590	2266.37611	-1204.58231	1794.16722	1
31298	C	75.19500	63.90380	80.72890	-550.03691	277.64046	675.29730	1
31299	H	74.55500	64.48980	80.03390	-774.65357	2594.63550	1619.90184	1

31300	C	76.09000	64.93880	81.32490	7.79610	-865.02069	-253.73457	1
31301	H	76.90300	64.44380	81.89790	1433.53814	-2310.02993	1549.53710	1
31302	H	75.62900	65.65480	82.03890	-744.74182	2230.49658	2097.85945	1
31303	H	76.67100	65.48180	80.54890	-1955.38732	-2377.68225	612.04428	1
31304	C	76.03300	62.90280	79.89590	-467.16410	-241.92754	736.73913	1
31305	H	76.48300	62.22980	80.65690	2592.36487	1538.50228	-908.75151	1
31306	H	76.84200	63.38880	79.30890	1488.71062	-1384.41660	2379.18426	1
31307	H	75.43400	62.30680	79.17490	2292.67334	-2130.57819	-71.58612	1
31308	C	72.43700	64.90980	81.66490	-228.38908	793.62649	412.34875	1
31309	O	72.81300	66.08780	81.57690	-439.33607	-585.87523	-280.75605	1
31310	N	71.36300	64.44380	80.99590	-331.23550	588.57350	522.19765	1
31311	H	71.19000	63.46780	81.10790	1191.13640	1458.11238	2520.42360	1
31312	C	70.42600	65.14580	80.24290	-630.80304	572.14959	359.06557	1
31313	H	71.03900	65.71780	79.56190	-2620.33195	-1450.00801	-966.06586	1
31314	C	69.50000	64.18580	79.47790	240.46550	7.58707	872.97383	1
31315	H	69.27400	63.33580	80.15590	9.75357	1080.59325	-2964.70159	1
31316	C	68.14600	64.84580	79.02290	712.03032	-190.34641	-523.32757	1
31317	H	67.51200	65.16380	79.87790	853.49834	-3009.34848	19.43103	1
31318	H	67.58600	64.15180	78.35890	-531.44131	2601.29329	-1719.11584	1
31319	H	68.45800	65.75480	78.46590	-668.27309	-2840.05866	1137.98900	1
31320	C	70.28000	63.43880	78.39190	-480.05697	-664.59104	378.32640	1
31321	H	70.44600	64.25280	77.65390	-157.73796	2039.21158	-2409.32655	1
31322	H	71.27200	63.03780	78.69290	-1948.46169	2082.57639	-1370.20572	1
31323	C	69.41000	62.39680	77.58790	17.97162	633.58027	665.91545	1
31324	H	68.96100	61.73580	78.35990	-2876.85571	571.04586	-1174.31559	1
31325	H	68.57700	62.83380	76.99690	967.41308	-2587.86645	1466.18965	1
31326	H	70.16900	61.86880	76.97190	-1513.70893	-2062.34964	-1827.05490	1
31327	C	69.70600	66.19980	80.98090	609.44405	-16.70266	-676.33114	1
31328	O	69.55800	67.36380	80.51690	438.77225	332.68944	566.19575	1
31329	N	69.14000	65.92480	82.22190	-565.76354	591.92886	254.63166	1
31330	H	69.22700	64.99080	82.55990	-2549.24282	-1668.76624	-772.17108	1
31331	C	68.75000	66.92180	83.19690	-553.61802	-541.41727	464.20669	1
31332	H	67.89500	67.41080	82.75390	-1207.12397	2125.27722	1997.96481	1
31333	C	68.34200	66.10180	84.47590	402.52788	-473.01077	649.93089	1
31334	H	68.06800	66.67780	85.38590	740.44075	-734.58255	-2966.71049	1
31335	H	69.24300	65.50480	84.73090	-2013.93705	-2057.91216	-1252.22635	1
31336	C	67.11800	65.15880	84.29590	-85.38393	-56.49113	-908.01565	1
31337	H	67.27600	64.54180	83.38490	-1075.94941	-2547.17962	-1478.83350	1
31338	C	67.17400	64.17980	85.52090	459.20280	-496.71331	-597.30686	1
31339	H	66.20600	63.64480	85.41390	2395.00573	1946.76772	-648.69311	1
31340	H	67.27400	64.75380	86.46590	-2870.93117	1261.97904	-352.99990	1
31341	H	68.06800	63.52580	85.43190	1292.24114	-769.86283	-2760.09977	1
31342	C	65.84000	65.91780	84.21390	866.54356	285.91912	-36.82296	1
31343	H	65.86700	66.56680	83.31290	2133.65322	-2052.04823	-1024.07491	1
31344	H	64.97100	65.22780	84.18490	2226.75670	-807.22742	-2060.41636	1
31345	H	65.68500	66.60280	85.07490	-1730.81883	-1786.23667	-1915.17407	1
31346	C	69.78900	67.93480	83.58990	-670.29428	606.73022	-198.57677	1
31347	O	69.52000	69.15080	83.59590	-330.35070	-484.44824	511.96013	1
31348	N	71.02500	67.45980	83.92190	-672.07486	467.28127	-253.14828	1
31349	H	71.29900	66.50280	83.86090	1262.67184	2420.98017	1577.21136	1
31350	C	72.04000	68.25880	84.44690	12.43229	436.79660	802.22291	1
31351	H	71.72900	68.65180	85.40390	-1704.57396	703.69995	2548.85363	1
31352	C	73.35000	67.44380	84.73490	-747.73798	-353.11062	370.24127	1
31353	H	74.10400	68.14980	85.14490	2986.32226	-683.18089	-699.23303	1
31354	H	73.20500	66.70780	85.55390	-706.77341	-2766.60467	1285.57814	1
31355	H	73.77200	66.98480	83.81490	2024.47140	-2202.73769	925.57183	1
31356	C	72.37500	69.33780	83.44090	-765.66384	-320.73747	-377.15137	1
31357	O	72.35400	70.52480	83.71590	532.53290	482.23522	338.36670	1
31358	N	72.52600	68.93380	82.15690	563.58768	-239.07913	564.69716	1
31359	H	72.48400	67.96680	81.91890	-315.95855	2492.69341	-1919.41216	1
31360	C	72.88600	69.73780	81.06290	277.12442	543.30803	-693.69608	1
31361	H	73.82700	70.20980	81.30690	-2880.59642	114.57366	-1277.81272	1

31362	C	73.15900	68.74380	79.88290	32.83451	918.25919	-120.50754	1
31363	H	72.24600	68.13780	79.70290	1997.62239	-771.53614	-2300.52515	1
31364	H	74.00200	68.08380	80.18090	-1463.26959	2603.11290	-1042.05540	1
31365	C	73.42400	69.35880	78.57890	801.24182	-407.45830	-41.64441	1
31366	C	74.73300	69.62180	78.20490	-893.76734	-158.74988	113.04118	1
31367	H	75.61300	69.41980	78.79790	508.12037	-2644.52821	1594.56967	1
31368	C	74.94800	70.16980	76.88990	499.63427	-134.24659	735.65698	1
31369	H	75.94500	70.40780	76.54990	-2064.62344	-749.49095	-2263.14144	1
31370	C	73.86900	70.43680	76.05490	-122.77894	-889.51032	-45.25455	1
31371	H	74.11800	70.79380	75.06590	-818.27239	2974.54039	-698.61427	1
31372	C	72.34100	69.62080	77.69590	-644.31167	12.26689	-658.08431	1
31373	H	71.31700	69.47980	78.01090	-920.47589	1701.27694	2488.71758	1
31374	C	72.56000	70.16080	76.43590	-555.43417	-645.96479	-313.91624	1
31375	H	71.70500	70.39580	75.81990	-2806.04596	438.92204	1368.67329	1
31376	C	71.85900	70.76280	80.73490	357.47623	-591.49051	-582.55264	1
31377	O	72.02600	71.98080	80.52490	247.04441	306.66018	683.73221	1
31378	N	70.56600	70.38080	80.67190	-579.58300	555.09696	-306.25047	1
31379	H	70.32800	69.41380	80.71090	1724.56623	2064.28517	-1650.72139	1
31380	C	69.44000	71.27380	80.50690	-835.47490	363.24477	-145.73606	1
31381	H	69.51600	71.89380	79.62590	-667.81711	-2403.13040	-1903.30049	1
31382	C	68.15900	70.43480	80.33790	502.38067	-163.76607	732.76827	1
31383	H	67.91400	69.83780	81.24290	-1466.97467	1442.45039	2389.77435	1
31384	H	68.37400	69.74180	79.49790	1816.99145	2245.60061	-1270.89991	1
31385	C	66.92100	71.17580	80.05790	-388.30195	-211.04770	-797.61654	1
31386	C	66.57200	71.44880	78.74590	-800.97779	459.52047	-55.84648	1
31387	H	67.31800	71.24980	77.98990	976.21728	1501.73331	2591.24119	1
31388	C	65.36200	72.05980	78.40290	-430.08116	577.60408	-582.32322	1
31389	H	65.06300	72.19480	77.37390	2875.39118	195.48732	1249.35418	1
31390	C	64.52500	72.43380	79.47390	282.46755	-504.53673	689.22144	1
31391	H	63.62600	73.01480	79.32790	-1616.90722	2089.60760	1734.11455	1
31392	C	66.02700	71.52980	81.08290	-420.82839	-430.47024	674.34376	1
31393	H	66.30100	71.35380	82.11290	-3038.49173	-800.74578	-132.08106	1
31394	C	64.89600	72.27080	80.79890	302.99812	579.14794	-650.73816	1
31395	H	64.14400	72.56780	81.51590	2264.12189	-325.04421	-2154.56069	1
31396	C	69.33500	72.26180	81.71990	784.36846	-86.35741	-452.03588	1
31397	O	69.08000	73.41680	81.52690	-375.40931	710.57247	44.89953	1
31398	N	69.63000	71.85980	82.96790	430.51046	-309.71384	643.31998	1
31399	H	69.70200	70.91080	83.26390	-1653.43755	-2656.48475	-185.58233	1
31400	C	69.74000	72.75980	84.02890	-877.00498	-101.46859	-230.38724	1
31401	H	68.80600	73.27580	84.19490	2216.93574	-1048.37009	1957.40170	1
31402	C	69.97200	71.99480	85.34890	-256.68655	537.20000	698.34506	1
31403	H	69.16700	71.24180	85.48590	1965.99118	1806.79777	-1683.51843	1
31404	H	70.95100	71.47480	85.41890	-259.22305	-3117.30883	-145.02417	1
31405	H	69.93600	72.73580	86.17590	-1650.29581	1803.93136	1989.73347	1
31406	C	70.81600	73.85580	83.78590	298.76513	629.84865	598.18438	1
31407	O	70.62400	75.02280	84.15090	-635.58151	-316.69472	-336.46006	1
31408	N	71.92800	73.46580	83.15890	218.04791	703.11088	-442.17699	1
31409	H	71.88900	72.59580	82.67490	-2321.00498	-1305.31715	-1672.86931	1
31410	C	73.00100	74.43080	82.80690	-57.87176	520.25350	-762.85840	1
31411	H	73.28100	74.87180	83.75190	559.57370	-245.86955	3078.40568	1
31412	C	74.19600	73.61780	82.23390	-180.62038	-412.71455	-793.04761	1
31413	H	74.96200	74.36980	81.94790	-92.60874	2314.60638	-2151.29943	1
31414	H	73.88900	73.19180	81.25490	-2499.72676	295.77553	-1900.56076	1
31415	S	74.87400	72.35080	83.38990	-393.14838	317.72489	-264.02820	1
31416	H	73.67600	71.91480	83.75190	2083.06396	-1789.53470	1509.03166	1
31417	C	72.62400	75.52980	81.86190	-617.84828	173.24234	647.19353	1
31418	O	72.81800	76.70480	82.13490	781.56233	-89.85070	6.95825	1
31419	N	71.91800	75.07780	80.72890	-225.81996	-514.55267	-624.13715	1
31420	H	71.92300	74.09580	80.55290	-2081.92484	-2329.56053	-289.94296	1
31421	C	71.54200	75.91280	79.63390	157.63009	299.97890	-856.44699	1
31422	H	72.31800	76.64380	79.46390	684.95589	2652.23441	1565.41695	1
31423	C	71.62200	74.98880	78.37290	-19.16385	-529.40110	-736.68663	1

31424	H	71.04500	75.42080	77.52690	542.31705	807.83626	2990.15788	1
31425	H	71.17500	73.99780	78.60090	1743.14932	-1652.35186	-2020.80999	1
31426	C	73.02200	74.78780	77.81290	62.58778	615.10980	676.46516	1
31427	C	73.70700	73.56580	77.87990	102.95425	676.54772	-624.14077	1
31428	H	73.23900	72.61380	78.08190	2247.06995	613.44003	2106.65650	1
31429	N	74.94100	73.72080	77.23790	658.84956	-421.62577	-293.43646	1
31430	H	75.57100	73.04880	76.91690	-2964.86390	-141.12964	-1066.19624	1
31431	C	75.03800	74.99780	76.86390	313.02434	-434.81760	719.63690	1
31432	C	73.88500	75.72880	77.20590	96.54637	-651.89619	-621.29519	1
31433	C	73.84600	77.15180	77.05090	597.78559	-444.76835	501.44887	1
31434	H	72.96800	77.73480	77.28890	-106.15578	3153.18740	185.43200	1
31435	C	74.99200	77.74080	76.45190	-389.32920	-643.44825	-508.91990	1
31436	H	74.97600	78.77380	76.13690	2073.48938	2376.23190	-16.63443	1
31437	C	76.13500	75.64780	76.26290	268.53610	378.30524	-797.76300	1
31438	H	77.00800	75.08280	75.96990	-1850.26531	-2067.97765	-1480.68584	1
31439	C	76.07400	77.02980	76.04390	260.67958	727.98424	491.87405	1
31440	H	76.95300	77.55880	75.70590	-2232.72839	1253.98075	-1851.49928	1
31441	C	70.21200	76.64580	79.76090	-793.79920	362.07573	288.10053	1
31442	O	70.11700	77.79280	79.22390	-400.33409	-234.68761	630.33244	1
31443	N	69.22300	76.15280	80.47990	-741.24064	408.51973	109.03059	1
31444	H	69.32500	75.27080	80.93290	-2385.54794	1979.04484	600.54779	1
31445	C	67.91700	76.79680	80.50690	-231.13086	-596.11514	632.51680	1
31446	H	67.50100	76.72480	79.51290	-2655.31807	603.14613	1584.40399	1
31447	C	67.04200	75.89380	81.32190	251.15121	-851.57276	-117.57591	1
31448	H	67.50300	75.63980	82.29990	1793.07574	-2427.22213	-842.71781	1
31449	H	67.00500	74.91080	80.80590	2389.90531	1507.23530	1394.91777	1
31450	C	65.64000	76.49380	81.61290	-713.56904	-478.64209	278.67245	1
31451	H	65.63400	77.50380	82.07590	-2855.88053	-375.62249	1260.57118	1
31452	C	64.73900	76.55180	80.32490	-188.03501	-374.37223	801.20039	1
31453	H	64.91700	75.65380	79.69490	2028.43009	-614.25876	2316.71116	1
31454	H	63.67100	76.57880	80.62790	-3053.05262	-742.70670	-106.29386	1
31455	H	64.89500	77.50380	79.77390	1266.09974	2163.19243	1919.10210	1
31456	C	64.90600	75.60280	82.61490	216.67778	499.21087	-743.93632	1
31457	H	65.60700	75.23780	83.39590	-1777.79673	1915.29319	1770.16835	1
31458	H	64.05500	76.15680	83.06690	1741.64802	-1235.95433	-2300.37142	1
31459	H	64.60100	74.61180	82.21590	1327.16901	-1905.20148	2104.93001	1
31460	C	67.88300	78.25880	80.97990	-723.03635	-403.94230	-368.47583	1
31461	O	67.19700	79.02380	80.29190	490.49678	489.81545	395.05214	1
31462	N	68.52100	78.78280	82.02490	-51.00370	850.01217	-125.09241	1
31463	C	69.31500	77.97980	82.97190	-774.98949	303.99729	380.77407	1
31464	H	68.96900	76.92580	83.03290	-430.94449	2339.22249	-2080.93609	1
31465	H	70.36000	78.03480	82.59890	-123.97192	-1695.74135	2632.73939	1
31466	C	68.47200	80.19080	82.39590	124.12718	-830.68618	-317.69041	1
31467	H	67.44000	80.42380	82.61490	-717.34741	-2300.81640	-2005.48565	1
31468	C	69.25900	80.17180	83.75390	-398.81389	606.00355	-572.00732	1
31469	H	68.88300	80.87580	84.52690	2878.28708	1229.05862	389.68089	1
31470	H	70.32300	80.40280	83.53390	1019.51249	2847.17474	-922.30550	1
31471	C	69.11600	78.74880	84.28590	827.29239	216.53143	326.01775	1
31472	H	69.94800	78.54280	84.99390	2721.75151	1591.02068	-132.11337	1
31473	H	68.10900	78.61380	84.73490	1976.91370	-1664.03139	1778.07679	1
31474	C	69.05500	81.12380	81.23090	627.35823	137.76917	647.00122	1
31475	O	68.57200	82.24780	81.04590	358.60191	685.68790	213.93279	1
31476	N	70.09900	80.67380	80.54090	-758.54922	-222.16292	281.43613	1
31477	H	70.39500	79.77580	80.85690	1830.71236	-1962.83504	-1626.27660	1
31478	C	70.60700	81.42980	79.40390	-216.14869	892.11939	124.28559	1
31479	H	70.77000	82.44380	79.73990	-1947.02819	-2346.87360	722.46979	1
31480	C	71.94100	80.76680	78.92290	437.53371	-724.08528	-309.56210	1
31481	H	71.86800	79.65880	78.87490	1431.06348	880.47266	-2669.08597	1
31482	H	72.71000	80.96280	79.70090	2496.92114	-1113.73247	1538.61149	1
31483	C	72.44600	81.21980	77.54890	549.14423	378.40562	-634.30371	1
31484	C	73.03200	82.49780	77.40790	124.14458	901.52227	-175.76119	1
31485	H	73.19700	83.12680	78.26990	2996.71480	-915.48562	-222.52130	1

31486	C	73.38000	82.91680	76.12890	-271.18549	701.42316	529.72930	1
31487	H	73.80300	83.90780	76.04790	284.63446	3059.16730	731.31612	1
31488	C	73.21100	82.08580	74.99290	-488.08263	-734.75426	181.82229	1
31489	O	73.66500	82.54480	73.75290	654.25750	-299.98294	-308.36401	1
31490	H	74.19700	83.33680	73.85990	-745.10778	2296.60879	2027.70026	1
31491	C	72.14500	80.45680	76.39290	-383.77614	-813.73955	-15.09869	1
31492	H	71.53000	79.57280	76.46990	-241.12036	-3097.26757	-398.45299	1
31493	C	72.59800	80.86680	75.14790	356.78016	-768.32861	-302.52187	1
31494	H	72.46700	80.20280	74.30690	2564.69602	-1617.25684	-800.64563	1
31495	C	69.60500	81.53480	78.26890	-280.25997	-719.02867	458.51051	1
31496	O	69.34000	82.63880	77.79490	696.42522	-320.44226	148.77178	1
31497	N	68.89900	80.39980	77.87590	715.42311	457.95506	43.41310	1
31498	H	69.15900	79.51980	78.26490	-1645.16304	-1998.49012	-1776.06391	1
31499	C	67.79400	80.35980	76.99690	791.33307	-82.05283	-439.38412	1
31500	H	68.02800	80.90180	76.09190	-813.16134	-1663.76118	-2536.38936	1
31501	C	67.37900	78.88380	76.66290	780.46474	168.88061	-441.99988	1
31502	H	67.35800	78.20080	77.53890	2469.71493	1484.61943	1272.97895	1
31503	H	66.31400	78.74980	76.37590	1801.83009	-957.56360	-2386.42008	1
31504	C	68.31100	78.32080	75.65290	-703.33047	516.66188	-308.45368	1
31505	C	68.11000	78.68280	74.28590	535.18122	557.29054	-499.72951	1
31506	H	67.23800	79.29980	74.12290	1010.96966	2099.20255	2125.93660	1
31507	C	68.99100	78.15880	73.25190	205.61353	-673.85665	553.40970	1
31508	H	68.92600	78.57780	72.25790	-1778.45392	-156.57054	2590.69908	1
31509	C	69.92600	77.15880	73.58790	-494.68005	127.30862	757.89504	1
31510	O	70.77300	76.70680	72.57590	617.45862	271.70118	-414.11308	1
31511	H	70.57700	77.24380	71.80390	-2377.46271	-1718.74210	1124.19934	1
31512	C	69.24800	77.30080	75.92290	394.97580	-430.87512	683.06177	1
31513	H	69.32500	76.81380	76.88390	2434.15303	2000.79207	-112.32641	1
31514	C	70.03300	76.73280	74.90990	269.00673	497.58553	-728.01785	1
31515	H	70.81500	76.02580	75.14390	1692.21359	2152.35017	1559.82241	1
31516	C	66.60900	81.16880	77.39390	-506.02908	552.16197	538.09591	1
31517	O	66.03000	81.91280	76.59390	-558.37943	-13.68226	-561.68809	1
31518	N	66.26200	81.14380	78.69490	-425.49705	477.98080	-567.92652	1
31519	H	66.72900	80.59280	79.38290	230.20985	-403.19818	-3111.32313	1
31520	C	65.22400	82.07880	79.20490	672.13341	-596.48050	-38.30277	1
31521	H	64.38800	81.88480	78.54990	-2064.80697	-1499.25703	-1827.54522	1
31522	C	64.68300	81.72780	80.60790	-832.24211	-26.10682	-370.78028	1
31523	H	65.60700	81.77480	81.22190	-1924.78910	1295.93246	2133.62466	1
31524	C	63.60600	82.80080	81.01090	505.97853	-379.22181	646.76423	1
31525	H	62.70300	82.86080	80.36690	-2006.84411	1146.51157	2144.99676	1
31526	H	63.25600	82.57980	82.04190	-2205.28657	-808.93042	2084.91315	1
31527	H	64.00900	83.83280	81.09290	-2809.39016	-717.57938	-1207.67864	1
31528	C	64.11400	80.29080	80.63890	611.92131	-575.54380	322.05916	1
31529	H	63.25500	80.13980	79.95190	2848.42307	614.97284	-1192.24904	1
31530	H	64.84000	79.61680	80.13490	-1851.03172	-2525.49661	-92.79165	1
31531	C	63.65900	79.83980	81.99690	532.39334	467.27198	-588.51413	1
31532	H	64.50200	79.89380	82.71890	2477.45324	-638.92472	-1825.89696	1
31533	H	63.43900	78.75180	81.95090	2383.03292	-165.25254	2045.56481	1
31534	H	62.80200	80.44580	82.35890	-733.46924	2945.38466	890.98692	1
31535	C	65.58000	83.61280	79.03390	-662.79844	-172.43368	596.00965	1
31536	O	64.77400	84.26080	78.37690	-449.09827	-82.16803	641.63233	1
31537	N	66.82900	84.06580	79.36490	-665.10694	239.64552	-471.68300	1
31538	H	67.45400	83.43180	79.81190	-2950.45726	-158.64659	1075.51871	1
31539	C	67.35028	85.39288	78.99975	259.20971	-642.76209	-282.71824	1
31540	H	66.77772	86.09561	79.60210	-1145.66105	-2906.75558	430.55774	1
31541	H	68.32927	85.16951	79.41645	-4440.90256	1430.59232	17.61092	1
31542	C	67.17880	85.63700	77.39992	-559.77246	-75.08083	611.46897	1
31543	O	66.42490	86.55492	77.03091	-13.08464	-528.00028	15.41130	1
31544	N	67.89100	84.89680	76.61290	355.29207	-646.66215	378.79087	1
31545	H	68.32900	84.14080	77.09390	886.72332	2678.80411	1418.76538	1
31546	C	67.85906	85.11249	75.16956	-563.73661	-459.73046	-35.26336	1
31547	H	68.33463	86.09061	75.01846	2896.54751	771.48897	-294.96595	1

31548	C	68.53600	83.92580	74.53290	-680.10604	-528.86219	-278.59119	1
31549	H	68.10500	82.98380	74.93690	-1569.82377	1834.36220	-2037.51178	1
31550	C	68.34900	83.93880	73.05490	-864.01320	304.02665	94.52486	1
31551	H	67.38300	83.53880	72.67890	554.86548	-3017.46245	612.11592	1
31552	H	68.68700	84.91880	72.65490	-2383.28337	1931.22675	752.53396	1
31553	H	69.02400	83.17980	72.60690	2568.34315	-607.25331	-1702.94691	1
31554	C	70.05800	83.94780	74.75490	-862.52604	31.12835	300.11181	1
31555	H	70.56200	83.01280	74.42890	-560.71396	2807.08195	1335.57787	1
31556	H	70.17300	83.76380	75.84390	1855.98036	1329.09483	-2176.63031	1
31557	C	70.86484	85.26118	74.39269	72.40894	503.49921	299.52093	1
31558	H	71.89487	85.30510	74.82148	-3303.78711	-608.71499	-3240.51170	1
31559	H	71.03246	85.39880	73.28193	1811.51702	-859.75277	3074.98940	1
31560	H	70.31850	86.20381	74.65225	34.79385	-57.99502	1007.48822	1
31561	C	66.28702	85.17255	74.58047	126.40894	1044.49645	-390.12336	1
31562	O	66.14558	85.83309	73.56797	165.07395	-101.90621	-9.64118	1
31563	N	65.47600	84.30180	75.09290	-417.80420	452.90614	-593.40036	1
31564	H	65.70400	83.60980	75.77290	-79.53137	-2414.24015	1993.47948	1
31565	C	64.05600	84.33580	74.67990	-313.54905	240.74974	-828.01889	1
31566	H	64.10600	84.16680	73.61490	-2583.92182	-1195.73997	-1329.41192	1
31567	C	63.18100	83.19080	75.19690	301.66284	-464.32204	711.36455	1
31568	H	62.22600	83.07180	74.64190	2743.92000	673.15508	1387.46085	1
31569	H	63.77500	82.27180	75.00590	520.71776	-1964.05298	-2386.06880	1
31570	O	62.80900	83.14980	76.55590	287.05027	178.05286	718.03026	1
31571	H	63.47300	83.61580	77.06990	2994.07496	50.58203	-960.33486	1
31572	C	63.31365	85.70988	75.19063	636.41923	225.63096	-712.60210	1
31573	O	62.32744	86.05758	74.58666	520.22286	170.11512	554.08920	1
31574	N	63.75120	86.06094	76.37257	-331.25846	669.18827	1040.01239	1
31575	H	64.55552	85.70538	76.92189	-1154.00041	-2200.40268	1245.14875	1
31576	C	63.38499	87.40821	76.78136	-278.36167	-23.91564	136.51349	1
31577	H	62.25573	87.35633	76.62901	996.56771	-256.30247	1729.12423	1
31578	C	63.92628	87.86305	78.18424	304.66963	-78.17432	-423.04538	1
31579	H	64.80036	87.29168	78.48415	3066.99945	-1191.81624	2321.62682	1
31580	C	64.11317	89.39956	78.42001	-12.47377	884.65162	497.66199	1
31581	H	64.49017	89.53435	79.46032	-101.88112	-1926.81792	886.87980	1
31582	H	63.18934	90.01294	78.35143	3259.19906	2132.14930	1232.76810	1
31583	H	64.88240	89.82599	77.72918	1457.52903	1349.79803	-666.15191	1
31584	C	62.75039	87.52143	79.24090	74.03162	60.41693	-805.83190	1
31585	H	61.87676	88.12716	79.00066	2167.20043	-974.60335	337.13197	1
31586	H	63.17596	87.79666	80.23874	-1180.49980	-165.25884	2015.24196	1
31587	C	62.44673	85.99018	79.14696	-144.68837	-798.79927	345.02784	1
31588	H	62.85170	85.55041	78.20294	2366.99118	3.26062	-1229.27061	1
31589	H	62.84107	85.45865	80.02264	1168.00212	-2540.41097	4774.61604	1
31590	H	61.35255	85.85505	78.92380	137.72247	-338.86348	249.93499	1
31591	C	63.91985	88.45525	75.66477	422.03400	-417.95057	464.63180	1
31592	O	63.25585	89.43078	75.41870	270.24386	1354.53565	-803.73223	1
31593	N	65.18352	88.19035	75.34546	383.36850	-533.35927	-242.76121	1
31594	H	65.69234	87.32942	75.73968	-1534.44320	-846.14643	-1224.64053	1
31595	C	65.90496	89.02341	74.41060	193.31727	-874.99058	-438.54441	1
31596	H	65.79992	90.08294	74.68576	-3290.57352	-1816.96472	1402.08841	1
31597	C	67.36743	88.55004	74.57693	677.56103	886.80517	369.63244	1
31598	H	67.60727	87.57846	74.02054	2144.75953	-1890.60809	527.69188	1
31599	H	67.49592	88.35087	75.67447	-390.87266	-4108.00079	-3098.87739	1
31600	C	68.56509	89.60491	74.19674	1123.55094	-436.48860	-79.77485	1
31601	O	69.00614	90.34926	75.13138	-272.89366	-432.82910	-528.90535	1
31602	O	69.08956	89.57797	73.05589	-393.15353	-516.17632	729.40503	1
31603	C	65.42558	88.90846	72.87046	-90.17122	-1260.60797	-21.98268	1
31604	O	65.70062	89.79728	72.04464	-725.71047	47.23064	64.42990	1
31605	N	64.85673	87.75816	72.56593	303.06223	-1125.78335	-306.46914	1
31606	H	64.79768	86.97118	73.22603	1669.96395	-2275.21755	-24.27306	1
31607	C	64.23810	87.76581	71.30825	-15.33425	-384.13754	493.62324	1
31608	H	64.74802	88.54828	70.70285	2512.97515	1619.59956	-2305.62682	1
31609	C	64.45328	86.30629	70.71298	-217.30989	-284.32519	-499.16699	1

31610	H	64.16654	85.53689	71.48312	108.98209	380.21548	482.28804	1
31611	H	63.80393	86.11353	69.80306	-1885.02464	520.35203	2704.24978	1
31612	O	65.92711	85.86875	70.64688	-203.16297	-980.59448	-107.43401	1
31613	H	66.13658	86.04259	71.59922	-3394.35511	-1063.90782	479.71471	1
31614	C	62.65047	88.14880	71.32520	215.57942	1020.27344	-477.41140	1
31615	O	62.08148	88.53732	70.32745	49.08693	313.88435	9.01721	1
31616	N	62.12919	88.09645	72.53803	595.25938	55.33551	-197.30929	1
31617	H	62.70860	87.66916	73.29659	-79.53403	-2137.63292	247.67776	1
31618	C	60.99300	88.97827	72.80795	-858.42677	-433.51551	-12.48697	1
31619	H	60.56228	88.61775	71.78299	-37.37306	-4251.48901	166.00852	1
31620	C	60.07945	88.52991	73.99627	637.43992	913.07155	344.46439	1
31621	H	59.08867	89.00618	73.81295	3515.88102	-616.83262	-1307.13838	1
31622	H	60.40331	88.97578	75.00209	-2769.44495	448.89870	-2929.35048	1
31623	C	59.80520	87.02140	74.04454	591.10317	489.54993	594.88080	1
31624	C	59.53191	86.24798	72.93565	-806.27782	478.58030	-1250.79810	1
31625	H	59.54106	86.70471	71.91584	-1169.23165	2357.37624	-1360.25097	1
31626	C	59.30100	84.85880	73.12290	21.54127	-598.25087	672.62821	1
31627	H	59.12100	84.20580	72.28090	1149.65641	2444.99098	1642.34120	1
31628	C	59.18800	84.30980	74.35190	547.62902	-513.43839	496.35454	1
31629	H	59.20900	83.23180	74.40590	-124.30327	-1393.97784	-2804.72221	1
31630	C	59.72903	86.47369	75.35581	517.06002	-376.43567	-627.79132	1
31631	H	59.97548	87.13537	76.20894	12.87989	776.82504	794.32489	1
31632	C	59.37000	85.13050	75.50108	104.41893	1037.27002	755.41193	1
31633	H	59.40800	84.60080	76.43090	498.10339	3094.15833	448.38382	1
31634	C	61.26294	90.52947	72.54647	22.60353	-292.12320	246.74294	1
31635	O	60.40898	91.43826	72.46970	-81.28272	534.84324	264.98421	1
31636	N	62.56698	90.74744	72.45073	-635.76453	190.56514	438.41106	1
31637	H	63.12452	89.91855	72.57686	-1954.76634	-1237.96537	1596.49702	1
31638	C	63.17045	91.97482	72.10388	218.83385	-274.04772	372.11157	1
31639	H	62.33615	92.72415	72.16788	-2798.41208	-2660.55969	-2609.08507	1
31640	C	64.33506	92.39762	73.08343	7.75344	-572.07179	-11.09079	1
31641	H	65.26187	91.97641	72.74510	-3140.57843	2528.14984	63.34382	1
31642	C	64.34487	93.99806	72.94220	356.60840	-316.13878	48.68205	1
31643	H	65.29222	94.46286	73.41059	1894.65113	-585.20359	-2318.16978	1
31644	H	64.26475	94.17630	71.88670	-192.70209	216.43808	-4486.40382	1
31645	H	63.51507	94.53959	73.45999	-2474.18383	-669.48739	-131.07898	1
31646	C	64.18884	91.99713	74.54338	1411.15931	150.89091	-186.58589	1
31647	H	64.23508	90.89610	74.71966	1175.82315	-58.47602	-1595.34535	1
31648	H	63.17518	92.34803	74.97427	-1595.04566	-741.45477	-471.57558	1
31649	C	65.37377	92.55723	75.39536	-442.89323	-442.65557	262.34232	1
31650	H	65.17488	92.48438	76.50839	2004.66736	-2284.97097	809.65113	1
31651	H	65.51346	93.68880	75.17294	-4.21681	3061.06483	3952.42087	1
31652	H	66.30495	92.00452	75.14545	-722.35907	-1359.35502	-2426.55308	1
31653	C	63.98325	92.01945	70.64308	-695.01178	-71.93545	-318.27274	1
31654	O	64.24358	93.11437	70.21238	973.58341	-128.48499	173.30730	1
31655	N	64.26577	90.81221	70.16434	-26.77037	80.78728	-550.40893	1
31656	H	64.09213	90.03879	70.78291	-2022.07043	458.34416	714.02263	1
31657	C	65.00578	90.78460	68.96435	178.90929	-35.45480	-153.19219	1
31658	H	65.45449	91.78757	69.03074	4834.00885	-94.84376	120.51295	1
31659	C	66.01031	89.53032	68.89951	-243.22064	890.39910	-518.57064	1
31660	H	65.49993	88.63416	68.45239	456.03286	47.63017	-3353.48534	1
31661	H	66.37855	89.20078	69.94249	2014.24530	2715.53811	485.53052	1
31662	C	67.18461	89.74020	67.99786	-468.41156	25.87698	-210.08086	1
31663	H	67.86993	90.47659	68.53077	957.17265	-1394.76118	-609.55881	1
31664	C	67.91479	88.43822	67.67358	-12.99497	-994.28457	416.23709	1
31665	H	68.63650	88.17521	68.57099	-2622.16488	-1740.97250	772.28123	1
31666	H	68.52783	88.41760	66.79088	-894.66762	-551.90688	1454.72965	1
31667	H	67.23412	87.60363	67.56874	-2641.62086	-1604.81414	974.49845	1
31668	C	66.74629	90.39935	66.69630	-199.41051	338.66657	150.11782	1
31669	H	66.18390	91.41634	66.72902	2339.21238	1283.40021	1996.88156	1
31670	H	67.64784	90.61119	66.21159	595.42049	-3160.76188	-112.58906	1
31671	H	66.15122	89.66405	66.01836	499.75933	4137.94545	-2761.94937	1

31672	C	63.86432	90.69255	67.80072	109.95291	-243.52605	239.60321	1
31673	O	63.96447	91.45239	66.85430	-347.90203	-662.10801	590.24893	1
31674	N	62.87761	89.84307	68.03317	114.29220	-227.44340	-458.89327	1
31675	H	62.64252	89.25650	68.84570	-1155.03863	-983.34974	644.92149	1
31676	C	61.82833	89.98457	67.02507	58.78319	312.26360	-566.56609	1
31677	H	62.36924	90.17120	66.05038	1353.04465	255.37544	1281.71865	1
31678	C	61.09980	88.56602	67.07241	208.72210	76.76030	-763.89428	1
31679	H	60.60793	88.48454	68.07742	-2317.86438	-261.37283	1228.87585	1
31680	H	61.88897	87.76594	67.02650	-37.48394	-979.11177	-1455.11873	1
31681	C	60.13386	88.23175	65.95114	-120.36327	-304.82985	384.98780	1
31682	H	60.66071	88.40843	64.97740	799.03338	-295.95692	-539.28412	1
31683	C	59.71619	86.77289	66.00256	1100.27025	707.04488	19.59146	1
31684	H	59.35941	86.45102	67.01401	-2402.68129	-231.95073	-1277.72158	1
31685	H	60.59765	86.05617	65.72905	-691.12313	-1723.13317	2100.41084	1
31686	H	58.98783	86.64220	65.26931	582.52860	-1315.35065	101.73990	1
31687	C	58.87488	89.06661	66.10870	-68.37617	-301.73411	-300.73235	1
31688	H	59.00912	90.12422	65.81222	-1024.29083	1108.52651	1695.88936	1
31689	H	58.01647	88.67888	65.48013	2276.79130	-1999.70726	-1431.16709	1
31690	H	58.57500	89.04804	67.22311	-779.65128	6.28594	582.07706	1
31691	C	60.89839	91.22236	67.39314	480.64314	858.42280	-468.39178	1
31692	O	60.15719	91.67618	66.54646	284.31400	-694.46904	702.24976	1
31693	N	61.10528	91.70190	68.64121	-418.03036	1074.17805	-314.35729	1
31694	H	61.80563	91.16771	69.09353	-428.95732	879.43722	-1019.52478	1
31695	C	61.23501	93.11801	68.89403	-1352.65635	-414.55781	833.47803	1
31696	H	61.90364	93.12008	69.76239	-185.26446	-1723.00729	515.44149	1
31697	C	61.78020	93.81238	67.61063	519.69290	-36.02981	-477.10368	1
31698	H	62.35264	93.07851	66.98272	-996.70680	498.43075	-2070.64331	1
31699	H	60.88214	94.06817	66.94340	-1400.77745	874.72162	-347.86397	1
31700	C	62.65985	95.02064	68.14391	-837.71447	236.71694	97.59893	1
31701	H	63.46533	94.59084	68.75861	-919.57894	499.29983	164.69748	1
31702	H	62.05903	95.80318	68.60093	3550.17842	1263.81311	-993.55236	1
31703	C	63.16478	95.74832	66.87895	394.63976	75.60415	503.28705	1
31704	O	62.31644	95.67266	65.77683	542.75419	-50.48204	-412.25143	1
31705	O	64.26992	96.25399	66.79930	300.01695	671.11713	-819.23067	1
31706	C	59.72286	93.68254	69.22343	141.02486	-438.21293	-1175.18830	1
31707	O	59.03792	94.27500	68.36901	222.87867	72.88133	309.23327	1
31708	N	59.32852	93.33975	70.43663	-285.70092	414.97017	-372.71210	1
31709	H	60.07260	92.89939	70.99237	492.50486	-2272.75291	656.65898	1
31710	C	58.03981	93.79089	70.85300	-273.05913	182.49901	-629.48639	1
31711	H	57.55441	94.38308	70.08783	4323.57141	2926.27380	934.60345	1
31712	C	57.04612	92.63245	71.30789	-33.28341	-641.27390	140.25604	1
31713	H	57.25443	92.50243	72.37684	-2813.70140	637.63799	595.64364	1
31714	C	55.53604	92.98087	71.11954	-304.29479	-22.54452	43.63330	1
31715	H	55.25488	93.84370	71.71986	-1278.31929	1713.86127	1505.82324	1
31716	H	55.26910	93.10996	70.08636	-1258.18942	-648.15622	1400.73926	1
31717	H	54.93777	92.09951	71.50691	-1042.92365	1015.77572	2793.84068	1
31718	C	57.48400	91.29418	70.64348	258.13039	451.19319	-92.48488	1
31719	H	56.95068	90.38405	71.00825	-636.11186	-877.23009	421.49436	1
31720	H	58.54256	91.19251	70.88732	-532.05696	-1602.72209	-2341.57509	1
31721	C	57.42295	91.44506	69.04063	758.07798	42.74056	320.75485	1
31722	H	57.97280	92.30099	68.61381	1059.54562	-2164.77165	1650.42433	1
31723	H	57.95757	90.58413	68.47954	3917.74453	-513.37794	-29.63070	1
31724	H	56.35511	91.46600	68.73274	1955.95247	-2814.38554	-2937.46900	1
31725	C	58.38686	94.64356	72.20456	-311.32354	-264.19517	-311.54628	1
31726	O	57.89853	95.73216	72.46825	-242.23382	497.93882	334.08852	1
31727	N	59.24623	94.04035	73.00431	370.19502	-43.95361	-370.05757	1
31728	H	59.62072	93.08237	72.91774	319.01422	3372.13725	213.09045	1
31729	C	60.37657	94.86641	73.51625	837.21770	-328.59592	456.41928	1
31730	H	59.92982	95.70421	74.12941	1115.49178	-3705.71975	302.94877	1
31731	C	61.24143	93.96420	74.42279	-103.58927	-423.32699	-276.39286	1
31732	H	61.96959	93.35508	73.82879	-206.79956	-872.43989	1568.11675	1
31733	C	61.96285	95.01162	75.32125	358.96263	-386.01415	-376.28016	1

31734	H	61.20582	95.59422	75.87747	-1437.93976	4706.52049	1536.67830	1
31735	H	62.55778	94.41420	76.06466	-669.94421	-1638.89293	759.80675	1
31736	H	62.82959	95.55581	74.76642	-2074.13761	934.61928	-1240.52315	1
31737	C	60.35661	92.98848	75.31496	-310.46252	-127.76958	-107.24427	1
31738	H	59.46679	92.67017	74.73473	-398.89485	-1409.96996	-2273.32184	1
31739	H	59.98468	93.58050	76.13249	-251.34703	-1687.75724	659.31152	1
31740	C	61.22997	91.77333	75.84869	1295.73570	365.74447	291.85903	1
31741	H	60.72813	91.03744	76.49319	-1054.97668	1163.59034	879.67261	1
31742	H	62.02388	92.19673	76.47513	-251.21439	2428.96325	-1336.03380	1
31743	H	61.68460	91.08494	75.07243	221.36072	-1040.61558	-2146.08975	1
31744	C	61.36513	95.31091	72.30212	820.69433	-605.78449	-773.03505	1
31745	O	61.74173	94.49788	71.46135	-389.33153	474.51938	189.37893	1
31746	N	61.70981	96.60064	72.37718	-185.97961	12.13205	218.30756	1
31747	H	61.44748	96.95763	73.21528	1837.23607	1239.62286	-1022.45403	1
31748	C	62.79787	97.02979	71.60633	57.62032	-180.29997	388.18373	1
31749	H	62.98510	96.21743	70.87505	-593.42177	309.63364	-1077.63074	1
31750	C	62.40802	98.43418	70.95660	91.71440	-486.18380	-82.12170	1
31751	H	63.34487	98.78058	70.40483	2476.67814	-1224.70120	-1231.15485	1
31752	H	62.13341	99.19957	71.78464	-2425.35846	1749.97406	571.05128	1
31753	C	61.32064	98.31647	69.88982	-374.79566	202.32272	707.10299	1
31754	H	60.81662	99.34007	69.75251	-2361.62100	-69.64523	-1710.92524	1
31755	H	61.77927	97.90556	68.89914	995.30591	2390.06976	-2245.85995	1
31756	C	60.13705	97.34092	70.38410	-523.90757	-38.96849	-792.82118	1
31757	H	59.87979	97.58030	71.42863	-474.78422	-6129.58756	326.94571	1
31758	H	60.52329	96.36481	70.29704	-223.48738	-373.51057	1762.11690	1
31759	C	58.91067	97.53812	69.40250	-711.65295	504.52543	578.49978	1
31760	H	58.83764	98.61591	69.29835	-3968.25484	-2668.57853	3731.28936	1
31761	H	57.96632	97.04113	69.73099	-2295.30060	561.20268	-3045.02074	1
31762	N	59.24660	97.03097	68.11157	-377.16150	461.47379	-39.12087	1
31763	H	62.89016	96.06045	65.00155	-1857.66472	2664.93784	1772.57708	1
31764	H	59.02331	96.01919	67.89392	-1035.92952	-2317.57691	1857.62228	1
31765	H	59.00666	97.57551	67.25984	-454.52173	-453.39168	1436.84556	1
31766	C	64.00854	97.36349	72.68564	283.56764	-379.54168	-256.30222	1
31767	O	63.78110	98.14762	73.57028	56.47926	-673.42456	-632.49450	1
31768	N	65.14061	96.72379	72.31878	-127.55499	-243.49196	-47.32239	1
31769	H	64.85775	96.07884	71.55655	-426.80007	-531.55025	-1591.27818	1
31770	C	66.38740	97.35422	72.61119	102.53849	-5.31452	-853.00016	1
31771	H	66.13425	98.37207	72.50725	-171.34118	1776.84173	-897.28037	1
31772	C	66.67179	96.90682	74.11297	531.79519	-1322.47561	-580.96002	1
31773	H	67.20221	95.94629	74.11355	-545.81719	1688.39989	949.88875	1
31774	H	65.75793	96.64403	74.71665	1232.28009	-528.54122	-278.17707	1
31775	C	67.56526	98.01543	74.72844	139.02470	-99.07839	-678.28044	1
31776	H	67.29779	98.20883	75.82925	730.14361	-274.92381	-3259.67352	1
31777	H	68.64587	97.74168	74.64605	1348.70046	92.03012	1416.69246	1
31778	C	67.50496	99.42921	73.92208	-289.44742	-141.02394	-159.14477	1
31779	O	68.38558	99.82198	73.20599	-213.28093	-398.55950	-538.52427	1
31780	N	66.25412	99.97947	74.04784	281.08008	-225.41462	-176.88430	1
31781	H	65.50490	99.34805	74.51162	-3066.42409	951.99732	-403.71574	1
31782	H	65.78451	100.57259	73.34888	2342.27137	-377.41480	-604.05010	1
31783	C	67.45673	96.84742	71.51001	142.52626	332.62826	-196.25048	1
31784	O	67.09440	95.87401	70.81927	275.81310	-24.26822	36.03707	1
31785	N	68.55316	97.57193	71.40717	-313.65089	581.73384	466.07373	1
31786	H	68.55614	98.43470	71.97707	-485.30328	-537.53526	-1238.88250	1
31787	C	69.48260	97.12493	70.36802	-542.63099	-459.39581	445.58644	1
31788	H	69.48650	98.05971	69.79235	1042.74778	1953.28140	-1325.56231	1
31789	H	68.95510	96.38205	69.62584	-228.48601	-2286.16545	3631.61124	1
31790	C	70.86229	96.72115	71.05922	-373.83913	656.41538	262.22079	1
31791	O	71.32272	97.27724	72.04693	202.98715	304.70047	-337.76162	1
31792	N	71.37085	95.67113	70.39314	82.44336	-61.55986	367.81464	1
31793	H	70.87501	95.29711	69.48907	324.91462	18.14171	1881.74124	1
31794	C	72.08688	94.63849	71.11333	253.88051	879.70506	146.42539	1
31795	H	71.42646	94.37959	72.04104	-3637.44076	-910.64565	-71.37864	1

31796	C	72.63859	93.40765	70.33111	197.34036	91.19336	361.02836	1
31797	H	73.00564	92.53647	70.88965	-682.80943	2372.63803	1259.17683	1
31798	H	73.54110	93.59650	69.66758	-1777.85440	-1332.26004	1648.45107	1
31799	S	71.21384	92.69129	69.21600	258.28826	-132.08136	68.30943	1
31800	C	73.41262	95.47106	71.64268	30.72375	145.79929	-355.93040	1
31801	O	74.01116	94.98845	72.57902	-937.30017	576.51062	1006.19232	1
31802	N	73.77530	96.54206	70.91459	-308.34098	-143.38976	56.05030	1
31803	H	73.13263	96.83460	70.14181	-5141.30794	2595.25499	453.74562	1
31804	C	74.95998	97.28686	71.18166	143.87585	513.62380	-377.72367	1
31805	H	75.75967	96.50985	71.49605	-10.53265	-1661.46358	2873.83015	1
31806	C	75.27033	97.97450	69.79960	-586.58174	-46.33716	210.47459	1
31807	H	74.49436	98.67473	69.46847	-1368.80538	-2143.18369	-1274.37184	1
31808	H	75.36063	97.15836	69.06615	690.33111	-726.65770	398.63057	1
31809	C	76.60637	98.73285	69.62837	802.30430	-540.38346	-1412.46149	1
31810	H	76.60329	99.81662	69.88039	1974.09799	285.28909	401.57035	1
31811	H	77.39046	98.29022	70.20193	-874.49758	165.65157	1149.52412	1
31812	C	76.87414	98.82058	68.04162	-169.66679	-320.43213	468.52164	1
31813	O	77.74443	99.65168	67.66963	50.81527	122.66693	-14.78509	1
31814	O	76.30773	97.99979	67.27245	25.95532	-92.34727	-175.28766	1
31815	C	74.81638	98.44944	72.27159	-136.44282	-260.67323	-168.20778	1
31816	O	75.71540	99.27062	72.46265	-171.57741	-684.57765	217.48997	1
31817	N	73.65399	98.49362	72.90835	-664.71502	169.73086	-172.33519	1
31818	H	72.86410	97.80186	72.73936	64.93634	1889.60674	944.07322	1
31819	C	73.77965	99.05473	74.24536	1161.00597	747.37563	775.52323	1
31820	H	74.67212	99.73846	74.28671	-116.27744	1166.01735	-1162.18758	1
31821	C	72.33627	99.68544	74.56502	-215.96704	-490.35807	12.99873	1
31822	H	71.50680	99.24432	73.92655	-1017.12025	21.57995	-422.24684	1
31823	H	72.10788	99.71145	75.66585	-1379.06376	-724.56760	1940.85291	1
31824	C	72.35919	101.17044	74.08485	-894.75836	159.00006	-867.43649	1
31825	C	71.24323	101.62901	73.38979	838.98586	683.20231	734.81902	1
31826	H	70.41794	101.00591	73.12259	881.05830	3277.50699	1802.92206	1
31827	C	71.24150	103.01099	73.06258	878.88851	-361.46341	194.45252	1
31828	H	70.45482	103.38828	72.40113	3116.22531	333.33093	-267.81212	1
31829	C	72.20632	103.89294	73.54963	178.13650	566.53874	-109.55858	1
31830	H	72.08646	104.97233	73.35091	-2246.01707	-3768.06117	2494.50745	1
31831	C	73.51618	102.00773	74.37854	283.19665	-241.33075	439.75346	1
31832	H	74.50282	101.65345	74.74930	-1547.79090	2832.48770	-227.43683	1
31833	C	73.34104	103.39013	74.26303	158.35412	-239.59130	261.54207	1
31834	H	74.17074	104.06480	74.45110	-1311.32847	7.37711	-1275.87987	1
31835	C	73.77914	97.89053	75.30971	-85.93793	-178.39923	-121.11204	1
31836	O	73.73880	98.24045	76.49818	-615.10321	-456.59132	614.21991	1
31837	N	73.78647	96.61334	74.92230	55.68682	185.81420	435.00344	1
31838	H	73.92977	96.38895	73.90962	2056.92508	2481.41061	4029.48314	1
31839	C	72.83828	95.77797	75.64072	-493.00319	-44.83442	110.41073	1
31840	H	72.37900	96.38316	76.44159	1813.40743	-944.63440	-2117.23638	1
31841	C	71.71945	95.39550	74.58701	-383.45554	339.31101	86.33041	1
31842	H	71.48376	96.31734	73.97432	568.40804	-2352.86765	-914.40117	1
31843	H	72.06034	94.57840	73.91612	494.41173	555.09355	2518.95584	1
31844	C	70.43090	94.93122	75.36220	446.10240	687.33399	-370.24251	1
31845	H	69.98195	95.81924	75.93636	3623.53583	506.47771	994.85858	1
31846	H	70.72842	94.16255	76.11116	634.47457	3134.12153	3387.46279	1
31847	C	69.39693	94.31247	74.31714	4.57325	-191.39315	831.96710	1
31848	O	68.24931	94.00412	74.56472	-222.82789	-800.83610	505.96161	1
31849	O	69.80200	94.18531	73.08335	94.46577	46.69691	-115.85655	1
31850	C	73.57183	94.46496	76.24687	-656.76431	-350.77684	301.90146	1
31851	O	72.99507	93.41319	76.64080	205.75415	-401.11114	429.08132	1
31852	N	74.88038	94.59034	76.21851	-152.87223	760.93919	46.65001	1
31853	H	75.10709	95.50931	75.89053	-1122.96151	-2234.81656	3269.24376	1
31854	C	75.60728	93.89065	77.23894	588.56361	-618.20111	-731.94640	1
31855	H	75.21976	92.83435	77.28996	531.78697	46.62915	789.45211	1
31856	C	77.11868	94.14826	76.90887	584.97133	-575.12453	604.68056	1
31857	H	77.50003	95.04313	77.36767	-3124.54131	-3266.39220	-1057.20523	1

31858	H	77.30569	94.36178	75.78322	2356.65786	885.96891	-721.68461	1
31859	C	77.97491	92.87012	77.35798	-127.10963	336.00849	-402.50898	1
31860	O	77.89583	92.25396	78.38867	-19.28456	-265.58399	413.46727	1
31861	N	78.90582	92.65876	76.34309	85.11352	-1130.28590	237.44596	1
31862	H	79.00811	93.03328	75.36135	2823.41417	-2734.84965	-1011.76675	1
31863	H	79.48126	91.81268	76.37125	-2738.87371	100.30051	640.22174	1
31864	C	75.23841	94.81580	78.56345	-1285.67683	-903.25114	-373.06961	1
31865	O	75.92662	95.76594	78.87538	86.34430	-634.28339	-871.58513	1
31866	N	74.11895	94.32531	79.09783	-10.26002	-38.14051	-34.50799	1
31867	H	73.62394	93.57443	78.59946	2603.66486	-271.14365	-2872.31652	1
31868	C	73.26063	95.09358	79.96175	325.26341	230.64200	68.72719	1
31869	H	73.90824	95.45983	80.82179	2579.01296	1033.72703	204.56603	1
31870	C	72.73907	96.28992	79.16382	-270.01410	-302.34508	-225.64305	1
31871	H	72.68926	96.09818	78.07250	-1114.71495	2361.64904	-178.57519	1
31872	O	73.84601	97.79644	79.07770	-151.39056	-826.93737	-985.67739	1
31873	H	73.81565	97.94730	77.99745	-1647.66836	4384.35586	-2142.88243	1
31874	C	71.35881	96.58558	79.71328	-1206.21182	-650.68738	840.41325	1
31875	H	70.75716	95.66376	79.71637	-815.33728	656.22312	-1663.70842	1
31876	H	70.82575	97.38060	79.09226	508.90887	2730.40274	3675.53137	1
31877	H	71.48408	96.91323	80.76882	-3877.13174	-556.56523	360.45437	1
31878	C	72.08657	93.94800	80.25044	-353.78796	-255.38235	-768.67508	1
31879	O	71.91370	93.57750	81.41821	76.94271	-147.82630	329.05676	1
31880	N	71.50399	93.57689	79.14174	-308.40928	-47.19138	-29.60974	1
31881	H	71.80242	93.93768	78.19988	705.37159	3091.16799	-769.63006	1
31882	C	70.62202	92.43406	79.28864	-155.58023	798.51274	184.63848	1
31883	H	70.24903	92.43037	80.38377	167.87405	-2458.63624	39.55667	1
31884	C	69.51154	92.23876	78.20879	535.61327	177.27989	-162.05933	1
31885	H	69.99214	91.80667	77.30740	1041.89278	-2310.90769	80.26781	1
31886	C	68.53854	91.08814	78.60611	122.74671	-329.06475	782.41668	1
31887	H	67.88853	90.83743	77.76730	-3171.19300	69.06663	-149.78031	1
31888	H	69.15754	90.15835	78.82731	2385.77719	2818.25187	1147.30000	1
31889	H	67.90425	91.37357	79.47656	1217.49617	-1689.75552	-1032.28431	1
31890	C	68.61776	93.54575	78.05267	355.94155	-78.38245	-1345.80386	1
31891	H	69.20560	94.40423	77.77613	-915.64322	952.11624	-674.62697	1
31892	H	67.88583	93.44099	77.20815	-615.76770	-2338.62315	-1522.91684	1
31893	H	67.97268	93.65140	78.92872	-777.92336	-2177.22810	-2226.08346	1
31894	C	71.41160	91.01023	79.12790	-373.40000	-177.16770	-304.63909	1
31895	O	71.17928	90.05844	79.84624	449.97338	-319.08345	-328.22405	1
31896	N	72.28085	91.13401	78.09175	-260.58395	231.42803	-480.60152	1
31897	H	72.39128	92.07331	77.69874	-1560.74515	1199.79651	635.49042	1
31898	C	73.15380	90.06471	77.83259	738.26734	170.25433	-421.93723	1
31899	H	72.41265	89.21544	78.08078	796.34900	-1159.12676	1975.67905	1
31900	C	73.70026	90.18369	76.32687	-868.49877	-1136.96565	-246.43941	1
31901	H	74.50091	90.89224	76.44531	4178.21107	-324.03005	637.58277	1
31902	H	72.93506	90.69489	75.66299	-757.42678	3619.03752	-3181.36364	1
31903	N	73.49920	88.30028	74.61820	372.21211	-339.17327	-399.88420	1
31904	C	74.14644	88.90611	75.64078	546.96166	427.76266	1186.51625	1
31905	C	74.01189	87.03227	74.51041	-187.09766	335.60945	-350.79668	1
31906	H	73.69088	86.25165	73.82777	562.95997	-1275.08952	-972.44838	1
31907	N	75.05588	86.96353	75.35652	325.23934	-599.63419	-479.72042	1
31908	H	75.55951	86.06595	75.40261	3356.02080	-2159.15350	-1190.44514	1
31909	C	75.17326	88.03172	76.12605	315.68667	40.72319	414.11553	1
31910	H	75.86924	88.00760	76.96261	-1875.68991	-1883.38428	-1381.25958	1
31911	C	74.44263	90.14502	78.82444	31.50150	1295.92445	-391.62421	1
31912	O	75.22482	89.22625	78.66560	-535.26266	-226.96915	-810.69402	1
31913	N	74.47407	91.16737	79.67256	184.00440	522.90376	-133.55142	1
31914	H	73.71011	91.92628	79.69020	-2916.21278	-830.60317	2327.91004	1
31915	C	75.36835	91.11327	80.76218	695.82324	-60.76217	-682.23971	1
31916	H	76.22190	90.87962	80.11202	-1323.78410	-471.22023	-418.52708	1
31917	C	75.75983	92.56176	81.41332	-478.17601	905.84007	281.59036	1
31918	H	75.77621	93.42621	80.67512	-759.86193	1050.25949	1518.82825	1
31919	H	76.84213	92.43413	81.67505	-467.21293	-1854.03328	-3333.60798	1

31920	C	74.76132	92.74607	82.62448	209.51832	171.79727	-349.52371	1
31921	H	73.81226	93.12445	82.18917	1718.06304	-2929.13636	-686.30224	1
31922	H	74.70383	91.79857	83.17447	-1264.04392	628.65473	-717.38070	1
31923	C	75.25177	93.85183	83.62851	615.05156	356.93183	655.05082	1
31924	H	76.36514	93.82316	83.68245	1842.54381	1550.21470	-2569.78742	1
31925	H	74.94657	93.56861	84.62414	-3245.27419	497.98919	-1703.68534	1
31926	C	74.69159	95.25236	83.17777	-750.78828	154.11450	-668.37142	1
31927	H	75.16346	96.10833	83.89142	-1691.44826	-867.88145	-1441.72556	1
31928	H	74.94895	95.36365	82.11855	-1479.93921	2312.75371	1506.58835	1
31929	N	73.27974	95.20993	83.20941	-875.32490	-311.26067	30.88866	1
31930	H	74.59103	97.14164	79.07823	-363.83088	1097.55898	1131.23163	1
31931	H	72.74628	94.73501	82.41515	-1876.92429	-64.03194	612.95983	1
31932	H	72.75966	94.93971	84.01908	-105.79757	2283.23631	1198.62913	1
31933	C	75.01043	90.03439	81.88402	494.11254	-215.74977	200.27307	1
31934	O	75.91820	89.59817	82.60653	-416.46862	-421.99504	-545.14865	1
31935	N	73.70278	89.85640	82.11745	328.10269	423.81097	86.31158	1
31936	H	73.04415	90.27982	81.40344	1451.58761	-4708.40550	1318.23460	1
31937	C	73.29256	88.78553	82.96994	-249.24731	-294.40611	-603.47033	1
31938	H	74.17190	88.60540	83.62719	3374.08418	1478.24308	-1288.46313	1
31939	C	72.03153	89.32596	83.76110	-371.20752	-292.20336	88.07879	1
31940	H	71.47438	88.49630	84.27337	695.29269	164.64411	1312.08770	1
31941	H	71.34109	89.93705	83.10799	2921.68852	4224.10333	987.27180	1
31942	C	72.72128	90.18275	84.83025	-732.84616	735.59404	103.36094	1
31943	C	73.21559	91.53354	84.70276	3.88306	492.88406	-104.98504	1
31944	H	73.08789	92.20695	83.86076	-2347.81419	1353.89625	-1157.33508	1
31945	N	73.67476	91.99685	85.86505	-982.48139	-889.25394	339.92215	1
31946	H	73.94672	93.00884	85.99228	928.58913	-338.97795	406.74865	1
31947	C	73.50601	91.07767	86.84340	557.45744	254.23056	-140.27046	1
31948	C	73.00170	89.81891	86.17742	-61.69165	-312.26200	-352.90585	1
31949	C	72.77171	88.64440	86.98916	767.21993	-1198.60660	272.10984	1
31950	H	72.54607	87.58689	86.56964	314.60631	-1110.38796	270.80666	1
31951	C	73.04445	88.80309	88.36424	-517.86379	-700.17753	412.00754	1
31952	H	72.94852	87.94195	89.01702	1022.63078	2527.85805	389.68150	1
31953	C	73.82958	91.06446	88.26480	504.20208	54.93273	-359.13994	1
31954	H	74.12173	92.03693	88.68627	-120.42950	-931.88370	-341.55282	1
31955	C	73.65670	89.92796	89.05295	-118.92140	-450.62725	1502.37669	1
31956	H	73.80556	89.87097	90.16866	789.65711	1651.13456	2378.24555	1
31957	C	73.07257	87.49181	82.06175	159.20747	51.76876	-179.77433	1
31958	O	72.91608	86.38140	82.61233	-38.28038	42.15966	390.05839	1
31959	N	72.87494	87.69231	80.74879	-171.52311	-174.23434	22.14837	1
31960	H	72.90920	88.64378	80.23392	-1459.63405	-556.91906	-1577.88250	1
31961	C	73.01776	86.54270	79.84626	20.84769	258.42549	-769.01025	1
31962	H	72.30207	85.79278	80.21784	333.75395	1490.78288	3247.21109	1
31963	C	72.48756	86.84847	78.42059	-70.18045	270.43638	28.37296	1
31964	H	73.19034	87.59183	77.98637	-2463.80550	-430.74215	-179.19044	1
31965	C	72.70929	85.63661	77.43286	257.20145	419.93148	-784.30999	1
31966	H	73.80065	85.37265	77.48083	-514.26138	-1887.86375	1361.14778	1
31967	H	72.46596	85.89941	76.41621	73.31204	2893.75565	702.24895	1
31968	H	72.24536	84.61226	77.62453	837.22991	-229.14934	104.07973	1
31969	C	70.95176	87.23079	78.56897	-512.74904	1438.02066	872.05429	1
31970	H	70.76244	88.16530	79.08735	-223.23662	-28.01260	-893.98251	1
31971	H	70.50227	86.54709	79.26871	-1946.98424	2033.22501	-635.06683	1
31972	C	70.25425	87.16961	77.17740	-105.93737	335.38717	135.50245	1
31973	H	69.14431	87.32761	77.32768	-2030.38659	-2611.13349	-2265.47232	1
31974	H	70.66177	87.98843	76.50250	244.09736	-5389.73490	2470.77988	1
31975	H	70.42162	86.10168	76.79615	-239.14761	-1474.25023	479.62032	1
31976	C	74.57601	86.00367	79.84154	691.61007	-355.98759	376.42376	1
31977	O	74.69720	84.81589	79.41228	-80.45605	-10.88249	-230.81472	1
31978	N	75.45131	86.87523	80.15273	228.01103	-582.17423	-757.00346	1
31979	H	75.15279	87.84443	80.29685	2255.53673	-1129.33427	1585.80288	1
31980	C	76.85247	86.52311	80.10244	317.98408	-160.20196	623.86652	1
31981	H	76.93072	85.75771	79.29357	2779.58868	-2379.28594	-1626.71919	1

31982	C	77.58702	87.88576	79.86311	-432.04021	-808.57855	-328.70974	1
31983	H	76.99462	88.44822	79.00800	1251.77819	-7.88728	156.40611	1
31984	H	77.48734	88.55109	80.78628	2080.39771	-2172.53655	93.26160	1
31985	O	79.04959	87.86697	79.64297	84.57059	288.57683	-23.78734	1
31986	H	79.08145	88.65338	79.09663	-610.60829	-1288.24916	-2076.02414	1
31987	C	77.24700	85.83816	81.58395	845.89122	163.82733	957.95371	1
31988	O	78.12970	84.97851	81.68414	456.30412	457.09585	-6.10522	1
31989	N	76.57705	86.37956	82.55747	-933.48075	37.24618	471.81041	1
31990	H	75.88897	87.06677	82.25134	-1790.10412	-139.44205	-86.77606	1
31991	C	76.50112	85.69650	83.83114	-780.63011	17.23448	250.33605	1
31992	H	77.58910	85.69476	84.11866	-468.53838	577.03759	-1748.47041	1
31993	C	75.67265	86.49720	84.88520	905.71200	-316.75861	206.66092	1
31994	H	74.61422	86.50090	84.48371	840.36576	-351.51489	-1664.46484	1
31995	C	75.59482	85.77076	86.28744	389.39583	172.99162	-476.05636	1
31996	H	74.79641	86.11451	87.02278	1993.53637	4.16961	635.72847	1
31997	H	75.51400	84.69780	86.20590	-1200.72439	-2363.71614	1664.19330	1
31998	H	76.59900	85.88452	86.78583	624.17545	281.43632	-122.75893	1
31999	C	76.21308	87.93173	85.20413	-467.42293	-230.43110	150.98491	1
32000	H	75.95709	88.59818	84.30851	8.59954	1539.59438	1498.76344	1
32001	H	75.69040	88.39776	86.05906	3480.94827	-3919.97123	-3150.80596	1
32002	C	77.77772	87.88812	85.38707	-160.96281	631.49502	91.43877	1
32003	H	78.19944	87.65822	84.38426	-562.41980	294.81435	3915.25566	1
32004	H	78.07738	87.16004	86.18527	-1576.99604	-602.73447	638.87565	1
32005	H	78.09869	88.91300	85.78785	1405.72694	-1619.17105	827.56117	1
32006	C	75.78700	84.21280	83.67290	788.53453	-28.49505	-468.88047	1
32007	O	76.22800	83.19180	84.17690	-757.40153	-34.54751	200.07716	1
32008	N	74.61500	84.11980	83.04490	571.12420	-174.38698	-602.00905	1
32009	H	74.13500	84.95480	82.78790	-336.47900	2883.14601	-1251.96788	1
32010	C	73.91400	82.81280	82.88690	-712.26382	404.45356	404.46614	1
32011	H	74.00400	82.22380	83.78790	629.73411	2167.38547	-2212.86146	1
32012	C	72.40500	82.98880	82.63790	730.54540	-290.89524	-460.61907	1
32013	H	71.80800	82.06780	82.46190	-1938.32127	-1704.82360	1777.66826	1
32014	O	72.05500	83.93480	81.60190	-710.49268	-61.66689	327.63637	1
32015	H	72.41500	84.72780	82.00590	2030.93150	-1563.18179	-1820.09708	1
32016	C	71.88900	83.50080	83.95390	613.14241	-345.10761	568.70575	1
32017	H	72.21200	84.53380	84.20790	2200.58367	-1924.14214	-1150.84564	1
32018	H	72.03100	82.81280	84.81390	1812.04637	99.49209	-2578.11935	1
32019	H	70.78500	83.62080	83.92590	-1619.98904	-2122.89556	-1645.60321	1
32020	C	74.57400	81.90580	81.81590	621.36775	-652.42880	43.16816	1
32021	O	74.51000	80.70880	81.83790	-640.77454	142.80220	435.59190	1
32022	N	75.20800	82.54480	80.80190	479.42188	691.08073	147.74909	1
32023	H	75.17800	83.52780	80.63590	-836.50066	-991.19347	2853.98741	1
32024	C	76.14000	81.91880	79.89590	163.05319	880.36338	221.42205	1
32025	H	75.54400	81.19980	79.35290	2580.55573	1369.68578	-1188.33998	1
32026	C	76.52300	82.92480	78.72290	280.39071	742.20958	-478.15948	1
32027	H	75.62500	83.11680	78.09690	2069.90502	-1547.28776	-1789.03978	1
32028	H	76.66500	83.94280	79.14390	2174.93594	-2252.88062	-190.11638	1
32029	C	77.84600	82.66780	77.99590	-612.71903	149.49584	653.33890	1
32030	H	77.88700	81.63180	77.59590	-1866.69941	2023.02840	-1551.88237	1
32031	H	78.72200	82.60580	78.67690	3007.42614	-846.25378	322.81626	1
32032	C	78.18500	83.71880	76.95690	-101.77697	-876.10774	169.16580	1
32033	O	77.71100	83.55580	75.80090	693.44839	14.69440	364.02734	1
32034	O	78.82900	84.76080	77.27790	525.75263	305.71765	500.00282	1
32035	C	77.35300	81.31380	80.52590	123.36138	737.97742	529.62648	1
32036	O	77.70100	80.15980	80.26390	-48.54966	749.62179	-288.64368	1
32037	N	77.95800	82.09480	81.38790	501.67043	656.29888	-226.06362	1
32038	H	77.75900	83.05180	81.58290	-1878.24704	-2203.52212	-1215.69784	1
32039	C	79.11300	81.64780	82.15290	-451.72930	511.53847	-624.07772	1
32040	H	79.84000	81.34180	81.41590	786.46122	-2544.78100	-1667.38510	1
32041	C	79.73600	82.80780	82.92590	556.34576	-691.52224	161.55164	1
32042	H	79.00500	83.27380	83.62090	2007.25997	-18.32550	2414.53703	1
32043	H	80.07200	83.58180	82.20390	1774.45048	-1959.34200	1683.81894	1

32044	H	80.64900	82.46280	83.45690	4.89799	2342.98725	-2123.25859	1
32045	C	78.82700	80.48580	83.13890	-363.70548	-587.65466	-592.04314	1
32046	O	79.55900	79.51980	83.22390	156.55684	298.84368	708.46807	1
32047	N	77.64800	80.51980	83.78290	450.85362	361.17242	614.63778	1
32048	H	77.05800	81.29980	83.58990	1785.81785	2084.84058	-1564.85080	1
32049	C	77.12500	79.38880	84.44290	-293.60047	-713.75831	456.65107	1
32050	H	77.86300	79.04080	85.15090	-2725.70752	-1193.98408	-1011.19579	1
32051	C	75.91800	79.80180	85.39390	-755.67903	-207.60385	-464.38306	1
32052	H	75.08100	80.21480	84.79090	1551.01874	-1142.61595	2474.92837	1
32053	H	75.49200	78.90680	85.89490	1947.33529	1938.80092	-1559.32333	1
32054	C	76.28200	80.82580	86.48490	-426.17957	94.76615	791.83861	1
32055	H	76.98000	81.55880	86.02790	3046.47485	540.40383	-608.32694	1
32056	C	74.98200	81.56780	86.85190	-735.89682	-299.14808	-439.07224	1
32057	H	75.18900	82.57080	87.28190	-2655.52362	-1209.65211	-1159.00628	1
32058	H	74.37200	80.96780	87.56090	451.53647	-2190.77408	2192.67946	1
32059	H	74.21300	81.76580	86.07590	-2690.99909	-1157.37042	-1132.11167	1
32060	C	77.11200	80.14080	87.64290	473.73493	-349.04518	-701.65537	1
32061	H	78.19900	80.15580	87.41590	-728.62184	-2421.76933	-1863.77431	1
32062	H	76.72400	79.10680	87.76490	768.93926	-709.12813	-2973.66066	1
32063	H	77.02300	80.76480	88.55790	-1919.19737	-2466.64293	215.29753	1
32064	C	76.81200	78.16480	83.60190	-21.86657	596.20934	691.69449	1
32065	O	76.88800	77.02780	84.09590	685.77157	-355.68646	-143.10498	1
32066	N	76.40900	78.34580	82.33290	119.22504	-314.95769	-777.09783	1
32067	H	76.25200	79.28280	82.02990	-478.80401	1320.79031	-2829.47174	1
32068	C	76.00000	77.24280	81.44990	225.06223	-697.55320	516.23294	1
32069	H	75.30300	76.60780	81.97590	-1973.89218	1245.50634	2110.95006	1
32070	C	75.34000	77.71080	80.16190	-748.50407	369.69860	-391.57026	1
32071	H	74.36600	78.17280	80.43090	-562.24139	2538.03136	-1799.47781	1
32072	H	76.02600	78.35680	79.57290	2902.51737	-1117.42707	419.38812	1
32073	H	75.07000	76.89780	79.45490	-1754.71165	-2484.24383	760.29744	1
32074	C	77.21500	76.45580	81.18090	252.45224	658.74784	582.07552	1
32075	O	77.05800	75.22780	81.01690	83.33404	485.42979	617.81627	1
32076	N	78.42600	76.99280	81.18490	356.89110	-61.57704	750.90182	1
32077	H	78.51000	77.98480	81.24190	2130.17501	-938.91419	2099.88886	1
32078	C	79.72500	76.37280	80.94990	788.92896	-201.80046	389.62549	1
32079	H	79.67100	75.84580	80.00890	-2581.97542	-1682.86945	-622.78098	1
32080	C	80.84500	77.40480	80.87490	-628.56068	623.96451	-262.44398	1
32081	H	81.81300	76.89780	80.67290	1828.90153	-2186.90516	-1321.96633	1
32082	H	80.83100	77.90280	81.86790	-791.59950	1518.76928	2634.40386	1
32083	C	80.72800	78.48680	79.85590	477.80854	146.41207	-774.89204	1
32084	C	79.79900	78.45180	78.78390	-186.36139	-144.81983	-889.98389	1
32085	H	79.19800	77.57480	78.59390	1922.91667	2027.93828	1447.30307	1
32086	C	79.71500	79.51180	77.92990	-492.38396	-663.59325	357.59285	1
32087	H	78.93100	79.51880	77.18690	-2293.43724	327.08747	2123.94736	1
32088	C	80.60300	80.61280	78.00890	-883.21266	142.28124	184.42038	1
32089	H	80.63700	81.41480	77.28690	-1403.63696	-522.56412	-2776.92815	1
32090	C	81.56500	79.61080	80.03390	-31.40913	730.79491	547.13444	1
32091	H	82.29100	79.66680	80.83190	-3116.11861	384.04947	218.86273	1
32092	C	81.49000	80.62980	79.09190	-433.29809	-314.65525	-745.85593	1
32093	H	82.21500	81.42980	79.14390	988.68604	1276.03345	-2717.25595	1
32094	C	80.06500	75.30780	81.89290	30.06506	-607.94728	-679.29995	1
32095	O	80.91900	74.45080	81.59690	671.74276	404.92641	107.45670	1
32096	N	79.44000	75.24380	83.07190	603.22251	-474.87754	-343.24358	1
32097	H	78.65900	75.82680	83.28190	104.67288	2703.62055	1615.59018	1
32098	C	79.63100	74.13880	83.98890	-67.91905	75.21585	896.44201	1
32099	H	80.68900	74.07380	84.19190	2816.28465	-1078.55727	868.70188	1
32100	C	78.87000	74.41180	85.37190	-411.35045	-598.79516	-547.98192	1
32101	H	78.83600	73.47280	85.96590	-1799.41308	-1136.35272	-2321.36606	1
32102	H	77.82200	74.75780	85.24390	739.07027	2943.04081	864.08794	1
32103	C	79.70500	75.33080	86.30090	17.38737	422.41305	803.13778	1
32104	C	79.44800	76.73280	86.29990	330.33177	-562.25603	-638.25219	1
32105	H	78.60500	77.12880	85.75290	2075.14118	1851.07090	1478.63196	1

32106	C	80.18400	77.60480	87.17890	-236.58297	844.69494	-293.29973	1
32107	H	79.91800	78.64980	87.23690	-66.28161	893.53631	-3029.90220	1
32108	C	81.22300	77.03480	87.99790	-583.98383	28.59610	-709.31061	1
32109	H	81.76900	77.73080	88.61790	25.78758	-2087.41420	2332.34975	1
32110	C	80.73400	74.83380	87.05290	-298.28421	456.99279	-748.17810	1
32111	H	80.89600	73.77180	87.15890	-2126.07529	-1143.85252	-2021.51953	1
32112	C	81.50200	75.61880	87.92690	-211.12842	896.73373	18.81755	1
32113	H	82.33500	75.21480	88.48390	-439.01408	2011.30671	-2399.85473	1
32114	C	79.16300	72.79280	83.47990	-513.98847	563.28423	-525.25282	1
32115	O	79.55200	71.72080	84.04290	545.12259	-423.33338	-378.43714	1
32116	N	78.30700	72.68380	82.44790	-841.16080	93.02246	43.43901	1
32117	H	77.94400	73.50180	82.00890	1036.56795	-602.87582	2895.56100	1
32118	C	78.01100	71.39980	81.79690	-313.03391	403.95598	-772.80076	1
32119	H	77.51000	70.87580	82.59890	1351.81266	1396.56266	-2488.67644	1
32120	C	77.14300	71.47680	80.57290	-600.38244	-464.42883	489.22919	1
32121	H	76.78100	70.46380	80.29490	-990.30154	-223.83569	-2987.37839	1
32122	H	76.21100	71.97380	80.91690	-391.31079	-1075.75395	2917.64515	1
32123	N	77.72300	73.44280	79.04490	337.46101	-758.98498	-30.92509	1
32124	H	77.43600	74.19280	79.63990	-1942.57870	-1976.43701	-1486.66530	1
32125	C	77.73900	72.10080	79.28290	339.17099	669.70393	520.80575	1
32126	C	78.21500	73.63280	77.79190	-506.36084	-638.44974	-405.63204	1
32127	H	78.09200	74.62580	77.35890	2923.32435	-596.40774	965.92021	1
32128	N	78.44100	72.46680	77.21390	484.34748	-372.07929	-579.52145	1
32129	C	78.16100	71.51680	78.14890	-694.38478	-575.78168	96.84530	1
32130	H	78.36500	70.47680	77.92590	1209.86376	1936.02027	-2182.17364	1
32131	C	79.20000	70.61280	81.39290	730.99432	487.67388	243.96631	1
32132	O	79.29400	69.44680	81.75690	-87.73488	53.18777	-794.82909	1
32133	N	80.23700	71.24080	80.70990	568.65566	442.03275	-457.38191	1
32134	H	80.12400	72.15080	80.31990	-1149.19080	-2394.92438	-1683.21211	1
32135	C	81.53600	70.68980	80.37790	257.92101	-771.53577	-399.56245	1
32136	H	81.30400	69.88380	79.69790	313.80498	-2645.80232	-1666.38811	1
32137	C	82.43700	71.71380	79.66390	590.85632	264.10046	-654.86117	1
32138	H	82.58700	72.59480	80.32390	633.69109	946.96046	2922.38254	1
32139	H	83.49300	71.39880	79.52090	1354.48972	-2162.45512	-1838.05205	1
32140	S	81.70000	72.38080	78.16590	93.93759	-437.53820	304.33494	1
32141	H	80.97600	71.33580	77.79290	1218.75458	-1554.97987	2426.47289	1
32142	C	82.28600	70.13480	81.59390	-540.95537	560.34492	478.41676	1
32143	O	82.97200	69.12480	81.49390	-436.97544	401.29361	519.70237	1
32144	N	82.03700	70.65580	82.81090	6.92897	-141.72959	817.85312	1
32145	H	81.50900	71.49380	82.92690	-1334.98503	1929.33994	2095.77522	1
32146	C	82.76200	70.16280	84.01490	-511.32706	520.73508	-571.55250	1
32147	H	83.68700	69.72280	83.67190	2439.99769	1701.14123	-1048.14856	1
32148	C	82.99500	71.37380	84.95390	746.08196	-506.40605	63.05231	1
32149	H	83.61300	70.98680	85.79290	-2662.15061	1499.21483	760.30728	1
32150	H	82.07200	71.89880	85.27890	-561.34361	-2062.54806	-2311.57713	1
32151	S	83.97900	72.63280	84.11290	-394.80544	180.15849	343.42411	1
32152	H	85.18200	72.12980	84.34390	-936.34414	715.88928	-2934.22292	1
32153	C	81.93800	69.10780	84.71990	-665.65083	510.81553	363.78887	1
32154	O	82.51800	68.29280	85.42290	-492.16268	-367.31411	-503.74206	1
32155	N	80.65300	69.10580	84.45990	617.90521	-121.47033	545.21300	1
32156	H	80.19800	69.73580	83.83490	-2558.13217	-1816.74297	-173.68841	1
32157	C	79.68700	68.14480	85.04490	-414.52547	264.89470	-784.01284	1
32158	H	80.05800	67.92580	86.03490	-1438.58887	-2764.59263	-369.76530	1
32159	C	78.28300	68.75380	85.06290	-348.08194	775.72935	349.02091	1
32160	H	77.45500	68.03180	85.23190	2179.52929	2193.51358	606.74686	1
32161	H	78.09100	69.16680	84.04990	1965.84540	-945.77438	-2269.15813	1
32162	C	78.00400	69.82480	86.20890	20.46080	210.97673	879.87689	1
32163	H	78.90500	70.47180	86.14290	-1125.66089	664.99288	-2875.08964	1
32164	C	76.81100	70.73680	85.85990	-443.58320	616.18741	512.05281	1
32165	H	76.67900	71.41480	86.72990	-1424.79755	2315.25916	-1611.09577	1
32166	H	77.14500	71.31780	84.97290	-1676.66972	748.06082	-2568.62275	1
32167	H	75.93600	70.06580	85.72890	2456.17085	1201.63001	1555.50272	1

32168	C	77.83700	69.07980	87.51390	258.42985	572.80388	661.21292	1
32169	H	76.86500	68.54180	87.53190	2629.80653	898.24513	1472.01065	1
32170	H	77.89600	69.81380	88.34590	1042.32787	-1649.69374	-2469.44381	1
32171	H	78.56200	68.26680	87.73190	99.20638	2305.71644	2140.81542	1
32172	C	79.65200	66.80780	84.29190	-500.73333	-486.16339	569.22402	1
32173	O	79.37600	65.74280	84.89590	479.31134	-528.27884	-325.00841	1
32174	N	79.98800	66.80280	82.99990	625.98910	-55.03591	546.19422	1
32175	H	80.13000	67.65680	82.50490	1398.48252	-2135.82713	-1833.02071	1
32176	C	80.27200	65.57980	82.21990	342.74488	-436.65578	-725.09988	1
32177	H	79.38000	64.97580	82.30090	1647.79262	1530.33545	-2214.94128	1
32178	C	80.25600	65.98080	80.69390	-336.76980	582.41517	618.17866	1
32179	H	80.91000	66.86380	80.53090	2643.58886	-525.27432	1597.33071	1
32180	H	79.24200	66.28180	80.35290	21.52088	-788.94404	-3053.08581	1
32181	C	80.67100	64.84780	79.76590	87.69388	874.45270	266.60516	1
32182	O	80.29900	63.70080	79.96890	487.10039	520.40840	334.49870	1
32183	N	81.33000	65.20580	78.66090	430.76865	-578.92711	-426.78536	1
32184	H	81.30100	66.17680	78.42390	-96.26643	2782.03926	-1499.52615	1
32185	H	81.92300	64.53680	78.21290	-1629.38720	-653.89863	2600.77792	1
32186	C	81.38000	64.62380	82.85090	822.06021	-1.71555	370.44026	1
32187	O	81.10700	63.45380	83.05790	-134.41042	790.04317	-29.38416	1
32188	N	82.53700	65.11480	83.31390	-341.44051	-711.53477	266.69754	1
32189	C	83.22100	66.26080	82.69590	540.24704	-101.19792	709.00807	1
32190	H	82.94100	67.16080	83.28390	1544.81404	-1998.31714	1848.09434	1
32191	H	82.92800	66.49280	81.64990	903.89387	-1193.80354	-2773.76113	1
32192	C	83.43800	64.25680	84.07790	-242.94054	-329.61239	-825.56006	1
32193	H	83.55400	63.29780	83.59490	2121.16200	-1220.28358	1951.41546	1
32194	C	84.69700	65.12580	84.13990	-798.72216	-116.28366	415.50703	1
32195	H	85.61200	64.50480	84.24490	2277.37313	703.09197	2036.64001	1
32196	H	84.61000	65.77680	85.03590	-1602.15424	-1244.30222	2387.95254	1
32197	C	84.69800	65.91280	82.85790	-750.90081	-514.67090	-28.40442	1
32198	H	85.34200	66.81680	82.82290	1911.05131	-1901.82905	-1619.59580	1
32199	H	85.02000	65.31480	81.97890	2190.61623	-1261.20420	1845.32405	1
32200	C	82.95000	63.89680	85.48290	695.77384	-6.39629	-597.50762	1
32201	O	83.29800	62.85680	86.07890	426.32927	-578.97091	-315.76325	1
32202	N	82.18500	64.85480	86.18890	644.68769	-451.75300	268.67899	1
32203	H	82.04200	65.79680	85.89690	-1850.39233	-2144.76892	-1369.00297	1
32204	C	81.67900	64.58180	87.53990	885.18049	215.51751	27.83933	1
32205	H	82.46700	64.31080	88.22590	1308.76511	1463.92789	-2476.02131	1
32206	C	80.99100	65.83580	88.13590	-476.49501	768.00857	-192.80664	1
32207	H	80.39700	66.35780	87.35590	2519.62588	1888.28779	118.89000	1
32208	C	80.07500	65.51980	89.33090	-485.06151	753.31383	204.15102	1
32209	H	79.23600	64.80180	89.20790	-1421.68854	-667.38069	2713.13365	1
32210	H	79.60200	66.50280	89.53890	-348.77910	1621.64979	-2691.26013	1
32211	H	80.59200	65.06380	90.20190	-2653.31743	1257.92388	1131.18289	1
32212	C	82.10400	66.82480	88.54790	341.92409	762.63975	372.39754	1
32213	H	82.94700	66.77280	87.82690	1058.79410	263.35229	2938.16362	1
32214	H	82.54800	66.39380	89.46990	210.72728	-1454.90537	2763.24008	1
32215	C	81.75600	68.27980	88.67090	768.35466	485.26227	-136.75340	1
32216	H	81.18400	68.37880	89.61690	-1082.60644	-2612.37751	1346.02031	1
32217	H	82.69900	68.86180	88.75190	-1627.89541	-1936.07157	1847.14214	1
32218	H	81.16100	68.59880	87.78890	-1719.07556	-495.14944	2574.44705	1
32219	C	80.71800	63.40580	87.53890	682.17196	537.64066	279.48266	1
32220	O	80.75900	62.52280	88.33690	-300.12631	296.78647	-685.28713	1
32221	N	79.82600	63.35580	86.53090	-568.42711	410.02799	-495.75557	1
32222	H	79.63700	64.12880	85.92890	1416.75869	-2154.69848	-1796.48571	1
32223	C	78.94800	62.20480	86.22690	-0.80874	447.29586	-811.77947	1
32224	H	78.49300	61.75780	87.09790	1784.28016	-1467.33777	2113.85473	1
32225	C	77.77100	62.67180	85.34990	-251.98514	-640.85157	-596.04353	1
32226	H	78.14500	63.09380	84.39290	-1174.26888	2073.92500	2058.90361	1
32227	H	77.13300	61.79380	85.11490	2691.69983	127.99970	1606.63939	1
32228	C	76.80000	63.71180	86.07290	-93.12231	-890.04852	82.95526	1
32229	H	77.33300	64.63980	86.37290	238.04181	271.25216	-3135.69076	1

32230	C	75.74100	64.25280	85.11390	504.71272	-673.69926	-325.77031	1
32231	H	76.09600	64.59780	84.11990	1285.52588	-2273.45529	-1742.29023	1
32232	H	74.99800	63.47780	84.82990	-1474.98661	190.47153	-2783.80236	1
32233	H	75.09800	65.00780	85.61490	2430.53964	-1717.99297	979.75472	1
32234	C	76.08600	63.16980	87.28090	-702.11459	-460.03929	-354.00922	1
32235	H	75.75700	62.14180	87.01690	-448.17259	-2532.19630	1786.50492	1
32236	H	76.70900	63.27280	88.19590	1109.71980	2073.17724	2092.16613	1
32237	H	75.17000	63.75080	87.51990	-1083.99224	-1731.52028	2376.17222	1
32238	C	79.71000	61.03980	85.48290	402.40153	578.96775	-597.12515	1
32239	O	79.10700	60.24680	84.78490	-166.13562	560.38761	534.22280	1
32240	N	81.05000	60.89580	85.67690	530.00166	-553.79255	-339.59497	1
32241	H	81.56300	61.63580	86.10390	1080.12050	-1547.55650	2496.23658	1
32242	C	81.67900	59.58380	85.48290	562.19458	-225.14508	660.63245	1
32243	H	80.94000	58.86180	85.16790	-1784.29206	946.60422	2409.05308	1
32244	C	82.84300	59.77880	84.44790	533.46562	-545.52844	467.32231	1
32245	H	83.72900	59.14880	84.67490	1886.79156	1329.26230	2124.54767	1
32246	H	83.19000	60.83380	84.42090	1054.86130	2839.92443	861.32795	1
32247	C	82.46800	59.21580	83.06090	631.25518	-57.63992	-660.13911	1
32248	C	82.09700	57.87180	82.98090	-622.58789	674.96096	-125.38789	1
32249	H	82.06500	57.29180	83.89090	-1047.11570	268.37778	-2971.18022	1
32250	C	81.76000	57.32380	81.74990	-209.27878	-389.29185	781.88943	1
32251	H	81.57400	56.26280	81.67190	1122.85843	2830.69296	-827.72698	1
32252	C	81.73300	58.12080	80.62590	785.25793	-435.25870	-36.25291	1
32253	O	81.35100	57.56780	79.39290	463.60845	624.56864	-161.83702	1
32254	H	80.98200	56.68280	79.44890	-2204.10587	-308.31719	-2245.17744	1
32255	C	82.57200	59.98580	81.93490	654.43870	-590.08328	-191.72200	1
32256	H	82.88300	61.01080	82.07090	2137.59112	-1732.24340	-1516.63137	1
32257	C	82.18800	59.43480	80.71690	-594.88777	-475.57251	-514.62977	1
32258	H	82.27300	60.00980	79.80690	-2941.38013	-982.75890	548.12677	1
32259	C	82.20300	59.06980	86.83590	536.18923	122.94024	712.20368	1
32260	O	82.67700	57.91880	86.94890	326.56715	41.84569	702.53403	1
32261	N	82.03300	59.88880	87.89690	-709.45916	-260.20504	-389.39020	1
32262	H	81.63800	60.79980	87.80690	-2289.90250	241.65332	2136.62994	1
32263	C	82.49000	59.51680	89.18790	-432.01079	-648.29885	-475.65635	1
32264	H	83.47100	59.07480	89.09290	-660.19624	-2934.85757	878.16350	1
32265	C	82.64400	60.75380	90.06890	592.43601	572.25670	-415.40702	1
32266	H	83.36700	60.50080	90.87390	1953.84494	-1216.49344	2123.96554	1
32267	H	81.69200	61.08180	90.53790	2703.34760	-852.70995	1342.00826	1
32268	H	83.13700	61.58380	89.51890	-2833.40110	-1362.16809	-34.38125	1
32269	C	81.62000	58.45680	89.91790	687.26219	514.37315	304.88254	1
32270	O	80.36400	58.52880	89.88090	469.97125	545.56725	-349.32487	1
32271	N	82.22900	57.62180	90.79390	-78.06647	-700.07091	436.85908	1
32272	H	83.21700	57.48780	90.80390	-2534.45505	1345.48651	1292.96103	1
32273	C	81.49200	56.95580	91.86190	-487.74723	594.32740	492.92487	1
32274	H	82.21900	56.51580	92.52890	413.54977	-2009.28391	-2389.21436	1
32275	C	80.59000	57.87080	92.75390	-493.02373	-647.93847	382.99562	1
32276	H	79.86600	58.38380	92.08590	1814.09800	1163.64728	2284.75869	1
32277	H	80.09300	57.24080	93.52290	2200.30492	-1689.83163	-1480.28349	1
32278	C	81.46100	58.86380	93.52190	-584.54069	617.34695	-362.48102	1
32279	C	82.52500	58.47380	94.32090	-98.18249	-748.52573	483.19915	1
32280	H	82.86400	57.44780	94.30990	2839.42747	-949.13249	941.11310	1
32281	C	83.30600	59.40880	95.01490	402.60370	474.92503	659.68400	1
32282	H	84.13400	59.10480	95.63690	2264.44592	-1678.40725	-1401.54481	1
32283	C	82.96400	60.78380	94.84590	563.53618	520.81291	490.47088	1
32284	H	83.47000	61.57380	95.38290	2292.18019	1114.29273	1838.64036	1
32285	C	81.16500	60.24680	93.35090	629.91120	606.60150	269.10958	1
32286	H	80.29800	60.48480	92.75290	-1224.70819	2171.61707	-1943.43482	1
32287	C	81.88600	61.18680	94.02290	-515.79364	745.35991	144.73327	1
32288	H	81.69100	62.24580	93.93990	-140.36455	-1675.54576	2640.01771	1
32289	C	80.76400	55.70980	91.43490	-504.13368	202.15456	-749.76495	1
32290	O	79.70800	55.31080	91.95290	-24.04880	620.50746	490.74085	1
32291	N	81.30300	54.90280	90.49790	-617.94624	149.99776	-575.33461	1

32292	H	82.18100	55.22180	90.14890	-1244.24897	2127.67709	1956.36366	1
32293	C	80.71900	53.68480	89.94390	606.73743	608.24122	-328.64632	1
32294	H	79.65100	53.83680	89.97990	2828.57808	-1163.01308	-710.46131	1
32295	C	81.27100	53.31280	88.53290	-566.72496	465.30192	-570.03452	1
32296	H	80.83700	52.33080	88.24890	1571.64029	-2681.14450	386.08336	1
32297	H	82.36400	53.11580	88.57390	1251.29217	-2231.22628	-1827.48263	1
32298	C	80.98500	54.38180	87.51690	-848.58501	360.39891	7.56375	1
32299	H	81.51500	55.32680	87.76390	2389.39941	-718.56295	-1917.34494	1
32300	C	81.53700	54.10480	86.08490	664.30825	-461.27398	383.71387	1
32301	H	81.59600	55.10380	85.60390	-973.36839	2736.89360	1225.83570	1
32302	H	82.55700	53.69280	86.23790	-2218.68294	-2214.42940	-258.37391	1
32303	H	81.03200	53.33780	85.45890	-1653.18365	-2498.36828	934.14481	1
32304	C	79.54200	54.65580	87.23390	-445.08200	564.28187	-588.99003	1
32305	H	79.04100	54.79480	88.21590	-1495.25218	-1948.69432	-1969.75943	1
32306	H	79.34300	55.38180	86.41690	-2627.20932	1281.52689	1180.39373	1
32307	H	79.14800	53.69780	86.83090	-883.05889	-2181.11443	2068.05600	1
32308	C	80.97300	52.63780	90.95190	-300.45171	237.06057	820.17798	1
32309	O	82.06500	52.10580	91.11790	-632.48614	143.58949	447.74637	1
32310	N	79.89800	52.16980	91.66690	695.23852	-379.35941	253.17018	1
32311	H	78.97800	52.45280	91.40590	-687.34199	2400.66023	-1941.01641	1
32312	C	80.08900	51.23780	92.72590	-243.31557	614.19983	629.12578	1
32313	H	79.15000	50.75680	92.95390	2209.77301	-2218.12726	-165.99322	1
32314	H	80.83200	50.52280	92.40490	-1671.63628	2615.64544	-591.45752	1
32315	C	80.71500	51.67880	93.95290	771.53138	-234.04793	-425.55402	1
32316	O	81.35700	50.96780	94.71090	237.91767	-636.89593	369.81865	1
32317	N	80.54900	52.96080	94.25390	207.66595	-712.12561	369.57726	1
32318	H	80.17900	53.60180	93.58590	2799.01513	242.41081	1400.35984	1
32319	C	81.11800	53.58680	95.39990	-689.22983	609.40018	4.10284	1
32320	H	82.06300	53.10980	95.61590	-2116.10288	-2261.78720	502.26495	1
32321	C	81.44900	55.05980	95.20090	13.22712	-462.95655	766.60318	1
32322	H	82.12800	55.25980	94.34390	-3145.38988	78.61417	91.53296	1
32323	H	80.47800	55.52680	94.93090	1233.87354	-2872.83124	226.10698	1
32324	H	81.73900	55.58780	96.13490	-2909.88232	-1174.94390	-180.56684	1
32325	C	80.21700	53.42580	96.59890	722.57576	-543.91465	-14.31545	1
32326	O	79.01700	53.23880	96.46890	630.15673	-296.38846	350.00582	1
32327	N	80.81200	53.47280	97.79790	-256.21939	554.04513	581.04554	1
32328	H	81.79700	53.59180	97.89590	-556.29506	1907.40031	2434.61085	1
32329	C	80.10400	53.53380	99.00590	-86.06844	675.09153	607.05965	1
32330	H	79.05200	53.39680	98.80390	-474.73009	2341.44897	-2070.90970	1
32331	C	80.72100	52.50880	100.05290	231.30024	-418.38753	-783.03436	1
32332	H	81.81400	52.47280	99.85790	1870.18237	-1418.88159	-2101.20900	1
32333	H	80.40300	52.62580	101.11090	2231.36854	-1188.38464	1855.90206	1
32334	C	80.28200	51.06780	99.72490	737.46104	395.91688	361.64887	1
32335	H	80.89900	50.69980	98.87790	-911.09701	-2092.13002	-2168.12451	1
32336	H	80.52600	50.40280	100.58090	1206.52354	-2434.32879	1558.03600	1
32337	C	78.78400	50.94080	99.35690	-221.11000	-398.13074	-795.02963	1
32338	H	78.65100	51.25080	98.29890	591.51460	654.94278	-3032.97955	1
32339	H	78.23800	51.66280	100.00090	-865.23786	2010.51577	2259.56210	1
32340	C	78.18400	49.58980	99.52590	655.34469	489.27378	-426.64145	1
32341	H	78.30600	49.19080	100.55490	2210.94800	2217.86409	-387.64965	1
32342	H	78.65300	48.87980	98.81090	2547.64178	-712.11268	1685.33403	1
32343	N	76.74200	49.65680	99.25790	415.52107	507.09784	533.15188	1
32344	H	76.66100	49.91580	98.25390	-1362.60350	755.65257	2727.73054	1
32345	H	76.41300	50.36980	99.93990	2244.36875	-1603.46919	1490.61514	1
32346	H	76.27200	48.73580	99.36890	-545.96965	484.29116	3053.14800	1
32347	C	80.22600	54.95980	99.62690	-376.54837	-85.41008	-835.83006	1
32348	O	81.26600	55.62880	99.55690	-513.21508	-289.15555	-530.60141	1
32349	N	79.06500	55.53180	100.15290	73.02384	-555.61903	-632.40519	1
32350	H	78.24600	54.96680	100.20890	2166.30014	2086.81452	942.43584	1
32351	C	78.96600	56.92180	100.51590	-586.38377	-542.21914	-432.24606	1
32352	H	79.79100	57.47180	100.08790	-1672.91489	-822.10614	-2540.29097	1
32353	C	77.72400	57.53680	99.83390	626.09372	211.63557	-644.87986	1

32354	H	76.80700	57.08980	100.27490	1414.79815	-2612.05168	-1018.31711	1
32355	H	77.67100	58.59880	100.15690	-2145.38231	725.53115	-2194.27525	1
32356	C	77.84300	57.42380	98.31090	-240.82968	-865.00068	50.38071	1
32357	C	78.61700	58.35580	97.58790	107.01682	-776.10337	436.51896	1
32358	H	79.29400	59.02580	98.09690	-523.11899	2303.11860	-2101.38569	1
32359	C	78.64100	58.25080	96.16690	851.79055	-126.76383	-307.09045	1
32360	H	79.20400	58.96380	95.58290	-2919.83167	1102.36809	412.40239	1
32361	C	77.93600	57.23580	95.50590	-630.18942	-481.52969	426.88746	1
32362	H	78.04600	57.12480	94.43790	1997.96235	263.06665	-2426.75801	1
32363	C	77.15700	56.45480	97.64590	578.79407	-606.71398	328.71700	1
32364	H	76.68800	55.65580	98.20190	-266.38515	-1279.88705	2846.65035	1
32365	C	77.20800	56.31680	96.28190	561.28466	459.04623	-572.47939	1
32366	H	76.74300	55.47580	95.78890	-2001.91674	2400.23580	428.33528	1
32367	C	78.97800	57.25380	102.00090	-764.49818	360.58731	333.63651	1
32368	O	79.06900	58.41480	102.47090	130.24651	460.28775	626.56437	1
32369	N	78.95100	56.16180	102.83090	544.39513	-546.36686	-342.38918	1
32370	H	78.58300	55.30280	102.48390	-2357.14231	1748.36662	-1154.28120	1
32371	C	78.88800	56.33080	104.26790	680.57491	-586.56676	-144.92238	1
32372	H	78.72600	57.37580	104.48790	2703.79390	387.34412	1563.45970	1
32373	C	77.73800	55.52780	104.91990	589.31152	-596.30820	-357.57514	1
32374	H	77.73700	55.67180	106.02190	-2145.97155	2298.80116	178.81571	1
32375	H	78.02200	54.47280	104.71790	858.87345	-2360.13672	-1892.73373	1
32376	C	76.39500	56.07880	104.37490	-382.48423	-443.83386	-696.97184	1
32377	H	76.33400	56.03080	103.26590	2426.22609	-1965.44537	-358.02120	1
32378	H	76.43600	57.17880	104.52490	2448.86545	853.34661	1785.87415	1
32379	C	75.12500	55.41780	105.00790	102.52979	-440.22752	-793.70981	1
32380	H	74.21200	55.89580	104.59090	-824.48515	-2222.68743	-2059.71800	1
32381	H	75.24900	55.59280	106.09790	-2540.14525	-773.47962	-1680.67059	1
32382	C	75.05000	53.89580	104.84890	-163.32800	-537.48876	-715.73298	1
32383	H	75.91600	53.36880	105.30390	2469.78929	-374.49775	-1925.19752	1
32384	H	74.88900	53.64780	103.77790	-1769.74189	2609.38066	96.25443	1
32385	N	73.87300	53.41980	105.56690	-546.32103	363.44572	-542.51098	1
32386	H	74.07600	53.58480	106.57290	2820.35617	-447.75867	-1335.62370	1
32387	H	73.01100	53.99980	105.60990	-235.99991	2593.47792	-1791.45915	1
32388	H	73.73800	52.42180	105.30890	1435.84397	1849.15444	2108.80301	1
32389	C	80.16700	55.94380	104.98190	-560.70932	-624.34960	316.12228	1
32390	O	80.39300	56.21780	106.18890	-468.43990	-340.24339	-536.17848	1
32391	N	81.09000	55.32780	104.18990	-618.85302	61.12308	554.41531	1
32392	H	80.83000	54.95680	103.30190	-1474.70260	1679.41001	2207.39620	1
32393	C	82.53200	55.16980	104.40690	226.97598	836.93629	299.75556	1
32394	H	82.59600	54.28380	105.02190	-3139.59480	-62.53534	57.01697	1
32395	C	83.29300	54.91580	103.09090	67.02435	753.82403	-536.72137	1
32396	H	82.81500	54.08480	102.53090	-1220.93896	-2194.25673	1868.57687	1
32397	O	84.67700	54.54080	103.24590	-721.20436	-100.97142	-307.62278	1
32398	H	84.78500	53.96080	104.00290	-300.16618	-2252.79782	-2180.49232	1
32399	C	83.23200	56.06680	102.10790	-552.77462	-364.72397	604.09919	1
32400	H	83.45200	55.63380	101.10790	-1789.52965	-2541.52033	407.56208	1
32401	H	83.82700	56.93980	102.45090	-1816.77045	-618.72992	2473.41509	1
32402	H	82.23100	56.54280	102.03790	1184.22351	2435.35339	-1632.45637	1
32403	C	83.20700	56.25880	105.24790	-479.70534	587.93305	-524.59919	1
32404	O	83.00500	57.44880	105.00190	553.33140	-557.71362	-62.93366	1
32405	N	83.99000	55.88980	106.24490	535.97578	249.44015	-626.12065	1
32406	H	84.16600	54.94980	106.52790	94.24078	-75.13878	3129.45763	1
32407	C	84.73700	56.88680	106.99290	828.39334	-375.44086	-112.51683	1
32408	H	84.96900	57.66880	106.28490	-1997.62984	1625.24185	-1822.00218	1
32409	C	83.91500	57.42980	108.20490	909.90033	130.88913	-75.33771	1
32410	H	84.21500	58.48080	108.40390	67.35161	-2959.56220	1026.20174	1
32411	H	82.85200	57.49980	107.89190	1206.34316	1407.06875	2537.98814	1
32412	O	83.89700	56.69080	109.40790	-22.53382	786.12027	123.22499	1
32413	H	83.44200	57.18580	110.09290	1301.95044	1820.04558	2210.78632	1
32414	C	86.04500	56.31880	107.48390	917.63767	-45.39540	-13.24045	1
32415	O	86.23700	55.11080	107.49890	231.63496	394.58535	-666.70978	1

32416	N	86.96200	57.19680	107.92490	600.44583	-107.49396	-606.35524	1
32417	H	86.55800	58.10780	107.88190	-188.58680	-3009.43680	852.63068	1
32418	C	88.24100	56.92680	108.44490	-36.34437	46.93780	-926.84107	1
32419	H	88.79900	56.31480	107.75190	-2305.97925	-384.33194	2078.49013	1
32420	C	88.99900	58.27680	108.62790	537.21340	282.37855	-707.74217	1
32421	H	88.48300	58.99280	109.30190	1626.38429	2521.91073	963.16930	1
32422	H	90.03800	57.98680	108.89590	2287.21325	-1509.30344	-1570.49678	1
32423	H	89.10200	58.71980	107.61390	-2184.71927	-1981.49967	1047.43683	1
32424	C	88.23700	56.08880	109.70490	645.63476	283.18038	574.40538	1
32425	O	89.01500	55.11480	109.84290	677.23446	-402.00685	77.73465	1
32426	N	87.28400	56.41280	110.61790	552.10341	470.72015	-467.81316	1
32427	H	86.91200	57.33580	110.56290	2031.94932	-1404.19530	1937.25401	1
32428	C	86.97200	55.47480	111.74990	-579.34132	-403.60153	-577.47953	1
32429	H	87.90700	55.26180	112.24790	2305.30646	499.27003	-2111.61159	1
32430	C	85.97400	56.15380	112.70390	-429.80708	343.46215	709.02082	1
32431	H	85.55200	55.42080	113.42490	-2647.64982	-427.95527	1609.52277	1
32432	H	85.16200	56.58080	112.07790	1396.94224	-1323.43221	2475.46296	1
32433	C	86.51500	57.41880	113.51390	-513.15254	597.85685	440.05693	1
32434	H	85.63700	57.75580	114.10590	-391.24881	-2858.48703	-1246.99831	1
32435	H	86.86800	58.20880	112.81690	3091.69406	302.81542	553.74552	1
32436	C	87.65700	56.97980	114.46190	-367.43622	550.91220	-642.56472	1
32437	O	87.51800	56.06080	115.23690	-556.36580	-224.00960	-513.06544	1
32438	N	88.78900	57.67580	114.32290	118.37500	844.45698	-21.88573	1
32439	H	88.76800	58.52780	113.79990	-1534.58681	-1692.37107	2131.50793	1
32440	H	89.56800	57.40480	114.88790	37.97872	-2343.57200	-2109.28252	1
32441	C	86.38100	54.13380	111.32290	189.03888	35.34435	-909.29419	1
32442	O	86.84900	53.05580	111.69790	-195.96565	-499.95573	552.91823	1
32443	N	85.41700	54.13580	110.31590	-568.46982	-489.00347	-379.16066	1
32444	H	85.05700	54.93680	109.84490	1275.32850	-2482.68913	1429.57713	1
32445	C	84.85500	52.81180	109.85490	424.05886	495.78782	-663.45005	1
32446	H	84.53200	52.34680	110.77490	307.24364	-718.53995	-3060.90627	1
32447	C	83.70500	53.01180	108.93090	-8.29458	-666.08801	-626.65204	1
32448	H	84.01300	53.65080	108.07590	1435.61263	-2791.68566	-124.44619	1
32449	H	83.34100	52.09480	108.41990	2246.11150	-1313.12220	-1783.77069	1
32450	N	82.20500	53.38680	110.95190	-126.67582	-103.77305	-838.62779	1
32451	H	82.76300	52.85980	111.59290	2117.85499	344.86873	-2323.70325	1
32452	C	82.52300	53.64980	109.61990	-538.58507	-352.92670	620.40431	1
32453	C	81.11100	54.09780	111.23090	-443.82078	129.83631	770.04170	1
32454	H	80.61100	53.96480	112.18990	525.18778	-1075.33595	-2919.53326	1
32455	N	80.67200	54.79180	110.20390	-663.54408	-486.01739	108.62602	1
32456	C	81.57800	54.50080	109.14890	-407.35767	180.76753	781.08490	1
32457	H	81.39700	54.85780	108.14190	-2402.51065	-1623.43899	1180.32516	1
32458	C	85.90800	51.89980	109.19590	-50.39442	509.03870	744.30720	1
32459	O	85.88900	50.70180	109.38790	753.45372	-246.61610	-38.37474	1
32460	N	86.82900	52.50780	108.42890	441.28187	-688.99297	178.53442	1
32461	H	86.68300	53.45680	108.15990	2069.66316	-2365.90214	-99.10149	1
32462	C	88.02200	51.87180	107.84890	688.27057	546.32583	-291.46500	1
32463	H	87.57200	51.13580	107.19990	-1838.69647	-2530.76370	217.86190	1
32464	C	88.70700	52.92580	106.97790	-737.48048	-511.89825	81.05634	1
32465	H	89.07900	53.71380	107.66690	1488.97869	-2236.34857	-1650.86987	1
32466	H	88.02500	53.45380	106.27890	1603.67476	-2647.15507	527.65388	1
32467	H	89.64100	52.60980	106.46590	-665.57603	1174.35123	2825.43346	1
32468	C	88.99100	51.29980	108.85590	662.34317	-493.32636	-405.75302	1
32469	O	89.45100	50.19180	108.67390	-261.65864	-69.91751	-757.06497	1
32470	N	89.27600	51.98380	109.97890	-423.34352	-542.58992	456.87433	1
32471	H	88.76800	52.80380	110.22890	-903.27617	-2817.07755	1027.70755	1
32472	C	90.10100	51.42580	111.06990	-677.77473	558.66479	219.57126	1
32473	H	91.01100	51.07180	110.60790	-930.47370	2658.46211	-1427.54856	1
32474	C	90.26000	52.46080	112.19890	-141.42683	-546.54111	-727.71421	1
32475	H	90.54900	51.99480	113.16490	-2804.08965	1362.00507	361.58139	1
32476	H	89.29800	53.00080	112.32690	-1958.27499	1892.76540	1553.92597	1
32477	C	91.46800	53.42280	111.91590	556.92658	-528.54979	476.48387	1

32478	H	91.24700	53.92980	110.95190	953.85793	-922.81861	2834.40017	1
32479	C	91.52600	54.66780	112.80790	-314.13062	-538.04038	636.84180	1
32480	H	91.94300	54.47580	113.81990	-1359.47703	-1631.34440	-2330.46367	1
32481	H	92.19500	55.45480	112.39790	-1471.88071	2661.92561	-823.05063	1
32482	H	90.49100	55.02780	112.99190	-1669.96531	1667.40647	-2095.75671	1
32483	C	92.83900	52.70780	111.87190	-392.29408	627.46774	-552.64167	1
32484	H	92.94400	52.02380	111.00290	-144.09324	-2003.28755	2396.47239	1
32485	H	93.60500	53.51180	111.82990	2256.54541	2163.60661	413.01939	1
32486	H	93.04000	52.07480	112.76290	1897.92658	1850.00731	-1731.33686	1
32487	C	89.46100	50.19980	111.71690	-546.91651	184.12374	683.72616	1
32488	O	90.15700	49.23380	112.03990	-660.86318	423.62098	-71.99281	1
32489	N	88.19500	50.21680	112.07190	512.32861	-563.11444	347.47432	1
32490	H	87.72300	51.07580	111.88590	-1717.65592	1965.25564	-1773.72234	1
32491	C	87.47100	49.11180	112.69890	402.48780	409.56070	700.32840	1
32492	H	88.04300	48.79080	113.55590	-2395.85916	-1912.79969	639.68946	1
32493	C	86.10000	49.48680	113.13590	610.31903	-195.95025	-669.58762	1
32494	H	85.43700	48.61080	113.30090	-2432.08034	-188.42573	-1991.48227	1
32495	O	85.50100	50.38680	112.30590	211.72794	666.25177	371.08771	1
32496	H	85.67800	50.08280	111.41290	-2035.97019	398.77427	-2375.60529	1
32497	C	86.15600	50.20880	114.52090	-417.50594	247.43368	-785.04234	1
32498	H	85.14000	50.56980	114.78890	-2904.16721	71.56657	-1199.41188	1
32499	H	86.84200	51.06980	114.37390	-865.02880	-2989.99615	366.57505	1
32500	H	86.58700	49.54880	115.30390	-2511.68353	-1559.78719	-1056.76324	1
32501	C	87.33200	47.86380	111.81290	744.80487	-522.76955	57.67122	1
32502	O	87.28100	47.98280	110.59890	402.39456	-495.03956	445.80702	1
32503	N	87.22900	46.69980	112.39890	-242.67095	620.68205	-540.68283	1
32504	H	87.31500	46.64780	113.38990	1729.62744	-1486.34161	-2184.69147	1
32505	C	87.00800	45.43480	111.73590	791.98919	-452.63825	20.66169	1
32506	H	87.60700	45.49580	110.83890	772.71066	2909.66433	-958.62063	1
32507	C	87.63800	44.22280	112.49690	-382.15012	-647.32428	485.21967	1
32508	H	87.57500	43.32580	111.84390	-1407.57220	-1571.94903	-2342.49959	1
32509	H	88.73700	44.38180	112.50190	-2504.94286	-1306.92374	1348.91369	1
32510	O	87.05400	43.98480	113.80390	460.02615	482.54226	422.14411	1
32511	H	87.22400	44.78680	114.30390	-836.52768	-2904.40762	-857.31163	1
32512	C	85.56100	45.12680	111.38790	-845.83549	-296.14054	-134.24093	1
32513	O	84.61300	45.60580	112.09190	51.26018	714.19071	-366.88753	1
32514	O	85.32200	44.42480	110.35290	-396.10698	256.28545	618.41111	1
32515	H	80.82215	98.05265	69.46570	-1722.80870	2452.96674	-1684.87021	2
32516	N	80.36465	98.52010	68.68823	-362.10539	-216.96359	-939.05573	2
32517	H	79.70288	99.08717	69.24899	793.58777	-572.78644	-678.75801	2
32518	C	81.37995	99.17447	67.92789	-247.41922	-586.37737	762.26364	2
32519	H	82.22606	98.47990	68.20366	-792.18825	-1465.38338	-1102.96003	2
32520	C	80.91617	99.26779	66.40562	-1446.47398	297.46796	413.82015	2
32521	H	79.81838	98.94535	66.42829	933.16259	1674.03979	-1699.15474	2
32522	H	80.82128	100.33868	66.23560	2559.92530	-1725.53957	-3090.14481	2
32523	C	81.89686	98.63764	65.42543	204.04462	-127.42867	-779.55184	2
32524	H	82.82619	99.20376	65.77706	-1023.56979	2490.45965	-697.12994	2
32525	C	81.99932	97.13863	65.63662	1328.18948	-19.92412	-110.78277	2
32526	H	82.98851	96.88823	65.19630	575.37954	-86.76769	594.43652	2
32527	H	82.00447	96.87207	66.72210	-4986.08861	875.61138	-177.77865	2
32528	H	81.22985	96.59493	65.01567	3284.46324	900.96957	471.67839	2
32529	C	81.67317	98.98721	63.95615	1443.09491	-251.67019	-1395.51788	2
32530	H	80.80320	98.43554	63.59032	-2188.07081	-994.37641	329.66289	2
32531	H	81.47005	100.13261	63.87146	1796.03379	-489.19527	-3889.84459	2
32532	H	82.54923	98.74141	63.28172	938.78437	1163.80595	-2139.71128	2
32533	C	81.36720	100.61475	68.64249	-568.39754	719.50790	-152.88643	2
32534	O	81.18925	101.71016	67.92438	-211.17050	578.47103	579.79453	2
32535	N	81.57417	100.60193	69.92777	-495.56841	-140.34125	360.58702	2
32536	H	81.74876	99.73052	70.37248	1585.51105	-2403.85695	1589.43725	2
32537	C	81.34943	101.86023	70.60495	-222.44344	180.56490	-834.46550	2
32538	H	80.49972	101.46272	71.20769	2274.24879	1423.83956	-2626.39297	2
32539	C	82.68625	102.23167	71.31382	-72.63979	288.66493	-31.98550	2

32540	H	83.45919	102.57313	70.58538	-993.03836	193.50043	691.66317	2
32541	O	83.31097	101.01211	71.96987	-651.55815	-213.83574	-136.12784	2
32542	H	84.21622	101.35098	71.99311	-97.20366	-1785.33276	-4312.75785	2
32543	C	82.16323	103.41307	72.20701	-190.18460	35.33660	132.54657	2
32544	H	81.44615	103.12806	73.06553	18.30012	294.59348	-637.80918	2
32545	H	83.02790	103.85200	72.71153	-483.48557	953.56155	-634.93430	2
32546	H	81.59398	104.20972	71.51267	-2699.48767	1983.42087	3014.69743	2
32547	C	80.92413	103.02302	69.44393	230.24359	-637.18080	-204.53045	2
32548	O	81.81256	103.94785	69.27852	393.37713	-170.71972	-110.09570	2
32549	N	79.61324	103.24130	69.55948	168.21611	-713.07586	-807.46838	2
32550	C	79.11014	104.36616	68.76986	239.77204	-199.65950	-800.84308	2
32551	H	79.59994	104.24805	67.82133	-1227.65396	-824.86734	-2016.77797	2
32552	C	77.56079	104.02099	68.77710	-494.27190	-559.92730	-454.26074	2
32553	H	77.06729	104.39698	69.64664	500.48235	346.73829	2546.55610	2
32554	H	77.11472	104.54293	67.97400	453.97900	811.93413	-3687.81404	2
32555	C	77.39436	102.47170	68.76093	-564.74566	-181.00082	1811.69772	2
32556	H	76.39729	102.10372	69.19543	-2723.17737	1024.80989	-2060.20368	2
32557	H	77.50159	101.99427	67.79109	401.01597	1003.54666	643.75039	2
32558	C	78.66566	102.13565	69.67556	55.38086	-150.25104	622.47815	2
32559	H	78.53834	102.08092	70.79047	-3772.05203	-3225.87574	533.23633	2
32560	H	79.23220	101.14256	69.40381	1978.96279	-1139.30071	1025.27563	2
32561	C	79.25617	105.81515	69.45009	-88.00949	-511.99841	-389.83817	2
32562	O	78.45850	106.65411	69.01811	579.26157	-682.93442	885.41586	2
32563	N	80.06917	105.94384	70.46710	-689.48689	-62.67373	240.71906	2
32564	H	80.49615	105.17939	70.98673	-244.53944	2993.47241	-1262.01247	2
32565	C	80.43575	107.24319	70.82954	-1615.67464	278.14047	318.83721	2
32566	H	79.62159	107.96036	70.65371	-385.64829	-1368.17626	151.00516	2
32567	C	81.02339	107.36820	72.34252	642.92233	1305.91022	129.05681	2
32568	H	81.69356	108.25622	72.16707	1701.65117	-1259.70170	-249.88813	2
32569	O	81.78311	106.25559	72.76033	1124.04312	119.15940	-738.92509	2
32570	H	82.75898	106.55532	72.63165	-2293.42208	-2897.66960	1653.37734	2
32571	C	79.80785	107.90939	73.13747	40.97404	275.30296	-315.41867	2
32572	H	78.95358	107.24088	72.87836	1058.86596	2189.41298	1434.79342	2
32573	H	80.01630	107.93807	74.30057	1826.93297	771.24140	1770.31698	2
32574	H	79.44226	108.95372	72.84265	904.07462	-369.26115	495.55603	2
32575	C	81.79909	107.61533	70.02913	-357.61219	-332.17751	-277.47885	2
32576	O	82.07780	108.80225	69.94427	592.78335	514.40552	-33.62968	2
32577	N	82.40289	106.60482	69.33947	-814.66403	142.49613	467.99801	2
32578	H	82.00819	105.66157	69.45346	-1114.30401	-633.12305	1457.93000	2
32579	C	83.82973	106.74723	69.30825	-760.71563	105.88001	-320.81898	2
32580	H	83.93605	107.92264	69.26814	2293.96351	710.66957	1571.93963	2
32581	C	84.51109	106.09508	70.48841	-259.52267	-277.23987	179.82183	2
32582	H	84.35139	105.02546	70.79433	-1509.95676	-2252.38337	-2581.51618	2
32583	H	85.57009	106.12045	70.31305	2152.29124	344.74115	43.40142	2
32584	O	84.21755	106.69329	72.09154	-229.43411	-242.12849	-43.06365	2
32585	H	84.45631	105.91246	72.56651	2104.79626	2180.70200	1353.67139	2
32586	C	84.48661	106.10285	67.93905	323.71157	-53.52646	344.63696	2
32587	O	85.42047	106.62991	67.38038	261.78404	133.27977	1098.16953	2
32588	N	83.88525	104.90646	67.78284	1046.68270	-26.56105	108.50046	2
32589	H	83.06874	104.69491	68.42264	976.17577	-370.94322	-1184.11672	2
32590	C	84.29941	104.17974	66.62140	-653.40921	55.02580	245.24670	2
32591	H	85.31623	104.52126	66.23102	1562.21855	-287.56173	-2298.48661	2
32592	C	84.23210	102.67315	67.10136	-235.65654	-223.03054	479.79405	2
32593	H	83.45891	102.44416	67.84449	923.54081	826.40461	2022.83954	2
32594	C	84.21435	101.56927	65.96810	-751.70911	353.61277	569.31867	2
32595	H	84.84425	101.92683	65.13039	3763.44150	803.38613	1037.97040	2
32596	H	84.58267	100.55869	66.34350	-2759.76564	-762.20860	666.54728	2
32597	H	83.19776	101.46065	65.49992	1291.06420	1789.94700	-1771.28515	2
32598	C	85.56259	102.42684	67.89431	-399.80690	-55.59636	-42.12613	2
32599	H	86.37703	102.42118	67.11878	116.10226	3550.84552	2519.27005	2
32600	H	85.70872	103.22670	68.66271	1130.14515	-312.84297	-918.65095	2
32601	H	85.59950	101.46935	68.46029	-323.85397	-1871.73780	-3988.71149	2

32602	C	83.00080	104.47872	65.61780	-1142.08583	364.90442	1753.85233	2
32603	O	81.85783	104.82239	65.95744	771.92526	-77.52817	-276.20418	2
32604	N	83.49704	104.35560	64.36052	-87.46003	-124.96520	-4.50417	2
32605	H	84.47428	104.16343	64.40215	1133.84163	1656.52833	-2654.62031	2
32606	C	82.99471	105.23329	63.37837	42.09818	331.40654	593.66963	2
32607	H	81.89612	105.08026	63.60421	-413.56921	1909.01411	1161.10416	2
32608	C	83.36047	106.78491	63.59483	-821.53400	-555.06023	-222.82849	2
32609	H	84.43178	106.88573	63.35042	-185.09017	1386.25234	-1070.63459	2
32610	H	82.74520	107.38578	62.88644	1934.56010	1217.63163	1995.40380	2
32611	C	83.15478	107.18230	65.09179	-72.98875	1007.10969	-1022.08812	2
32612	H	82.13801	106.77431	65.39837	-2334.25761	2217.41653	-4593.18065	2
32613	H	83.88882	106.62449	65.70713	2557.64583	1707.73928	369.87527	2
32614	C	83.37536	108.75597	65.27136	424.12674	-81.33255	-83.27374	2
32615	O	82.68451	109.55471	64.68191	-398.24704	-139.76508	609.65246	2
32616	N	84.30769	109.14695	66.21889	-252.41521	478.92912	604.72119	2
32617	H	84.77621	108.45025	66.87334	-1237.74354	-304.06024	-384.81466	2
32618	H	84.38156	110.12849	66.36659	-4561.04276	1185.85213	1255.40731	2
32619	C	83.35456	104.90578	61.81964	261.68233	-827.32746	84.77432	2
32620	O	83.82762	105.71189	61.03600	257.28369	-167.23181	-16.52289	2
32621	N	82.99958	103.64526	61.59715	-328.33042	-153.45361	-566.14718	2
32622	C	83.02846	103.11120	60.24967	259.97891	-927.04375	356.45171	2
32623	H	84.00787	103.44067	59.78909	-1940.63466	272.45527	-3246.17264	2
32624	C	83.02962	101.55640	60.42674	166.16917	-43.04040	378.33286	2
32625	H	82.47867	101.24737	59.52897	-2.16145	3171.53329	-4548.51945	2
32626	H	84.07371	101.13149	60.37172	-76.81197	3504.52170	2378.83500	2
32627	C	82.31278	101.28836	61.80873	93.97130	310.60895	464.40221	2
32628	H	81.24702	101.20655	61.69370	520.63330	-1032.32572	10.74193	2
32629	H	82.50196	100.30409	62.22660	-1674.83005	1801.50204	1326.99758	2
32630	C	82.81775	102.58699	62.57812	112.17731	446.56470	-190.58200	2
32631	H	82.11303	102.94583	63.40878	430.61373	2099.68538	-1749.35786	2
32632	H	83.81301	102.54015	63.03563	703.58234	-342.75310	3692.76274	2
32633	C	81.76623	103.49065	59.26706	101.88861	-141.27321	-834.01307	2
32634	O	81.75589	103.68648	58.07426	-805.25184	-279.38208	-71.86663	2
32635	N	80.65706	103.46888	60.01745	-111.48782	-158.69762	-103.55293	2
32636	H	80.80634	103.24214	60.98193	-116.69406	320.28076	-5658.83667	2
32637	C	79.74138	104.60697	59.84332	-207.49935	399.80654	-943.48097	2
32638	H	80.18810	105.12481	58.97738	-692.75824	3185.11890	-1020.17880	2
32639	C	78.24472	104.17416	59.65955	119.40178	583.22459	233.47652	2
32640	H	77.86968	103.38793	60.38468	2790.28611	-1235.93734	-436.82161	2
32641	C	77.40568	105.47151	59.48217	192.33257	163.96249	856.16500	2
32642	H	76.35298	105.14503	59.27617	-1378.88970	4362.91328	-1289.77859	2
32643	H	77.46832	106.05380	60.43836	-920.02341	-3166.45322	1359.63902	2
32644	H	77.78904	106.13238	58.66968	873.58158	-0.53138	2176.58568	2
32645	C	78.21873	103.64099	58.17629	-481.92560	103.80138	69.50683	2
32646	H	77.26911	103.32302	57.83571	-1386.00575	-76.80329	-81.77763	2
32647	H	78.51440	104.43226	57.43523	-441.44576	120.39197	-1374.47699	2
32648	H	78.92034	102.76973	58.20636	632.68587	-2796.69591	-1598.17214	2
32649	C	79.95384	105.42767	61.22926	106.21536	206.32759	768.73877	2
32650	O	79.96559	104.97916	62.36583	28.71869	-389.11397	-357.93512	2
32651	N	79.97371	106.69002	60.81335	-327.29353	-450.31307	-547.65144	2
32652	H	80.28518	106.86426	59.84295	-1002.26390	284.09907	43.35368	2
32653	C	80.13735	107.77186	61.70709	572.11748	290.39355	-248.31784	2
32654	H	80.54746	107.14966	62.53153	-1790.19070	412.38101	2272.99909	2
32655	C	81.19650	108.81595	61.01164	-44.78165	85.99515	-324.94739	2
32656	H	81.37373	109.56973	61.81921	424.74761	2108.23265	-441.90162	2
32657	H	82.09081	108.22494	60.87149	720.04050	-2428.86923	-224.80960	2
32658	C	80.77571	109.66301	59.79630	1316.38518	294.38043	-1098.76047	2
32659	H	79.73512	109.98855	60.02284	-5560.84232	-2626.15249	-781.87239	2
32660	H	81.33477	110.62977	59.78319	383.78834	-161.19252	-1981.20107	2
32661	C	80.72165	108.88736	58.42023	-4.64935	112.57809	194.91871	2
32662	H	79.97819	108.02160	58.48764	-2791.30064	-2255.02493	-2189.95102	2
32663	H	80.29496	109.46454	57.58257	2112.56239	-2405.04947	465.42201	2

32664	C	82.12616	108.27147	57.97407	-193.96844	-670.62433	311.32578	2
32665	H	82.32728	108.31660	56.79662	1411.98200	-633.37159	1467.66748	2
32666	H	82.88722	108.77950	58.53761	1823.64782	2127.01899	-1331.60367	2
32667	N	81.91714	106.92913	58.46632	-221.56041	-460.27877	88.28827	2
32668	H	82.15860	106.19806	57.85459	112.88911	179.13741	-1666.61003	2
32669	H	76.73171	108.28985	58.15167	1703.22780	-1487.75943	-46.40517	2
32670	H	82.49667	106.60055	59.23268	1218.92618	626.11583	-1083.73460	2
32671	C	78.69778	108.33260	62.12692	-324.13154	-37.65883	-309.96996	2
32672	O	77.68697	107.59007	62.17517	-339.38433	-32.63882	178.39908	2
32673	N	78.75699	109.66182	62.21439	-291.37413	-133.32833	-39.33079	2
32674	H	79.61043	110.18933	62.08505	1718.47239	-37.95484	-1947.96525	2
32675	C	77.54936	110.25146	62.69155	601.48599	846.25465	608.70721	2
32676	H	76.99627	109.37542	63.29197	-1032.46796	-2150.51828	-1912.79926	2
32677	C	77.70835	111.57753	63.59729	130.58678	298.43566	431.26394	2
32678	H	78.54257	111.37126	64.35523	-1010.65324	-1361.87726	-474.27170	2
32679	H	78.18755	112.37495	62.93687	-398.69490	1499.18089	2511.10270	2
32680	C	76.35979	112.00872	64.26304	412.28499	257.52543	193.95855	2
32681	H	76.41625	111.24477	65.12723	-160.89585	-1548.76795	69.43531	2
32682	H	76.47927	112.93264	64.88905	-553.63910	626.51950	945.67730	2
32683	C	75.05642	112.03213	63.37507	-103.44680	93.93538	130.58324	2
32684	H	74.97541	112.88164	62.67769	489.97984	3033.61726	-914.44519	2
32685	H	74.99108	111.17019	62.68706	-488.32046	-1224.53196	1946.72478	2
32686	C	73.84509	112.05100	64.38282	-163.57920	-1247.54711	-494.87443	2
32687	H	73.87035	112.75105	65.24217	306.78583	488.45920	-2091.65456	2
32688	H	72.85420	112.25465	63.84985	920.38046	1833.83538	-208.74551	2
32689	N	73.85578	110.60975	64.90083	717.05145	-31.56555	314.75999	2
32690	H	74.55328	110.06699	65.50119	-329.57964	719.69917	1787.41788	2
32691	H	72.95732	110.49969	65.47422	421.01128	1781.92838	-846.51534	2
32692	H	73.67780	109.94187	64.00525	956.37744	71.70507	-3634.90758	2
32693	C	76.74312	110.46523	61.32540	-648.38703	-119.86110	-441.12770	2
32694	O	76.84675	111.44923	60.59872	-18.65939	-541.64020	-427.58682	2
32695	N	76.21453	109.26360	60.89048	-56.49688	381.87614	-137.23701	2
32696	H	76.21555	108.50810	61.66153	-210.22255	-3150.88112	1739.11990	2
32697	C	74.89665	109.49768	60.23084	-68.56014	703.26449	-408.19563	2
32698	H	74.85703	110.58596	60.02827	-331.07078	1765.42448	42.37446	2
32699	C	74.93771	108.74021	58.89815	267.87650	111.23751	-1296.83700	2
32700	H	74.99922	107.65901	59.07129	-1073.13854	-4912.93823	615.71867	2
32701	O	76.42902	109.23614	58.04165	-347.17158	-124.09891	64.85074	2
32702	H	76.79209	109.67062	58.86915	-167.86846	-673.85787	-3097.66766	2
32703	C	73.72359	109.22538	58.11811	-219.64396	211.48239	435.96944	2
32704	H	73.67209	108.61046	57.16347	1438.98244	1558.46560	-666.48312	2
32705	H	72.72332	109.13647	58.71531	-1333.57173	-2445.60160	-188.14793	2
32706	H	73.71606	110.32958	57.89242	-2327.61301	3480.28895	-1166.12419	2
32707	C	73.81870	109.05266	61.34045	-957.86091	725.35972	-249.80515	2
32708	O	73.84988	109.47415	62.48890	-694.16353	285.50630	599.63370	2
32709	N	73.07674	108.04871	60.85402	-623.07067	77.49988	4.64075	2
32710	H	73.24653	107.90223	59.81490	-3233.60423	-2716.36180	2501.49206	2
32711	C	72.85289	106.85050	61.63235	-97.91918	-117.38421	656.56389	2
32712	H	72.59265	107.23812	62.58988	550.81812	820.65804	1429.08376	2
32713	C	71.70905	106.18540	60.81379	294.97571	353.67349	249.84318	2
32714	H	70.88699	106.89762	60.58533	-1302.42048	1721.97937	2852.03260	2
32715	H	72.15525	105.92317	59.80707	1343.20437	849.56190	437.75662	2
32716	C	71.17787	104.98632	61.63634	1188.04146	-388.28108	372.20414	2
32717	C	69.85215	104.54478	61.46440	-640.87025	-809.93665	350.92364	2
32718	H	69.16442	105.03124	60.73553	-1712.67339	-109.88558	-799.97681	2
32719	C	72.00598	104.18710	62.53181	856.49879	735.12272	384.34779	2
32720	H	73.02974	104.53555	62.58530	-1006.96105	-1424.90921	852.77113	2
32721	C	69.45846	103.33838	62.08041	1697.46814	423.97032	86.83519	2
32722	H	68.42922	102.98258	61.83923	363.43309	744.74858	-625.57009	2
32723	C	71.62927	103.02014	63.18053	-872.33096	1019.39745	467.72340	2
32724	H	72.34154	102.53409	63.87596	1651.20755	982.44947	3759.68045	2
32725	C	70.27406	102.59525	63.02256	692.13691	-180.37761	435.72034	2

32726	O	69.80279	101.42353	63.55399	12.71728	375.23242	244.42712	2
32727	H	68.74319	101.67797	63.86070	590.40140	378.68277	2243.78418	2
32728	C	74.28951	106.01969	61.70900	-66.11665	-596.12993	-583.41315	2
32729	O	74.70947	105.26776	60.85837	-167.71200	342.91977	-278.24590	2
32730	N	74.97533	106.41744	62.82892	374.74238	-49.25944	-277.66275	2
32731	H	74.36793	107.04587	63.33683	1852.15925	721.56201	2504.77141	2
32732	C	75.54913	105.24437	63.52058	-514.46145	-97.22408	-359.52164	2
32733	H	74.67112	104.58968	63.81890	-575.59940	-285.03260	-2869.58998	2
32734	C	76.71835	104.70921	62.68871	302.54447	881.88048	426.12846	2
32735	H	76.40486	104.39868	61.66796	424.37839	2415.17530	-2939.09658	2
32736	H	77.55494	105.42452	62.58106	1159.34383	-2539.20383	261.03256	2
32737	C	77.11613	103.44564	63.57641	-426.83460	-189.70790	-284.58570	2
32738	H	77.68881	103.75440	64.51064	1039.51070	1388.30078	1234.69286	2
32739	H	76.20391	102.90905	63.95770	1919.85507	-293.75634	1555.60421	2
32740	C	78.13498	102.46758	62.84872	171.21741	50.77475	-543.30707	2
32741	H	77.62312	101.77560	62.09768	-1529.53774	-1855.36815	-1123.34697	2
32742	H	79.07909	102.94113	62.41158	4717.06897	-2704.93813	21.52905	2
32743	N	78.27212	101.81142	64.11049	298.18470	553.47645	896.18646	2
32744	H	77.57032	101.11341	64.23703	-859.25753	110.68558	3642.49857	2
32745	C	79.15489	102.15063	64.95534	-357.88198	901.31862	889.69542	2
32746	N	80.06741	103.14150	64.58634	-512.50367	-495.10753	19.34060	2
32747	H	79.95935	103.71128	63.69596	1997.08118	2526.08655	2923.47569	2
32748	H	80.77394	103.54132	65.17231	-994.04408	449.97619	-1969.52393	2
32749	N	79.11999	101.40611	66.13500	301.52636	-210.71778	-19.19699	2
32750	H	78.46103	100.60188	66.37910	3320.14592	-751.92475	1222.02221	2
32751	H	79.68750	101.64367	66.95438	164.10125	-782.11155	-906.28227	2
32752	C	76.09950	105.85388	65.00835	-298.72548	265.91294	-531.69628	2
32753	O	75.95521	105.13422	65.98003	-434.64710	-96.07774	159.54846	2
32754	N	76.93562	106.81573	64.88364	-243.87339	100.61097	-241.22865	2
32755	H	77.19060	107.19074	63.93462	1213.67290	2200.92692	-360.40496	2
32756	C	77.59061	107.37970	66.02849	69.89259	426.38634	153.76746	2
32757	H	77.53178	106.59702	66.74705	-2669.48639	517.52929	-58.88960	2
32758	C	79.02240	107.76764	65.44469	193.60668	-74.25999	738.52014	2
32759	H	78.94835	108.10465	64.42965	784.78485	4319.67770	-2020.19232	2
32760	C	79.71310	108.80897	66.41911	100.05027	-128.92068	-514.93474	2
32761	H	80.84298	108.65775	66.40530	-3304.48276	-1357.25270	484.63195	2
32762	H	79.50024	109.82871	66.19099	-1861.47189	334.25911	-2228.51195	2
32763	H	79.40649	108.62677	67.52017	3208.74646	242.91313	1753.49153	2
32764	C	79.71434	106.37438	65.45317	-397.95732	-690.17645	-83.46030	2
32765	H	79.19619	105.57736	64.79178	-1290.20540	-813.66840	537.58206	2
32766	H	80.70854	106.55088	64.97732	530.60170	-505.91681	1440.10567	2
32767	H	80.01992	106.05525	66.46537	-1353.78699	-638.27320	-638.07928	2
32768	C	76.64901	108.49764	66.69080	-800.09975	621.46328	-355.73009	2
32769	O	76.13449	109.39548	66.04364	238.83799	371.67426	-14.66455	2
32770	N	76.32054	108.17953	67.98375	-273.74490	-102.86358	-315.07790	2
32771	H	77.03990	107.47625	68.38302	773.68378	-71.07982	-173.92481	2
32772	C	75.78271	109.30754	68.73386	551.68812	452.95268	-215.05779	2
32773	H	75.16064	109.86053	68.02716	-3049.79366	-4211.34487	267.95301	2
32774	C	74.82339	108.64971	69.86353	-157.06009	180.66977	290.00359	2
32775	H	75.45621	108.00969	70.59655	1618.80402	-193.92917	-1557.70278	2
32776	H	74.33943	109.43876	70.52176	648.80358	154.81119	1463.66343	2
32777	C	73.62176	107.90724	69.36977	-616.27396	559.67943	1093.28200	2
32778	H	74.10765	106.92689	68.97334	1174.79681	-2469.85111	-738.41432	2
32779	C	72.46942	107.56082	70.32885	673.14909	-209.04313	-79.14929	2
32780	H	72.64787	106.60185	70.91711	-2144.26675	-1469.64673	253.17676	2
32781	H	72.17408	108.35553	71.07835	1906.47272	574.74690	-1346.21634	2
32782	H	71.56343	107.25366	69.79214	-71.37993	539.90747	2621.78151	2
32783	C	73.07118	108.66467	68.16297	-962.64665	-299.93624	-766.39534	2
32784	H	73.73295	108.51165	67.25032	-370.60976	-984.44500	-1946.91248	2
32785	H	72.12260	108.24181	67.75175	1418.00086	-2267.32226	-366.72047	2
32786	H	72.99787	109.76613	68.30534	152.40516	-1886.31741	-4963.28247	2
32787	C	76.98729	109.98392	69.48658	188.11000	178.55317	263.82267	2

32788	O	77.27079	110.07328	70.65321	564.15732	-722.51131	122.82518	2
32789	O	77.90566	110.37859	68.49286	192.88755	-41.69767	406.59763	2
32790	H	77.34710	110.11440	67.69072	-904.69670	-572.46502	-176.23615	2