

Theoretical study on epoxide ring-opening in CO₂/epoxide copolymerization catalyzed by bifunctional salen-type cobalt(III) complexes: influence of stereo-electronic factors

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Table S1. Relative electronic-energy (ΔE , in kcal/mol) of alternative local minima for RPO and SPO epoxide complexes for each group of considered stereoisomers of **1a** and **1b**. Dihedral angle ζ [in °] describes rotation of epoxide around $O_{(PO)}-Co$ bond, (see Figure 7 in the main manuscript). The relative electronic-energies of RPO/SPO complexes were calculated with respect to the lowest-energy RPO/SPO structure, while the numbers in parentheses correspond to the relative electronic-energy values calculated with respect to the ‘global minimum’ epoxide complex.

Stereoisomer	1a		1b	
	ζ	ΔE	ζ	ΔE
SS- δ -trans-RPO(out)	327	7.66	330	7.86
	135	1.19	134	1.17
	211	0.00	206	0.00
SS- δ -trans-RPO(in)	146	3.04	154	3.36
	154	3.22	278	17.97
	266	10.23	66	3.72
SS- δ - Λ -cis- β_1 -RPO	66	3.70	146	3.08
	295	10.49	344	15.21
	153	13.96	140	8.40
SS- δ - Λ -cis- β_2 -RPO	213	7.99	212	7.25
	310	5.65	307	2.74
	34	4.75	31	2.44
SS- δ -trans-SPO(out)	71	0.18 (1.06)	142	0.24 (1.16)
	143	0.23 (1.12)	262	6.19 (7.11)
	267	5.96 (6.85)	66	0.00 (0.92)
	67	0.00 (0.88)	---	---
	69	0.25 (1.14)	---	---
	141	0.21 (1.10)	---	---
SS- δ -trans-SPO(in)	209	2.55 (3.44)	207	3.44 (4.35)
	---	---	131	4.14 (5.05)
SS- δ - Λ -cis- β_1 -SPO	147	8.01 (8.89)	145	6.56 (7.47)
	263	13.99 (14.87)	266	12.61 (13.52)
	71	7.32 (8.21)	72	5.75 (6.67)
SS- δ - Λ -cis- β_2 -SPO	326	2.89 (3.77)	242	1.90 (2.82)
	246	4.91 (5.80)	318	0.92 (1.84)
	322	2.79 (3.68)	---	---

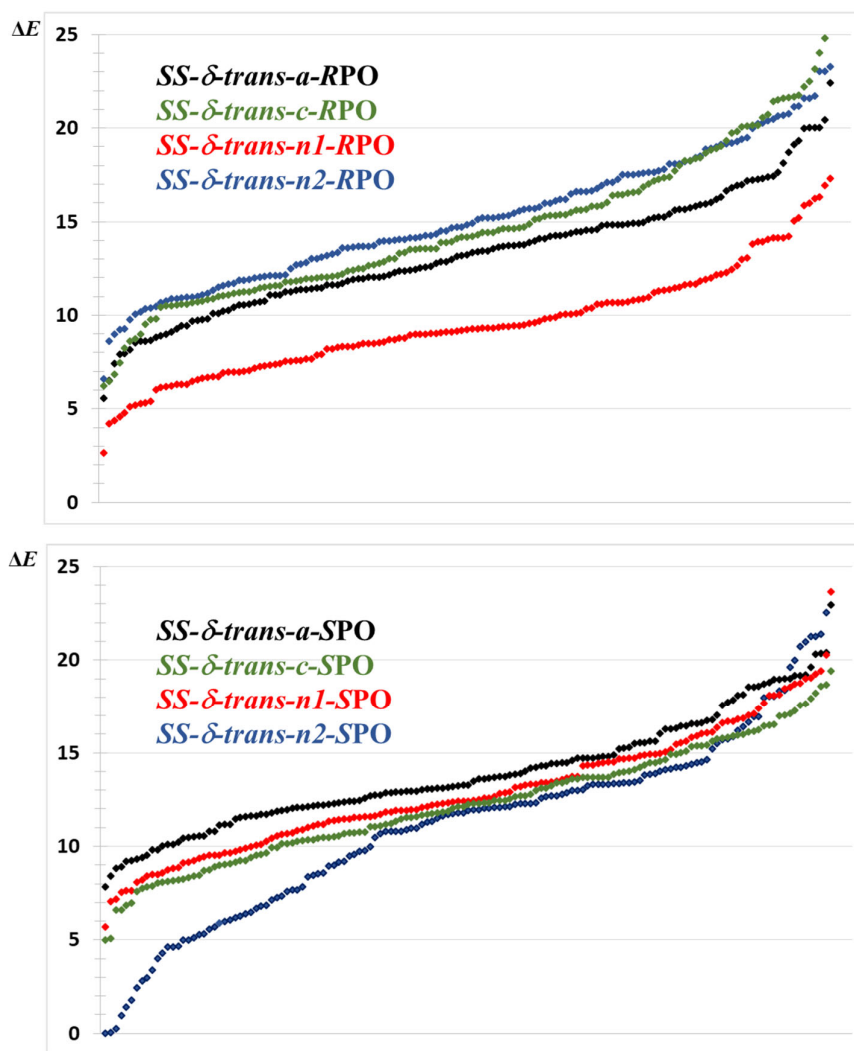


Figure S1. Relative electronic-energies [in kcal/mol] for all optimized geometries of RPO (top) and SPO (bottom) complexes 2, with respect to the 'global minimum', *SS- δ -trans-n2*-SPO geometry.

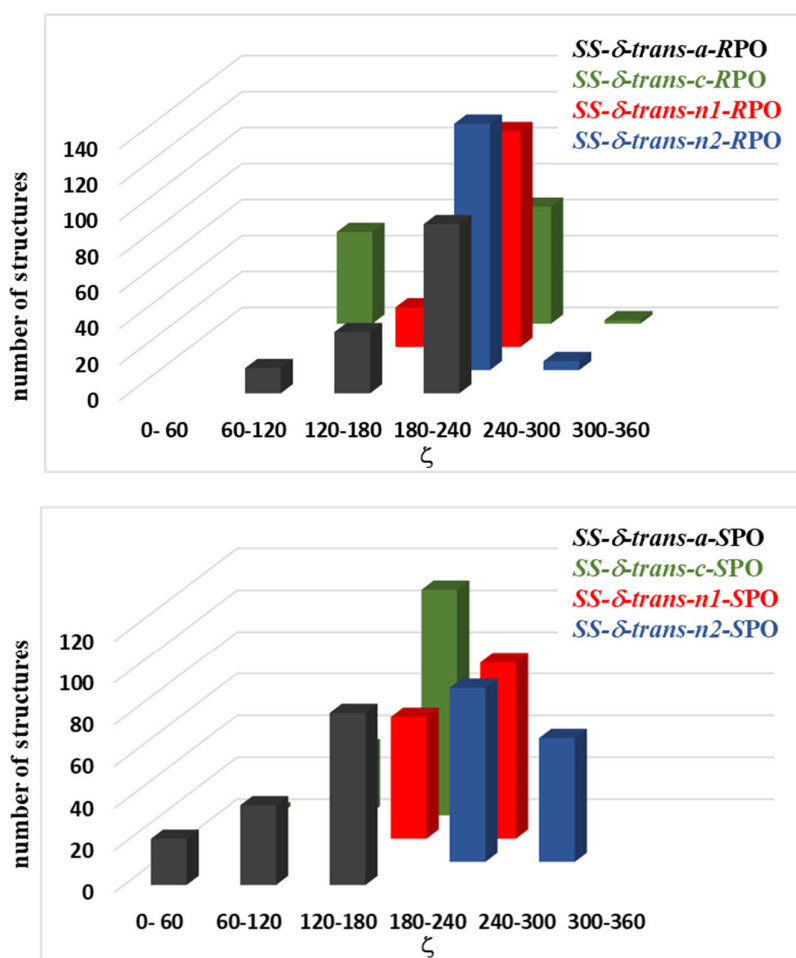


Figure S2. Distribution of dihedral angle ζ describing the epoxide orientation in all optimized geometries of RPO- and SPO- complexes with **2**.

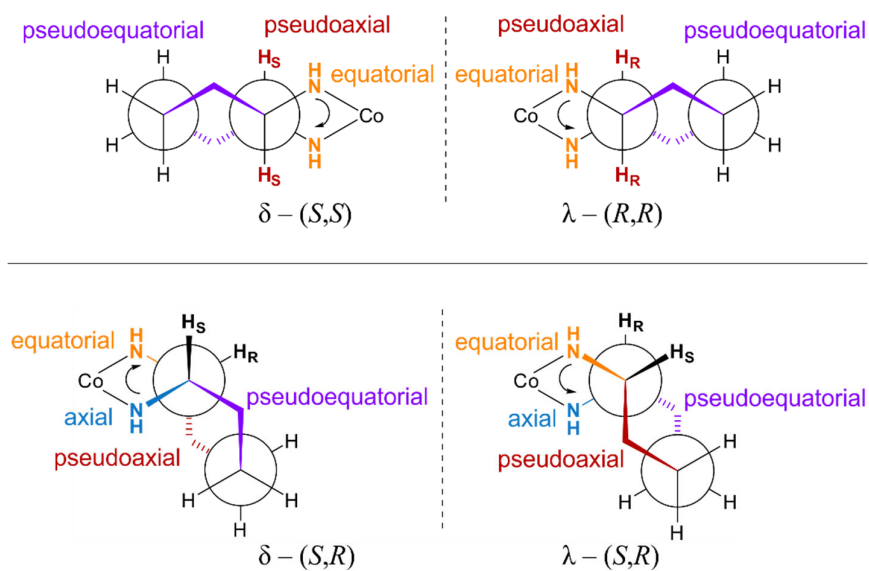


Figure S3. Chelate conformation of *trans*-1,2-cyclohexanediamine ligand, presented as a Newman projection along $\text{CH}_2\text{-CH}_2$ bonds of cyclohexane ring. Arrow depicts the direction of the measured angle. H_S / H_R label indicates hydrogen atom connected to asymmetric carbon atom of *S* / *R* configuration.

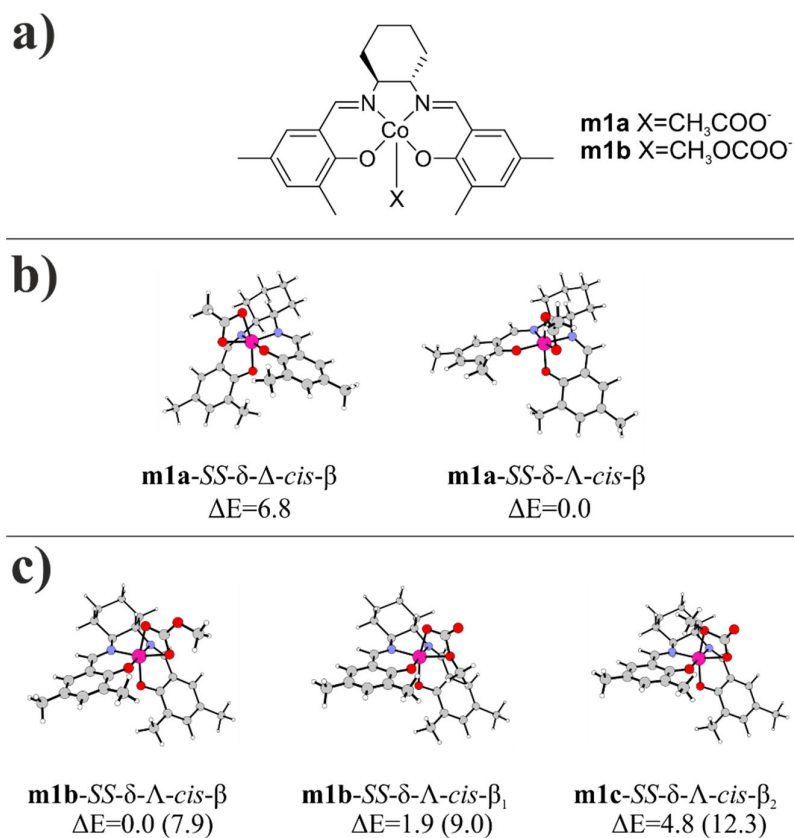


Figure S4. Comparison of electronic-energies of isomeric δ - Λ -*cis*- β and δ - Δ -*cis*- β structures for model catalyst complex. **Part a:** structures of the model for the catalysts **m1a** and **m1b**. **Part b:** DFT-optimized molecular structures of **m1a**- δ - Δ -*cis*- β and **m1a**- δ - Λ -*cis*- β , and their relative electronic-energies (ΔE ; in kcal/mol). **Part c:** DFT-optimized molecular structures of alternative δ - Λ -*cis*- β isomers of **m1b**, and their relative electronic-energy values. In parentheses ΔE values obtained for the corresponding δ - Δ isomers are provided. Please note that all the δ - Δ isomers are higher in energy than the corresponding δ - Λ by ca. 7–12 kcal/mol.

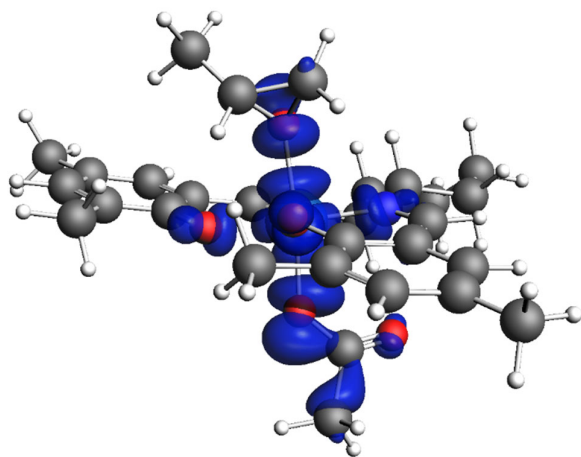


Figure S5. Contour of LUMO density for **1a** ($\rho^{\text{LUMO}} = 0.001$ a.u.).

Optimized geometries of the structures presented in the manuscript (xyz-format)

H	-2.508394	2.347420	-3.366099	74			
H	-3.877827	1.246787	-3.540540	1a-cis-B1-RPO	ksi=295		
H	-3.820371	0.696664	-1.130915	C	2.762563	0.483858	1.365504
H	-3.916140	2.447946	-1.329177	C	1.447304	0.611381	1.928443
H	-1.462523	2.666452	-0.882546	C	1.283070	0.658244	3.338759
H	-2.251915	1.782631	0.434909	C	2.353638	0.560368	4.207129
H	-0.670416	0.884916	1.652147	C	3.644645	0.430335	3.636361
H	4.506025	0.340015	4.305475	C	3.871773	0.400166	2.269898
H	0.268992	0.757569	3.736639	C	0.271853	0.693860	1.119751
H	5.991413	0.068804	2.474319	N	0.233437	0.547463	-0.172333
H	5.545745	1.159912	1.135880	Co	1.728217	0.039878	-1.241290
H	5.275327	-0.568125	0.958719	O	1.731002	1.982791	-1.904108
H	-0.566792	-1.844546	-3.683526	C	2.018261	3.093911	-0.991759
H	3.291180	-5.780256	-1.597434	C	2.862536	2.898032	-2.187956
H	0.701946	-3.872487	-4.453526	C	4.272296	2.398966	-2.093596
H	2.617867	-3.773363	1.130298	C	2.175344	0.568334	5.704909
H	3.921125	-2.878694	0.359490	C	5.249462	0.254585	1.687449
H	3.979925	-4.671350	0.404334	O	3.033085	0.475959	0.082755
H	2.505129	-0.382571	6.151878	C	-1.050251	0.553169	-0.905884
H	2.764596	1.368771	6.177770	C	-0.706530	0.499312	-2.412020
H	1.832678	-7.095912	-3.531256	C	-1.964096	0.256960	-3.238491
H	1.543840	-6.063442	-4.949020	C	-2.947148	1.412785	-2.978919
H	1.122400	0.718192	5.978146	C	-3.259890	1.578952	-1.483041
H	3.196674	-6.320512	-4.351334	C	-1.987038	1.730301	-0.630998
H	1.232033	3.851750	-0.980606	N	0.382549	-0.468611	-2.476290
H	2.415863	2.776930	-0.027139	C	0.267695	-1.650073	-2.999294
H	2.619101	3.493089	-3.072062	C	1.144350	-2.737375	-2.668935
H	4.929028	3.264736	-1.915252	C	1.237828	-3.874013	-3.500575
H	4.380440	1.680176	-1.274691	C	2.009099	-4.970761	-3.141145
H	4.575657	1.926452	-3.034246	C	2.675076	-4.925831	-1.893869
C	3.165593	-0.237362	-3.668560	C	2.599745	-3.841401	-1.028717
C	4.255686	-1.021924	-4.395144	C	1.826286	-2.706477	-1.411466
O	2.391359	0.514752	-4.280437	O	1.726112	-1.710458	-0.551308
H	3.900001	-2.053831	-4.530485	C	3.324166	-3.799155	0.286887
H	4.449016	-0.577075	-5.377280	C	2.150630	-6.173587	-4.040579
H	5.174507	-1.067007	-3.797832	O	3.170909	-0.492883	-2.377533
74				H	-1.571483	-0.391499	-0.660293
1a-cis-B1-RPO	ksi=153			H	-0.272922	1.468684	-2.698109
C	2.688712	0.560218	1.591850	H	-2.430829	-0.701352	-2.954995
C	1.348825	0.565259	2.109541	H	-1.709521	0.200199	-4.306783

H	-0.768869	0.672286	1.759649	C	1.132728	0.587183	3.513967
H	4.337113	0.578773	4.590502	C	2.177206	0.588280	4.417475
H	0.100794	0.590100	3.876883	C	3.494733	0.585205	3.891709
H	5.906294	0.493933	2.814262	C	3.771062	0.579287	2.535203
H	5.384729	1.471890	1.412719	C	0.203667	0.566808	1.260070
H	5.315728	-0.279898	1.308397	N	0.217388	0.449457	-0.036021
H	-0.314944	-1.789680	-3.673201	Co	1.781561	0.094172	-1.056401
H	3.751500	-5.560834	-1.658051	O	1.781063	2.166209	-1.380238
H	1.083678	-3.710836	-4.479379	C	3.092753	2.764788	-1.641539
H	2.911094	-3.739379	1.145297	C	1.965499	3.104170	-2.530460
H	4.128910	-2.694449	0.425340	C	1.813859	2.590427	-3.927196
H	4.351038	-4.476053	0.389529	C	1.948387	0.574812	5.908096
H	2.323129	-0.356114	6.362360	C	5.174925	0.564294	1.999058
H	2.468673	1.408523	6.404004	O	3.004589	0.558439	0.324781
H	2.373116	-6.890375	-3.682214	C	-1.036274	0.397262	-0.814283
H	2.105065	-5.802734	-5.062838	C	-0.627753	0.473946	-2.301695
H	0.879243	0.655215	6.145695	C	-1.824557	0.220387	-3.211253
H	3.736848	-6.013427	-4.393490	C	-2.893851	1.287869	-2.920028
H	3.406493	3.461755	-0.862734	C	-3.288733	1.310011	-1.434920
H	3.828150	2.031216	-1.975283	C	-2.073369	1.478946	-0.506101
H	1.442082	4.037447	-2.296852	N	0.526135	-0.415672	-2.382535
H	2.415280	3.217014	-4.604351	C	0.483233	-1.582517	-2.951049
H	2.152095	1.544921	-4.021821	C	1.399456	-2.638344	-2.631370
H	0.767778	2.664019	-4.257998	C	1.589564	-3.726236	-3.510762
C	3.565819	-0.555108	-3.328646	C	2.428370	-4.781656	-3.183517
C	4.854831	-1.334422	-3.569908	C	3.073747	-4.743906	-1.924329
O	2.797129	-0.297907	-4.271179	C	2.907617	-3.707527	-1.014433
H	4.643616	-2.392982	-3.352972	C	2.050142	-2.619917	-1.357752
H	5.165227	-1.241861	-4.616475	O	1.858142	-1.678916	-0.451567
H	5.651885	-1.008483	-2.890839	C	3.619820	-3.661877	0.307238
74				C	2.670956	-5.930303	-4.130782
1a-cis-B2-RPO ksi=310				O	3.407539	-0.250458	-2.060308
C	2.000751	0.477029	1.871019	H	-1.487210	-0.601155	-0.657101
C	0.600508	0.314956	2.123909	H	-0.260079	1.493653	-2.486363
C	0.093957	0.508503	3.436288	H	-2.240685	-0.783313	-3.024137
C	0.911012	0.848538	4.498210	H	-1.514151	0.258015	-4.265949
C	2.293861	1.003833	4.230806	H	-2.500810	2.277190	-3.208552
C	2.846838	0.832866	2.972183	H	-3.781202	1.109115	-3.544305
C	-0.332092	-0.016443	1.094509	H	-3.801036	0.365737	-1.184450
N	-0.063463	-0.223939	-0.158401	H	-4.012291	2.116920	-1.249062
Co	1.652135	-0.134091	-0.884849	H	-1.605797	2.466311	-0.652100
O	1.602624	1.755541	-1.315112	H	-2.395410	1.425399	0.543619

H	2.509758	-3.318927	-4.858008	C	0.371695	1.054264	5.891822
H	4.181779	-2.830524	0.761331	C	4.317322	1.002851	2.711287
H	4.731623	-4.517796	0.489230	O	2.568152	0.325431	0.701807
H	3.045072	-4.155230	0.951869	C	-1.114948	-0.553985	-1.144951
H	0.843725	0.367905	6.611553	C	-0.558683	-0.110588	-2.520215
H	0.560444	2.078331	6.249399	C	-1.489268	-0.528686	-3.651057
H	4.030312	-5.064788	-5.489028	C	-2.868428	0.109101	-3.417653
H	5.518091	-5.072724	-4.518627	C	-3.442540	-0.301477	-2.054503
H	-0.712408	0.882348	5.925753	C	-2.496231	0.051102	-0.894581
H	4.285314	-6.315021	-4.252024	N	0.797398	-0.662163	-2.498071
H	3.944120	1.797312	-0.920685	C	1.158806	-1.684624	-3.219780
H	5.412865	0.697062	-1.281751	C	2.220107	-2.571624	-2.849135
H	2.994946	1.361801	-3.152306	C	2.811582	-3.423659	-3.811934
H	5.411308	-0.578877	-3.524096	C	3.764038	-4.365089	-3.459920
H	3.962355	-0.573631	-4.557234	C	4.100214	-4.474143	-2.087256
H	5.086784	0.808030	-4.604752	C	3.529834	-3.687504	-1.097109
C	0.711297	2.692754	-1.073818	C	2.568770	-2.691666	-1.461612
C	1.324224	4.091038	-1.135978	O	2.031615	-1.972724	-0.500478
O	-0.490865	2.537866	-0.815575	C	3.902119	-3.812264	0.352900
H	2.086728	4.159293	-1.922096	C	4.431469	-5.248990	-4.483701
H	0.538641	4.837690	-1.294196	O	3.500332	-0.135226	-1.725084
H	1.815552	4.293928	-0.173049	C	4.395078	1.009265	-1.522443
74				C	3.845863	0.740354	-2.864234
1a-cis-B1-SPO ksi=147				C	4.623982	0.056734	-3.948313
C	2.147137	-2.608744	-1.506309	H	-1.185394	-1.658184	-1.177637
C	1.737893	-2.501997	-2.873964	H	-0.476914	0.983931	-2.484977
C	2.087907	-3.507473	-3.802633	H	-1.593331	-1.627049	-3.677012
C	2.854760	-4.600920	-3.428947	H	-1.073501	-0.213890	-4.620610
C	3.251164	-4.693220	-2.072906	H	-2.772045	1.206077	-3.459259
C	2.917177	-3.745073	-1.114880	H	-3.556542	-0.183079	-4.224371
C	0.874632	-1.420687	-3.250267	H	-3.631867	-1.389032	-2.057327
N	0.803868	-0.310292	-2.581143	H	-4.415259	0.185044	-1.891516
C	-0.355868	0.574374	-2.620749	H	-2.375053	1.139155	-0.797549
C	-0.998974	0.387156	-1.228861	H	-2.920414	-0.330618	0.045683
C	-2.073981	1.452794	-1.008038	H	-1.381730	-0.078319	1.401110
C	-3.126464	1.361161	-2.127586	H	2.960969	1.272583	5.055851
C	-2.501324	1.440934	-3.529444	H	-0.980343	0.383221	3.597180
C	-1.392300	0.391873	-3.723460	H	4.747475	0.083851	2.285535
N	0.109992	0.358682	-0.253511	H	4.854531	1.253749	3.634681
Co	1.821841	0.080488	-1.027717	H	4.495737	1.798739	1.972111
O	3.573444	-0.218457	-1.810697	H	0.580531	-1.921489	-4.121686
C	3.888701	-0.265499	-3.084663	H	4.852956	-5.211417	-1.790953

H	2.922739	-5.415826	-5.432246	O	3.292167	0.288340	-4.028003
H	4.359611	-5.778522	-4.451084	C	3.264837	-5.663593	-4.418179
H	1.200900	-1.092611	6.305912	C	3.362120	-3.843765	0.316598
H	2.843734	-6.645486	-4.150302	O	1.806307	-1.745504	-0.569367
H	2.771777	2.003637	-3.228662	C	-0.117339	0.347682	1.027634
C	1.724729	3.967644	-2.984803	C	0.874311	0.248212	2.047898
H	3.974144	2.041667	-1.030416	C	2.280810	0.289968	1.759199
H	5.566201	-0.884238	-4.306372	C	3.193237	0.201898	2.863805
H	5.846589	-1.026459	-2.527171	C	2.698899	0.063184	4.149741
H	4.786907	-2.181205	-3.353374	C	1.313257	0.018974	4.449668
H	3.141150	3.643127	-0.568642	C	0.431374	0.121733	3.391695
H	1.383136	4.596492	-2.151851	O	2.799582	0.420370	0.566701
H	2.390988	4.564330	-3.625489	C	0.842725	-0.146097	5.872439
H	0.856929	3.678196	-3.594168	C	4.665634	0.237432	2.565918
74				O	1.845093	2.106458	-1.297216
1a-cis-B1-SPO ksi=263				C	3.166450	2.752752	-1.200113
C	2.116981	-2.957170	-1.721658	C	2.466613	2.759932	-2.494581
C	1.888740	-2.733946	-3.117274	C	5.116689	-1.131376	-3.338717
C	2.326541	-3.676657	-4.071742	H	-1.469474	-0.614755	-1.226829
C	3.010425	-4.822606	-3.689810	H	0.025663	1.604788	-2.668698
C	3.228149	-5.029867	-2.307308	H	-1.825927	-0.620942	-3.674787
C	2.798889	-4.144763	-1.325773	H	-0.920869	0.503150	-4.711000
C	1.098522	-1.600851	-3.496319	H	-2.074955	2.446347	-3.682641
N	0.978291	-0.545877	-2.745420	H	-3.278153	1.309980	-4.296308
C	-0.175790	0.343638	-2.827205	H	-3.669387	0.405814	-2.029892
C	-0.892472	0.106326	-1.475716	H	-3.872530	2.158875	-2.001553
C	-2.075640	1.062690	-1.308323	H	-1.591432	2.443637	-1.005451
C	-3.028518	0.952561	-2.510371	H	-2.557835	1.324900	-0.029232
C	-2.303689	1.158349	-3.847090	H	-1.159306	0.412986	1.369184
C	-1.132869	0.176293	-4.003043	H	3.415768	-0.024109	4.972114
N	0.165759	0.165203	-0.448298	H	-0.646030	0.091117	3.578629
Co	1.897831	-0.303027	-1.099759	H	5.256152	0.061430	3.474143
O	3.627835	-0.701200	-1.820070	H	4.958619	1.208160	2.137709
C	4.023556	-0.270116	-2.994035	H	4.924224	-0.517294	1.809196
O	3.437794	0.533231	-3.740995	H	0.211927	-1.561444	-4.112204
C	3.523864	-5.817060	-4.701297	H	3.863976	-5.545166	-1.763121
C	3.056952	-4.365658	0.137562	H	1.765417	-3.395819	-4.840926
O	1.674711	-2.146596	-0.777185	H	3.869530	-2.916479	0.619332
C	-0.090349	0.517951	0.781454	H	4.037759	-4.696219	0.462195
C	0.854519	0.592019	1.844379	H	2.501651	-3.955762	0.992786
C	2.238561	0.235274	1.680557	H	1.214022	0.665228	6.516893
C	3.096087	0.342150	2.832360	H	-0.253994	-0.145977	5.929121

H	6.007586	-1.049610	-2.557395	C	2.575803	0.788125	4.033161
H	5.109076	-1.921370	-3.812680	C	1.212103	1.147455	4.208251
H	3.410142	3.214139	-2.288301	C	0.382782	1.039303	3.111666
H	3.081932	3.905977	0.192840	O	2.789249	-0.171428	0.574103
H	1.516915	4.760942	0.067523	C	0.711393	1.620385	5.549933
H	1.661808	3.308786	1.092650	C	4.540007	-0.038592	2.669433
74				O	2.416790	1.696642	-1.169335
1a-cis-B2-SPO ksi=326				C	2.441203	2.716896	-2.214112
C	2.441104	-2.398945	-1.737225	C	1.605034	2.911459	-1.011072
C	2.146208	-2.113126	-3.111385	C	5.337802	-0.921186	-3.415954
C	2.682849	-2.928424	-4.135725	H	-1.266455	-0.934554	-1.503386
C	3.510862	-4.003816	-3.855507	H	0.199359	1.379545	-2.831142
C	3.763969	-4.296257	-2.493124	H	-1.520788	-0.855708	-4.025767
C	3.248524	-3.545022	-1.446154	H	-0.600934	0.350014	-4.949880
C	1.154206	-1.121588	-3.420551	H	-1.923717	2.192362	-3.906127
N	0.815109	-0.162200	-2.611998	H	-3.007763	1.035796	-4.682501
C	-0.511356	0.458588	-2.605494	H	-3.499158	-0.045113	-2.504995
C	-1.134845	-0.122397	-1.315634	H	-3.843383	1.682689	-2.401073
C	-2.477020	0.542552	-1.011678	H	-1.698684	2.095840	-1.218519
C	-3.411812	0.391935	-2.223686	H	-2.626649	0.841336	-0.383455
C	-2.776011	0.919667	-3.518338	H	-1.119644	0.797744	1.039635
C	-1.428594	0.233278	-3.800531	H	3.249990	0.861619	4.892271
N	-0.091268	-0.015738	-0.269661	H	-0.676278	1.298025	3.203971
Co	1.638651	0.168909	-0.940910	H	5.091696	0.098073	3.608221
O	3.433351	0.349354	-1.873776	H	5.014445	0.560993	1.878899
C	4.428207	1.263868	-1.296990	H	4.633117	-1.086200	2.347444
C	4.669067	-0.188982	-1.255374	H	0.527741	-1.655052	-4.429898
C	4.119121	-4.851235	-4.945567	H	3.775292	-5.923383	-1.991929
C	3.523352	-3.873821	-0.005691	H	2.137792	-3.480042	-5.130423
O	1.993716	-1.697792	-0.718737	H	3.494955	-3.460045	0.580966
C	-0.361699	-0.179096	0.987516	H	3.730427	-5.217757	0.295153
C	0.574879	-0.160473	2.068245	H	2.119743	-4.554395	0.682878
C	1.962806	0.137883	1.881842	H	1.244896	2.523981	5.883417
C	2.808634	0.148241	3.036688	H	-0.360196	1.857408	5.511328
C	2.270994	-0.140354	4.282087	H	3.269307	-5.510351	-5.724396
C	0.902806	-0.442028	4.483140	H	4.618838	-5.916464	-4.643238
C	0.082489	-0.436873	3.369511	H	0.858295	0.854175	6.326770
O	2.513773	0.415355	0.723877	H	3.099445	-6.818527	-4.532550
C	0.378250	-0.756153	5.862152	H	0.535232	2.714143	-1.122372
C	4.267642	0.460563	2.851282	C	1.993561	3.773423	0.153460
O	1.636336	2.085794	-1.148799	H	2.005200	2.402472	-3.161068
C	0.781163	2.980377	-0.708038	H	5.816734	-0.325375	-4.200689

C	2.476065	-2.672977	-1.553382	O	-0.396974	2.793403	-0.369923
C	2.187769	-2.517081	-2.951263	C	1.400144	4.376060	-0.635861
C	2.733379	-3.418941	-3.896870	H	-1.285747	-1.203369	-1.501993
C	3.576470	-4.449097	-3.517370	H	-0.369305	1.534393	-2.439233
C	3.852732	-4.592108	-2.134421	H	-1.592058	-0.846150	-3.961182
C	3.326117	-3.756039	-1.161154	H	-0.969197	0.637776	-4.715263
C	1.205468	-1.557190	-3.356431	H	-2.614787	2.006208	-3.429950
N	0.866615	-0.525016	-2.637782	H	-3.458394	0.765680	-4.366957
C	-0.458513	0.095944	-2.705639	H	-3.669947	-0.672727	-2.359440
C	-1.106383	-0.367201	-1.379623	H	-4.355508	0.920297	-2.024724
C	-2.456372	0.317402	-1.165796	H	-2.283808	1.598782	-0.780150
C	-3.366945	0.059039	-2.378247	H	-2.945016	0.082903	-0.128741
C	-2.706256	0.474258	-3.700751	H	-1.410683	-0.340338	1.261653
C	-1.354098	-0.232297	-3.893429	H	2.940993	-0.137403	5.147405
N	-0.085866	-0.153728	-0.329359	H	-0.982641	-0.657828	3.480904
Co	1.661915	-0.068096	-0.977532	H	4.743627	-0.266360	2.175388
O	3.534502	-0.113338	-1.748775	H	4.798682	0.443074	3.811396
C	4.010009	0.862828	-2.737687	H	4.405378	1.450160	2.390479
C	4.502981	0.931943	-1.350373	H	0.595925	-1.236723	-4.358224
C	4.185330	-5.395800	-4.521772	H	4.398833	-5.153624	-2.249440
C	3.627326	-3.924766	0.301180	H	2.434677	-2.690845	-5.173944
O	1.975343	-1.915750	-0.602849	H	2.590915	-4.110610	0.527924
C	-0.393433	-0.121319	0.930652	H	3.955612	-3.010114	0.521041
C	0.510368	0.047927	2.023867	H	4.206967	-4.727784	0.080545
C	1.911283	0.275067	1.834582	H	0.560813	0.073568	6.562163
C	2.725625	0.456263	2.999514	H	-0.703312	-0.944602	5.840010
C	2.145229	0.397259	4.256367	H	5.218659	-4.791486	-4.934337
C	0.762176	0.171533	4.460979	H	3.852647	-5.912342	-4.826165
C	-0.026377	0.006890	3.337180	H	0.865433	-1.649378	6.283629
O	2.505651	0.334509	0.669447	H	3.777490	-4.526965	-5.937399
C	0.190661	0.119059	5.856235	H	4.440376	-0.676807	-0.305103
C	4.197960	0.688121	2.806628	C	5.587287	-0.894635	-2.207609
O	1.685872	1.828192	-1.370411	H	4.073682	1.767963	-0.399007
C	0.833630	2.782786	-1.061943	H	2.194693	4.505394	-1.380110
O	-0.364970	2.652410	-0.777780	H	0.620672	5.135739	-0.761697
C	1.487909	4.163228	-1.083004	H	1.843436	4.498325	0.363512
H	-1.248762	-1.461723	-1.467024	H	4.920485	1.871806	-2.058402
H	-0.319991	1.182411	-2.629442	H	5.196634	-1.890365	-2.454516
H	-1.516273	-1.321593	-3.962197	H	5.710021	-0.319076	-3.134031
H	-0.876230	0.089856	-4.831127	H	6.574160	-1.021138	-1.738045
H	-2.547796	1.564892	-3.704070	74			
H	-3.371365	0.244969	-4.546103	1a-cis-B1-SPO ksi=246			

C	0.448790	-1.356229	1.399142	H	-3.620095	-1.014404	-2.425715
C	-0.925702	-0.826517	0.962487	H	-4.315558	0.599117	-2.244550
C	-2.018423	-1.829168	1.324969	H	-2.270455	1.391088	-1.025139
C	-1.998417	-2.072504	2.843999	H	-2.944267	-0.063790	-0.256974
C	-0.612896	-2.505865	3.343868	H	-1.452773	-0.219183	1.193469
C	0.489097	-1.520003	2.917959	H	2.791342	0.527850	5.130118
N	-0.798065	-0.439109	-0.446984	H	-1.100343	-0.165505	3.449456
Co	0.848808	0.409573	-0.768520	H	4.653306	-0.150475	2.257980
O	1.507535	-0.905739	-1.946304	H	4.709819	0.799585	3.770859
C	1.240866	-2.194464	-1.958938	H	4.380177	1.590538	2.203358
O	0.614478	-2.865013	-1.125914	H	0.658701	-1.747342	-4.288731
C	7.562918	0.524981	1.262652	H	4.514822	-5.402779	-1.814401
C	4.573676	2.760162	-2.167781	H	2.478690	-3.284677	-4.952021
O	2.455809	1.384164	-1.085543	H	2.717146	-4.179473	0.864620
C	-1.679735	-0.706214	-1.359333	H	3.992440	-2.980206	0.729874
C	-1.585661	-0.278774	-2.724182	H	4.373314	-4.713242	0.462560
C	-0.647918	0.728095	-3.124515	H	0.324684	1.076835	6.382925
C	-0.630058	1.123695	-4.498627	H	-0.884551	-0.103282	5.834841
C	-1.500118	0.515989	-5.393001	H	5.285126	-5.340123	-4.511279
C	-2.430664	-0.481094	-5.012620	H	3.913458	-6.440691	-4.306904
C	-2.462361	-0.849939	-3.677634	H	0.682404	-0.656108	6.463844
O	0.175789	1.332354	-2.299979	H	3.848236	-5.163733	-5.540700
C	-3.333288	-1.119664	-6.038731	H	4.023118	1.676988	-0.713713
C	0.364062	2.169153	-4.921490	C	5.837144	0.401561	-0.922574
O	0.138273	1.977479	0.355707	H	3.241091	1.571756	-3.044578
C	1.044913	2.933489	1.017668	H	2.253524	4.234084	-1.865769
C	0.355803	3.326733	-0.222945	H	0.724642	4.937384	-1.217145
C	1.789169	-2.842637	-3.229129	H	1.982454	4.321622	-0.113137
H	-3.164693	-1.618586	-3.342563	H	4.620693	0.394337	-3.512109
H	-1.451673	0.814353	-6.444986	H	5.769765	0.003081	0.097789
H	0.130154	3.145876	-4.469923	H	6.181372	-0.395114	-1.594276
H	1.370602	1.902020	-4.569036	H	6.578143	1.214478	-0.924638
H	0.376271	2.284948	-6.012786	74			
H	-2.549621	-1.313244	-1.084416	1a-trans-SPO ksi=71			
H	-1.107929	0.115319	1.513066	C	3.604722	1.135882	-0.504847
H	-1.836912	-2.769479	0.779956	C	3.782174	0.249699	0.607632
H	-3.007496	-1.452598	1.025038	C	5.074398	0.073658	1.170098
H	-2.749556	-2.831523	3.107788	C	6.186851	0.733558	0.680989
H	-2.296008	-1.143448	3.359326	C	5.992223	1.614308	-0.411957
H	-0.374143	-3.500914	2.933972	C	4.756495	1.830061	-1.001443
H	-0.621263	-2.608282	4.438951	C	2.696835	-0.475455	1.194310
H	1.465837	-1.901172	3.248175	N	1.459847	-0.463614	0.792414

O	1.601794	-0.951627	-1.957966	H	0.340062	-0.539490	3.402080
C	1.233149	-2.215116	-1.959068	H	0.578793	-2.329544	0.899931
O	0.506100	-2.811317	-1.151066	H	5.179762	-0.615592	2.012919
C	7.637339	0.446738	1.440572	H	6.858501	2.145725	-0.818147
C	4.843592	2.591646	-2.204479	H	5.534836	3.178613	-2.492708
O	2.655759	1.310526	-1.156429	H	3.897530	3.590199	-1.911526
C	-1.602760	-0.516335	-1.405048	H	4.103227	2.233931	-3.010787
C	-1.480530	-0.130989	-2.780133	H	2.951948	-1.099056	2.060498
C	-0.465324	0.783300	-3.210933	H	-4.014338	-1.842989	-5.571449
C	-0.412724	1.125758	-4.597708	H	-3.944532	-0.368787	-6.562034
C	-1.330150	0.561317	-5.473549	H	8.021024	1.478259	1.568044
C	-2.342270	-0.338838	-5.062016	H	7.525955	-0.128750	2.144151
C	-2.403490	-0.658637	-3.715619	H	0.946638	3.259048	-1.138276
O	0.397654	1.356173	-2.399957	C	-0.864526	4.195127	-0.252249
C	-3.295967	-0.934678	-6.067881	H	2.096673	2.652818	0.971034
C	0.663760	2.070190	-5.053961	H	-2.751792	-1.654793	-6.805458
O	0.496282	2.065417	0.318505	H	8.241241	0.060373	0.529927
C	0.761693	3.387389	-0.274155	H	2.599403	-2.252546	-3.670356
C	-0.628705	2.930253	-0.123995	H	2.121753	-3.862827	-3.003785
C	1.802423	-2.937956	-3.179515	H	0.963969	-2.899420	-3.954189
H	-3.166130	-1.355176	-3.356120	H	0.657604	3.265502	1.983506
H	-1.256787	0.817989	-6.534907	H	-0.570426	5.240311	-0.427836
H	0.505171	3.080141	-4.645427	H	-1.523481	3.883392	-1.073202
H	1.643285	1.738870	-4.681056	H	-1.419070	4.139489	0.693500
H	0.691168	2.138625	-6.148962	74			
H	-2.510925	-1.058118	-1.118798	1a-trans-SPO ksi=143			
H	-0.976217	0.298744	1.464715	C	3.768139	1.068078	-0.510777
H	-1.901600	-2.530076	0.740943	C	3.881796	0.219677	0.638435
H	-2.980167	-1.136097	0.975234	C	5.146719	0.037825	1.258454
H	-2.823811	-2.514414	3.066716	C	6.292262	0.652881	0.789855
H	-2.251472	-0.861868	3.310890	C	6.162595	1.489809	-0.346721
H	-0.499168	-3.349322	2.894086	C	4.957034	1.710097	-0.992386
H	-0.686121	-2.440367	4.397957	C	2.760468	-0.461135	1.205184
H	1.445254	-1.879610	3.212520	N	1.539600	-0.434058	0.758668
H	0.416687	-0.443225	3.361691	C	0.477610	-1.266605	1.359641
H	0.547374	-2.246646	0.861135	C	-0.860013	-0.654498	0.915398
H	5.202146	-0.618600	2.131685	C	-2.019438	-1.576905	1.280625
H	7.056973	1.984032	-0.738877	C	-2.019994	-1.812498	2.800629
H	5.826663	2.975317	-2.505635	C	-0.668821	-2.339795	3.302845
H	4.175871	3.445539	-2.012851	C	0.498499	-1.432117	2.879011
H	4.397233	2.039248	-3.044066	N	-0.703542	-0.288535	-0.497719
H	2.968632	-1.061100	2.099910	Co	1.001769	0.437446	-0.830725

C	-0.369495	0.596856	-3.519395	H	-4.032085	-1.585716	-5.578349
C	-0.339589	0.940201	-4.912152	H	-3.846334	-0.154080	-6.615139
C	-1.421998	0.619576	-5.714840	H	8.078568	1.401405	1.766395
C	-2.583781	-0.034586	-5.230196	H	7.555624	-0.203780	2.321356
C	-2.618423	-0.359427	-3.887425	H	-1.090728	2.536780	-1.031386
O	0.661832	0.939032	-2.793372	C	-1.532525	3.389874	0.980327
C	-3.724949	-0.359631	-6.161037	H	1.235117	3.322195	-1.253535
C	0.887745	1.625381	-5.442417	H	-2.761292	-1.538649	-6.817411
O	0.923353	2.054590	-0.423239	H	8.352695	-0.019184	0.745106
C	-0.308081	2.714752	0.005815	H	2.752669	-2.498099	-3.501379
C	0.774850	2.482353	0.980658	H	1.918944	-4.002932	-2.950144
C	1.338325	-3.462985	-3.290756	H	1.079052	-2.831249	-4.000964
H	-3.492331	-0.870655	-3.473840	H	1.184925	4.086415	0.449500
H	-1.371323	0.877341	-6.777353	H	-2.134124	4.243114	0.634381
H	1.014400	2.617494	-4.982897	H	-2.226292	2.589733	1.273387
H	1.789500	1.053908	-5.180142	H	-0.956024	3.700702	1.860679
H	0.833058	1.745545	-6.531886	74			
H	-2.631762	-0.843090	-1.338042	1a-trans-SPO ksi=267			
H	-1.036104	0.155080	1.259342	C	3.728299	0.928708	-0.533678
H	-2.031793	-2.574827	0.315438	C	3.635057	0.458413	0.819614
H	-3.067981	-1.169909	0.658975	C	4.644538	0.794508	1.762033
H	-3.001458	-2.715307	2.622322	C	5.720348	1.595090	1.429403
H	-2.359524	-1.119072	3.019086	C	5.797436	2.059029	0.090099
H	-0.708057	-3.631734	2.391032	C	4.857551	1.748801	-0.878101
H	-0.886246	-2.869997	3.976339	C	2.545830	-0.349975	1.264565
H	1.287399	-2.276488	2.879000	N	1.461638	-0.592686	0.585042
H	0.302608	-0.829337	3.169826	C	0.378712	-1.448990	1.089662
H	0.425428	-2.383318	0.507120	C	-0.929125	-0.765593	0.651091
H	4.547098	0.409800	2.781614	C	-2.127905	-1.669912	0.934668
H	6.640266	2.696391	-0.195108	C	-2.162819	-2.030734	2.428373
H	5.817048	2.917426	-2.414663	C	-0.846082	-2.662419	2.896927
H	4.035556	2.779302	-2.577742	C	0.361144	-1.763307	2.582492
H	5.049492	1.409625	-2.995855	N	-0.723174	-0.338530	-0.745683
H	2.632963	-0.772966	2.272593	Co	1.073977	0.118654	-1.127669
H	-4.529712	-0.886418	-5.631333	O	1.470469	-1.466100	-2.080231
H	-4.154042	0.552259	-6.605243	C	0.838524	-2.617436	-2.119562
H	6.850399	3.059706	2.563109	O	-0.061395	-3.041037	-1.376194
H	6.573876	1.525010	3.415159	C	6.783421	1.968314	2.432556
H	0.647906	1.631886	1.654519	C	4.955253	2.249106	-2.290922
C	1.744267	3.539659	1.416418	O	2.870358	0.665259	-1.479957
H	-1.186889	2.067901	0.002511	C	-1.663170	-0.432880	-1.642928
H	-3.394712	-0.999743	-6.993696	C	-1.537104	-0.066146	-3.015212

O	3.183126	-0.070126	-1.476696	H	7.777945	1.620586	2.112613
O	1.212905	-1.721521	-1.928020	H	2.371203	-3.214195	-3.557975
C	0.275228	-2.641684	-1.909709	H	1.238798	-4.525569	-3.041775
C	0.492275	-3.649446	-3.039053	H	0.695550	-3.243772	-4.156077
O	-0.694634	-2.753007	-1.143053	H	-0.432188	3.702980	-0.441304
H	-3.484823	0.633765	-2.982695	H	1.412835	3.981257	2.367764
H	-1.167677	1.879827	-6.380894	H	2.738245	3.096245	1.568142
H	1.958915	0.771617	-5.192644	H	1.821261	4.334045	0.663603
H	1.209079	1.946826	-6.320275	74			
H	1.840500	2.459281	-4.727693	1a-trans-RPO ksi=327			
H	-2.503043	0.151667	-0.964951	C	-0.061224	0.931436	-3.286338
H	-0.599185	0.536809	1.495300	C	-1.340759	0.668229	-2.694605
H	-2.268975	-1.859717	0.610531	C	-2.524505	0.850283	-3.459228
H	-2.915429	-0.246566	0.994536	C	-2.490550	1.280270	-4.771919
H	-3.142478	-1.767530	2.962702	C	-1.217653	1.543089	-5.340756
H	-2.117361	-0.374754	3.316260	C	-0.029122	1.385190	-4.647731
H	-1.151883	-3.213464	2.651467	C	-1.477800	0.255048	-1.336124
H	-1.072232	-2.427128	4.232775	N	-0.498435	-0.004853	-0.517231
H	1.132539	-2.384108	3.036447	Co	1.330391	-0.074722	-1.009018
H	0.543097	-0.739475	3.350732	O	1.781687	1.827548	-0.345714
H	0.149117	-2.287766	0.715580	C	1.543523	2.443429	0.959323
H	4.981779	-0.662437	2.701653	C	0.756065	2.874384	-0.214091
H	7.478809	0.709516	-0.515488	C	1.035497	4.127976	-0.986579
H	6.619328	1.086393	-2.696937	C	-3.746760	1.468431	-5.585783
H	4.884245	1.535958	-2.751732	C	1.312509	1.657960	-5.266696
H	5.363576	-0.105599	-3.147725	O	1.084639	0.820349	-2.668978
H	2.773755	-1.240782	2.352468	C	-0.743822	-0.380479	0.890094
H	-3.870309	2.516468	-5.900341	C	-2.115311	-0.963503	1.229873
H	-3.727624	0.856638	-6.500619	C	-2.172039	-1.306951	2.727479
H	8.393270	-0.531578	1.773388	C	-1.029130	-2.238395	3.150028
H	7.948636	1.117658	2.239332	C	0.346115	-1.661234	2.774508
H	1.096657	1.778780	1.699368	C	0.369731	-1.366157	1.277969
H	2.390048	3.044208	1.297808	N	1.608925	-0.823058	0.704612
H	-0.252766	2.463722	-0.299349	C	2.752529	-0.851084	1.327526
H	0.389138	4.941772	-0.626422	C	3.998445	-0.409081	0.790396
H	2.084265	4.431099	-0.877532	C	5.124148	-0.369425	1.657151
H	0.821540	3.962017	-2.050572	C	6.372322	0.029185	1.220105
H	-4.637285	1.183450	-5.010370	C	6.499366	0.387763	-0.147539
H	7.302577	-0.263608	3.150091	C	5.445087	0.354768	-1.044134
H	-0.091331	-3.311483	-3.907511	C	4.141772	-0.048245	-0.591892
H	1.545843	-3.707061	-3.332396	C	7.563694	0.090100	2.143738
H	0.114733	-4.629762	-2.726935	C	5.598486	0.742316	-2.487320

H	1.442488	1.843489	-6.369497
H	1.499245	2.825008	-4.879659
H	-2.688841	-0.112588	-1.383116
H	-0.979890	1.070776	1.158888
H	-2.583493	-1.497974	0.699026
H	-3.261887	0.145449	0.675542
H	-3.572150	-0.925311	2.927003
H	-2.600040	0.546677	3.007598
H	-1.546830	-2.337925	3.059724
H	-1.554101	-1.199499	4.411002
H	0.702943	-1.386998	3.338731
H	0.085548	0.270565	3.219887
H	-0.163545	-1.844230	0.986821
H	4.690557	-1.591393	2.271072
H	7.310536	0.120364	-0.672729
H	6.475016	1.318642	-2.544681
H	5.055819	2.315121	-2.121789
H	4.825933	0.854690	-3.072324
H	2.424397	-1.310723	2.187921
H	-3.496648	0.806811	-6.974913
H	-2.836995	-0.834373	-7.066105
H	7.874618	-2.111418	0.975203
H	8.074171	-0.592594	1.863359
H	2.176278	3.102939	-1.493562
H	0.979260	4.290279	-0.689423
H	2.852149	2.218213	0.724335
H	2.399783	4.194987	2.327246
H	0.674220	4.127378	1.873271
H	1.425309	2.779515	2.776097
H	-4.117537	-0.459918	-5.893861
H	7.058018	-1.886944	2.536108
H	0.394306	-3.062360	-3.790199
H	2.094826	-3.089229	-3.272856
H	0.919927	-4.289047	-2.606635

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1a-cis-B1-RPO ksi=213

C	2.726197	0.349885	1.493455
C	1.410087	0.583921	2.015193
C	1.243270	0.908274	3.389315
C	2.311820	1.003518	4.258958
C	3.606105	0.766553	3.729004
C	3.835396	0.450922	2.400883

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1a-trans-RPO ksi=135

C	-0.129588	0.964193	-3.439713
C	-1.368243	0.374199	-3.026511
C	-2.360992	0.063057	-3.987926
C	-2.167167	0.292837	-5.339921
C	-0.936385	0.871375	-5.733806
C	0.065814	1.209550	-4.836011
C	-1.653921	0.137438	-1.642834
N	-0.773847	0.195191	-0.692030
Co	1.072640	0.428745	-0.952939
O	0.850987	2.256845	-0.037856
C	1.590001	3.388229	-0.620298
C	1.978718	2.871536	0.703793
C	1.588658	3.531928	1.992143
C	-3.209391	-0.066630	-6.369744
C	1.374038	1.805265	-5.274740
O	0.825924	1.325809	-2.615888
C	-1.089938	0.055795	0.733598
C	-2.468730	-0.481634	1.108344
C	-2.601743	-0.494193	2.641152
C	-1.461581	-1.269504	3.317261
C	-0.076207	-0.765511	2.875516
C	0.010574	-0.819576	1.350770
N	1.287220	-0.392246	0.737481
C	2.430471	-0.752511	1.243121
C	3.720318	-0.494870	0.678961
C	4.855985	-1.010044	1.359307
C	6.144115	-0.809224	0.898492
C	6.300407	-0.049258	-0.287473
C	5.233335	0.484143	-0.992365
C	3.896272	0.263242	-0.525337
C	7.347952	-1.379104	1.606822
C	5.418149	1.283762	-2.251450
O	2.923069	0.800227	-1.219301
O	1.330979	-1.164010	-1.927024
C	0.675443	-2.299805	-1.813033
C	1.064444	-3.255623	-2.940144
O	-0.173022	-2.623680	-0.969943
H	-3.296906	-0.384185	-3.641305
H	-0.758728	1.051880	-6.798604
H	2.213251	1.217422	-4.876091

H	5.468304	0.923229	1.069960	C	0.238414	0.537604	1.201620
H	5.271155	-0.791875	1.385785	N	0.194393	0.240593	-0.064075
H	-0.455213	-1.651768	-3.929708	Co	1.719352	-0.179619	-1.124586
H	3.363889	-5.842289	-2.318107	O	1.815071	1.862908	-1.345127
H	0.855438	-3.533000	-4.939287	C	2.294489	2.588751	-2.549233
H	2.564425	-4.327500	0.664570	C	3.185747	2.434098	-1.386980
H	3.850578	-3.268619	0.098811	C	3.431157	3.515046	-0.378883
H	3.981203	-5.041944	-0.152827	C	2.131234	1.338972	5.718185
H	2.480537	0.518869	6.364748	C	5.214287	0.199080	1.859143
H	2.701706	2.237566	5.999028	O	3.007184	0.069186	0.249450
H	1.913501	-6.844473	-4.507004	C	-1.072098	0.259625	-0.824608
H	1.785571	-5.586055	-5.755280	C	-0.676120	0.453983	-2.308555
H	1.074785	1.524096	5.953807	C	-1.886280	0.321937	-3.225948
H	3.369345	-6.008762	-5.070625	C	-2.927938	1.380285	-2.829148
H	2.414760	1.929703	-3.414984	C	-3.322481	1.251791	-1.351157
H	1.763740	3.536223	-2.679259	C	-2.105246	1.309858	-0.411823
H	3.929441	1.638119	-1.452621	N	0.429740	-0.481275	-2.477508
H	4.356003	4.054121	-0.631486	C	0.339906	-1.569582	-3.180039
H	2.600633	4.232645	-0.353846	C	1.200162	-2.697665	-2.976908
H	3.552818	3.075896	0.620920	C	1.344936	-3.686775	-3.974091
C	3.352268	-0.490927	-3.529136	C	2.116947	-4.819414	-3.760965
C	4.480000	-1.360989	-4.072056	C	2.737706	-4.962704	-2.496979
O	2.622980	0.163525	-4.297949	C	2.610098	-4.031549	-1.473857
H	4.120688	-2.401142	-4.092096	C	1.825846	-2.860546	-1.699396
H	4.743135	-1.051822	-5.089460	O	1.673906	-2.014209	-0.698114
H	5.355168	-1.328009	-3.412045	C	3.295278	-4.185270	-0.145751
74				C	2.304621	-5.867209	-4.829726
1a-cis-B2-RPO ksi=34				O	3.269117	-0.558588	-2.220408
C	2.160836	0.308077	1.724166	H	-1.519249	-0.749620	-0.748588
C	0.782458	0.114221	2.057828	H	-0.263909	1.469723	-2.410739
C	0.380684	0.117338	3.418756	H	-2.327197	-0.684171	-3.128104
C	1.280633	0.294570	4.453898	H	-1.579741	0.448914	-4.274548
C	2.640121	0.483512	4.106003	H	-2.511569	2.384880	-3.012747
C	3.091885	0.497192	2.795347	H	-3.818108	1.288000	-3.467838
C	-0.231079	-0.068050	1.066168	H	-3.846162	0.292692	-1.200309
N	-0.056594	-0.118115	-0.218274	H	-4.035154	2.043730	-1.078655
Co	1.611096	-0.043114	-1.050840	H	-1.631874	2.304812	-0.453428
O	1.617981	1.854425	-1.419616	H	-2.436270	1.150130	0.623960
C	0.849524	0.295691	5.899969	H	-0.701454	0.793365	1.706744
C	4.542549	0.694278	2.453210	H	4.467821	0.832813	4.400426
O	2.633009	0.330269	0.501026	H	0.228122	1.083858	3.756706
C	-1.182161	-0.346827	-1.152996	H	5.967576	0.264197	2.654383

H	1.388463	-0.468017	6.481572	C	-0.681246	0.110034	-2.543541
H	1.048535	1.267621	6.378133	C	-1.694946	-0.229736	-3.628078
H	3.399343	-5.078366	-5.835456	C	-3.021804	0.473299	-3.296440
H	4.920562	-5.250663	-4.935308	C	-3.537726	0.061864	-1.909962
H	-0.225538	0.091312	5.992586	C	-2.506428	0.330483	-0.800963
H	3.585502	-6.373375	-4.632613	N	0.644211	-0.506794	-2.610947
H	4.448751	-0.851329	-0.531428	C	0.924916	-1.522459	-3.371775
H	5.177568	-1.044397	-2.241155	C	1.952617	-2.479326	-3.073144
H	4.070670	1.559548	-0.882613	C	2.419712	-3.362175	-4.075076
H	5.182435	1.065828	-3.753906	C	3.292164	-4.399157	-3.784236
H	4.285845	2.524432	-3.240094	C	3.667364	-4.576885	-2.430824
H	5.913503	2.208177	-2.592034	C	3.220233	-3.758234	-1.402840
C	0.784933	2.802342	-1.056667	C	2.359634	-2.656785	-1.709501
C	1.436197	4.184176	-1.109267	O	1.963515	-1.894575	-0.711229
O	-0.395855	2.673164	-0.698597	C	3.609831	-3.981433	0.031439
H	2.191389	4.243081	-1.902402	C	3.824682	-5.321682	-4.853045
H	0.668933	4.954217	-1.245607	O	3.323463	0.014174	-2.137559
H	1.939511	4.359615	-0.146779	C	4.582080	-0.457749	-1.539085
74				C	4.375459	0.984136	-1.758050
1a-cis-B1-SPO ksi=71				C	4.972669	1.734455	-2.909038
C	2.169264	-2.651553	-1.396985	H	-1.324042	-1.442990	-1.215305
C	1.904057	-2.628947	-2.802982	H	-0.539417	1.197517	-2.487244
C	2.362541	-3.676636	-3.630812	H	-1.857788	-1.320418	-3.673445
C	3.100883	-4.733571	-3.117233	H	-1.320142	0.089626	-4.612444
C	3.348341	-4.745750	-1.724127	H	-2.867664	1.564189	-3.320612
C	2.900990	-3.752460	-0.861933	H	-3.771684	0.238741	-4.065977
C	1.067558	-1.586985	-3.326803	H	-3.789261	-1.012998	-1.925378
N	0.912189	-0.446033	-2.731054	H	-4.469268	0.598619	-1.678895
C	-0.220124	0.443596	-2.956076	H	-2.312711	1.405722	-0.685340
C	-1.011131	0.359030	-1.630484	H	-2.894427	-0.050675	0.154992
C	-2.084826	1.447507	-1.596105	H	-1.257229	-0.158423	1.439690
C	-3.017339	1.282629	-2.809626	H	3.373120	0.623043	4.906514
C	-2.248939	1.253613	-4.140854	H	-0.679819	-0.028265	3.642947
C	-1.139320	0.186939	-4.144167	H	4.935144	-0.167746	1.892641
N	-0.014852	0.378119	-0.537809	H	5.146627	0.825097	3.359891
Co	1.767112	0.056265	-1.115616	H	4.680541	1.574587	1.807360
O	3.549302	-0.264510	-1.747365	H	0.289159	-1.713240	-4.245494
C	3.919509	-0.030190	-2.988907	H	4.341580	-5.400963	-2.177336
O	3.307012	0.634238	-3.839916	H	2.081109	-3.208936	-5.103418
C	3.635457	-5.834640	-3.999268	H	4.025657	-3.065099	0.475799
C	3.181038	-3.770589	0.614320	H	4.344282	-4.792010	0.119499
O	1.719881	-1.740513	-0.553968	H	2.730020	-4.235069	0.641957

H	3.839716	2.106551	-0.900451	C	-0.379136	0.413734	0.710574
C	3.597736	3.591736	-2.542367	C	0.502665	0.336248	1.833085
H	1.810698	2.694767	0.398414	C	1.932193	0.361190	1.694841
H	5.696050	-0.257826	-4.204788	C	2.721188	0.272345	2.888124
H	5.932748	-0.671614	-2.462174	C	2.092313	0.154073	4.117478
H	5.036277	-1.773130	-3.520643	C	0.683361	0.130308	4.270423
H	1.304312	3.944216	-0.890940	C	-0.081313	0.230900	3.123620
H	2.796588	4.234414	-2.930548	O	2.574275	0.489081	0.558449
H	4.432014	4.226805	-2.210124	C	0.062275	-0.017857	5.636923
H	3.945963	2.932820	-3.348280	C	4.217280	0.281277	2.747859
74				O	1.854706	2.023586	-1.655315
1a-cis-B2-SPO ksi=322				C	1.903580	3.072744	-0.618466
C	2.556359	-2.508298	-1.530769	C	3.116108	2.757474	-1.395467
C	2.278605	-2.369616	-2.930854	C	5.245209	-0.712564	-3.315778
C	2.867471	-3.256925	-3.862400	H	-1.499367	-0.633910	-1.610511
C	3.729078	-4.267063	-3.465858	H	0.196544	1.458340	-3.042187
C	3.967681	-4.413951	-2.077592	H	-1.587226	-0.818524	-4.070921
C	3.403206	-3.586225	-1.117083	H	-0.565878	0.228494	-5.081419
C	1.248517	-1.461350	-3.349723	H	-1.794024	2.241700	-4.321146
N	0.847009	-0.447433	-2.642308	H	-2.945442	1.072476	-4.972172
C	-0.510861	0.096285	-2.713898	H	-3.582826	0.341910	-2.698668
C	-1.119332	-0.381394	-1.374416	H	-3.759299	2.094314	-2.820576
C	-2.507642	0.219932	-1.159319	H	-1.591191	2.432838	-1.617951
C	-3.409151	-0.115202	-2.359581	H	-2.667771	1.396493	-0.665258
C	-2.785279	0.318306	-3.694226	H	-1.450931	0.493454	0.939806
C	-1.393499	-0.306505	-3.887866	H	2.717818	0.065900	5.011128
N	-0.104305	-0.089577	-0.336509	H	-1.172598	0.210820	3.195692
Co	1.629315	0.086487	-1.003117	H	4.704391	0.099868	3.714306
O	3.430571	0.235993	-1.926973	H	4.573120	1.243725	2.349275
C	4.347528	1.298536	-1.491184	H	4.540820	-0.482783	2.026312
C	4.681821	-0.110037	-1.212029	H	0.502671	-1.785125	-4.245445
C	4.388494	-5.192366	-4.458186	H	3.932762	-5.569650	-1.303266
C	3.662497	-3.762106	0.352774	H	2.145104	-3.632186	-4.701377
O	2.057278	-1.733572	-0.592837	H	3.641154	-2.821147	0.923649
C	-0.401606	-0.058935	0.925212	H	3.844333	-4.603395	0.880752
C	0.502303	0.170140	2.008753	H	2.250376	-3.862064	1.194029
C	1.889961	0.458954	1.808802	H	0.371388	0.795733	6.311127
C	2.700969	0.691321	2.966116	H	-1.034143	-0.007374	5.577107
C	2.130432	0.619742	4.227645	H	3.349869	-5.676857	-5.047594
C	0.761408	0.331396	4.443197	H	4.734498	-5.884944	-3.955031
C	-0.024306	0.117983	3.325383	H	0.362951	-0.964144	6.112787
O	2.473016	0.531139	0.636342	H	3.254212	-6.819912	-3.689790

H	5.785734	-0.463438	-3.026264	C	0.199552	0.265350	5.841845
H	6.648139	-0.878276	-1.518808	C	4.160026	0.993857	2.767412
74				O	1.546207	1.971444	-1.396312
1a-trans-SPO-in ksi=209				C	0.626668	2.865668	-1.113418
C	5.138031	0.148310	1.312690	O	-0.565492	2.660771	-0.840367
C	3.904398	0.208244	0.611517	C	1.188671	4.286630	-1.148617
C	3.838153	0.867204	-0.659238	H	-1.193432	-1.484128	-1.441550
C	5.052514	1.413011	-1.197637	H	-0.434322	1.189987	-2.658321
C	6.224706	1.321698	-0.464719	H	-1.488290	-1.404906	-3.937606
C	6.300303	0.698672	0.806502	H	-0.943530	0.029655	-4.834379
C	2.771605	-0.437020	1.197575	H	-2.694428	1.416316	-3.716193
N	1.575636	-0.497437	0.690982	H	-3.440876	0.034426	-4.530346
C	0.494947	-1.281026	1.319357	H	-3.596127	-1.202917	-2.387361
C	-0.826415	-0.601409	0.919073	H	-4.388234	0.367441	-2.226248
C	-2.017383	-1.466357	1.321415	H	-2.388546	1.305195	-1.037671
C	-1.979654	-1.711510	2.838737	H	-2.963248	-0.177312	-0.240464
C	-0.644245	-2.319504	3.287759	H	-1.451483	-0.210929	1.199826
C	0.557209	-1.473524	2.833469	H	2.774191	0.793313	5.095622
N	-0.698902	-0.253248	-0.503211	H	-1.088588	-0.102533	3.445555
Co	1.043379	0.334610	-0.921570	H	4.674782	0.152145	2.277973
O	1.451968	-1.129420	-2.034833	H	4.654140	1.192300	3.727003
C	0.962114	-2.350640	-2.007226	H	4.296668	1.866385	2.111297
O	0.239644	-2.881466	-1.151229	H	0.714439	-1.694418	-4.279380
O	2.753618	1.012090	-1.372847	H	4.628310	-5.218966	-1.741061
C	5.005284	2.042429	-2.563209	H	2.629458	-3.131287	-4.922231
C	7.610543	0.634005	1.551494	H	2.731649	-3.995835	0.890661
C	-1.638789	-0.447242	-1.376961	H	4.038725	-2.830106	0.799883
C	-1.542335	-0.100059	-2.764828	H	4.385969	-4.567285	0.532570
C	-2.526054	-0.590447	-3.657531	H	0.320103	1.223759	6.370205
C	-2.493205	-0.298059	-5.011683	H	-0.871723	0.024351	5.826179
C	-1.447467	0.535507	-5.475405	H	5.484529	-5.087654	-4.438219
C	-0.467921	1.059730	-4.642690	H	4.161166	-6.246646	-4.238274
C	-0.490285	0.740749	-3.250159	H	0.708071	-0.503017	6.444452
O	0.433613	1.271934	-2.478805	H	4.051695	-4.981539	-5.481615
C	0.640985	1.937451	-5.151944	H	4.461019	-0.453250	-0.198995
C	-3.513572	-0.854543	-5.974023	C	5.670466	-0.893089	-2.023053
O	0.643066	2.007907	0.260285	H	3.934402	1.914345	-0.693804
C	0.964347	3.441857	0.021143	H	1.948618	4.395708	-1.931913
C	1.843082	3.824656	-1.129525	H	0.375603	5.006232	-1.293308
C	-0.409936	2.941543	-0.161012	H	1.669903	4.488952	-0.180382
C	1.372783	-3.114166	-3.265580	H	4.818221	1.809370	-2.333387
H	-3.315456	-1.233830	-3.259037	H	5.349986	-1.938815	-2.118062

C	6.013575	1.332880	0.158196	H	-1.399102	0.771393	-6.543044
C	4.876725	1.570698	-0.598177	H	0.535045	2.967537	-4.776891
C	2.452781	-0.568698	1.378873	H	1.612137	1.574367	-4.786792
N	1.281642	-0.527581	0.814439	H	0.648412	1.968676	-6.249010
C	0.162824	-1.354499	1.316103	H	-2.566894	-0.928769	-1.050116
C	-1.121634	-0.754772	0.728932	H	-0.876045	0.358720	1.465327
C	-2.307074	-1.682357	0.986376	H	-1.964221	-2.420677	0.773549
C	-2.462116	-1.896375	2.502264	H	-2.964252	-0.975975	1.050359
C	-1.167725	-2.406700	3.149899	H	-2.812485	-2.368303	3.129561
C	0.031702	-1.497627	2.832158	H	-2.137872	-0.752802	3.362140
N	-0.825692	-0.398337	-0.665489	H	-0.545272	-3.331620	2.862219
Co	0.900622	0.329092	-0.828785	H	-0.628221	-2.432642	4.381720
O	1.617546	-1.058651	-1.881778	H	1.486352	-1.983937	3.124042
C	1.268496	-2.327662	-1.895990	H	0.551534	-0.491007	3.336536
O	0.456598	-2.916478	-1.168048	H	0.498644	-2.255945	0.805424
C	7.302094	0.262087	2.069527	H	5.156254	-0.362441	2.279896
C	4.889694	2.458095	-1.811138	H	7.138395	1.741552	-0.897321
O	2.590372	1.207347	-0.971354	H	6.010561	2.329081	-2.897371
C	-1.660741	-0.561631	-1.643839	H	4.363338	2.935979	-2.574748
C	-1.441090	-0.114888	-2.986660	H	4.565917	1.346093	-3.292271
C	-0.372525	0.782455	-3.309973	H	2.949620	-0.933964	2.158825
C	-0.250588	1.225274	-4.665310	H	-4.263470	-1.461784	-5.450090
C	-1.154916	0.771623	-5.614069	H	-4.043138	-0.052097	-6.510393
C	-2.217987	-0.113031	-5.309607	H	7.990678	1.640479	1.786822
C	-2.344118	-0.531691	-3.995769	H	7.502264	0.087115	2.497605
O	0.483578	1.258571	-2.437430	H	-0.752151	2.757537	-1.180482
C	-3.160751	-0.580284	-6.390522	H	-3.038033	-1.492707	-6.735115
C	0.876288	2.160190	-5.004373	H	8.386046	0.126731	0.956696
O	0.149188	1.964899	0.165754	H	2.328838	-2.755330	-3.662034
C	1.007960	2.846748	0.976710	H	1.414773	-4.186309	-3.043730
C	0.561681	3.288761	-0.355887	H	0.598654	-2.941044	-4.027131
C	1.995356	-3.069731	-3.017500	H	1.190122	3.917851	0.980154
H	-3.152993	-1.213328	-3.717945	H	1.672858	4.890395	-1.349111
H	-1.033329	1.110445	-6.647522	H	2.899327	3.691704	-0.867910
H	0.751744	3.131180	-4.500197	H	1.617512	3.222385	-2.014729
H	1.832550	1.751387	-4.647688	H	-1.168538	3.106229	0.606804
H	0.933268	2.334510	-6.086413	74			
H	-2.606059	-1.077540	-1.441645	1a-trans-SPO ksi=67			
H	-1.304038	0.206222	1.245791	C	3.640998	0.940722	-0.234908
H	-2.128632	-2.641484	0.474575	C	3.634468	0.094074	0.921334
H	-3.234687	-1.252537	0.580697	C	4.832222	-0.105599	1.658528
H	-3.284857	-2.600108	2.695553	C	6.025652	0.491728	1.298597

C	0.279013	-2.111704	3.642531	H	-2.749974	-0.939971	2.971161
C	1.210564	-1.080561	2.982252	H	-0.951065	-3.421474	2.778006
N	-0.543283	-0.537763	-0.299511	H	-1.296322	-2.489373	4.239145
Co	0.952825	0.431842	-0.897492	H	0.942333	-1.932433	3.268005
O	1.629818	-0.930364	-2.010179	H	-0.105920	-0.502450	3.289198
C	1.518746	-2.233171	-1.859446	H	0.289512	-2.341480	0.843584
O	1.055715	-2.865592	-0.899755	H	4.796047	-0.762488	2.532322
O	2.406098	1.516032	-1.492074	H	6.947765	1.812956	-0.149111
C	4.247746	2.881273	-3.012400	H	5.902616	2.824949	-2.019475
C	7.851795	1.154165	0.106592	H	4.222908	3.323637	-1.676527
C	-1.483375	-0.991145	-1.068259	H	4.511312	1.916898	-2.690069
C	-1.585041	-0.708989	-2.470180	H	2.563847	-1.166219	2.292265
C	-2.491331	-1.465593	-3.251508	H	-3.963735	-1.202178	-5.973368
C	-2.640155	-1.249496	-4.612008	H	-3.627595	0.268831	-6.912920
C	-1.864978	-0.220889	-5.198761	H	7.722246	1.207734	2.445710
C	-0.975068	0.563882	-4.478804	H	7.131618	-0.396698	2.931311
C	-0.810574	0.332377	-3.077302	H	1.285528	3.170575	-1.164315
O	0.021962	1.107401	-2.420682	C	-0.567160	4.249646	-0.572009
C	-0.139942	1.635206	-5.122170	H	2.027175	2.482558	1.101788
C	-3.572452	-2.083829	-5.455203	H	-2.634840	-1.178453	-7.151020
O	0.199705	2.028581	0.142666	H	8.073264	-0.205400	1.437899
C	0.244614	3.329812	-0.567188	H	2.957076	-2.602151	-3.254469
C	-1.043777	4.092679	-0.547785	H	2.128268	-4.118865	-2.730650
C	1.078874	3.108572	0.626827	H	1.361569	-3.030075	-3.915055
C	2.021755	-2.958510	-3.106798	H	0.496344	3.212445	1.869620
H	-3.068734	-2.253558	-2.759990	H	-0.167861	5.265193	-0.708012
H	-1.958320	-0.042456	-6.274522	H	-1.119755	3.975873	-1.480062
H	-0.411326	2.633129	-4.744849	H	-1.258726	4.254305	0.280384
H	0.920696	1.491221	-4.871091	74			
H	-0.261919	1.629584	-6.212859	1a-trans-SPO ksi=69			
H	-2.244854	-1.647823	-0.633062	C	5.412405	0.570720	0.440411
H	-0.699431	0.201508	1.615970	C	4.042359	0.623930	0.069755
H	-1.171205	-2.807137	1.282390	C	3.643003	1.386380	-1.076476
H	-2.452252	-1.596556	1.520828	C	4.660262	2.083526	-1.807311
H	-1.818393	-2.679452	3.696597	C	5.982019	1.986669	-1.400482
H	-1.538228	-0.936132	3.705693	C	6.394149	1.231974	-0.274273
H	0.585487	-3.120817	3.320886	C	3.105841	-0.100548	0.872833
H	0.397308	-2.078517	4.735570	N	1.828779	-0.209647	0.651006
H	2.254301	-1.316805	3.233738	C	0.989818	-1.111590	1.470392
H	1.003795	-0.067701	3.368020	C	-0.473181	-0.773952	1.146801
H	1.170835	-2.122821	1.073585	C	-1.400293	-1.831696	1.740366
H	5.687279	-0.025175	1.315470	C	-1.191761	-1.886025	3.264065

C	4.553830	2.683334	-3.090209	H	6.742145	2.513606	-1.985610
C	7.954531	1.203853	0.367181	H	5.123508	3.292377	-3.530469
C	-1.426671	-0.793052	-1.133383	H	3.584452	3.713321	-2.730180
C	-1.500225	-0.555057	-2.545403	H	3.672856	2.256341	-3.710805
C	-2.457704	-1.271448	-3.304263	H	3.523108	-0.615544	1.747700
C	-2.583038	-1.097237	-4.673028	H	-4.119684	-2.810188	-4.839940
C	-1.731049	-0.151670	-5.291911	H	-4.311913	-1.459041	-5.978995
C	-0.787016	0.590743	-4.595306	H	8.273839	2.153366	0.294493
C	-0.644317	0.397850	-3.186488	H	7.991909	0.553535	1.015112
O	0.241965	1.132894	-2.549746	H	0.757067	3.498344	1.594964
C	0.122504	1.577816	-5.271189	H	-3.020582	-2.646111	-6.224677
C	-3.574178	-1.887611	-5.491057	H	8.452167	0.695244	-0.694271
O	0.593231	2.132353	0.049704	H	2.800815	-2.384357	-3.620163
C	-0.633617	2.866902	-0.353923	H	2.384904	-3.954261	-2.828778
C	-1.470215	3.359946	0.788318	H	1.170750	-3.072817	-3.793897
C	0.695595	3.409632	-0.677237	H	0.751377	3.222555	-1.527886
C	1.889601	-3.093068	-3.095140	H	-0.861188	5.134887	-0.847853
H	-3.093032	-1.996537	-2.788234	H	-1.747955	3.649473	-1.263882
H	-1.808162	-0.005521	-6.373752	H	-1.498385	4.087989	0.451476
H	-0.085482	2.605057	-4.934385	H	2.141012	2.904009	0.497319
H	1.169474	1.374758	-5.004771	74			
H	0.006857	1.538695	-6.361823	1a-trans-SPO ksi=141			
H	-2.233616	-1.383211	-0.685344	C	5.503895	0.607210	0.570210
H	-0.559872	0.388846	1.544176	C	4.161055	0.621276	0.107701
H	-1.270308	-2.572791	1.218055	C	3.832654	1.311915	-1.103744
H	-2.451756	-1.264363	1.452862	C	4.892453	1.971590	-1.810316
H	-1.911850	-2.391890	3.629893	C	6.183643	1.917305	-1.311201
H	-1.485833	-0.678226	3.641686	C	6.525223	1.238385	-0.114921
H	0.447300	-3.030195	3.241805	C	3.182251	-0.071514	0.885421
H	0.348266	-1.987489	4.665298	N	1.921370	-0.199049	0.595446
H	2.257866	-1.368823	3.171245	C	1.022536	-1.045920	1.406909
H	1.113669	-0.021426	3.313188	C	-0.412740	-0.604029	1.079053
H	1.128978	-2.064915	1.001789	C	-1.421909	-1.581895	1.675000
H	5.724658	0.067347	1.495623	C	-1.220861	-1.653231	3.198300
H	6.976796	2.415997	-1.877024	C	0.226218	-2.002036	3.572349
H	5.457066	3.080872	-3.570422	C	1.238261	-1.044668	2.919757
H	3.856300	3.515495	-2.909237	N	-0.460680	-0.380917	-0.371348
H	4.041984	2.003464	-3.786491	Co	1.116551	0.442420	-0.989874
H	3.548865	-0.541659	1.806435	O	1.694682	-1.013433	-2.042066
H	-4.150968	-2.575318	-4.858574	C	1.437154	-2.292949	-1.874347
H	-4.286531	-1.228078	-6.010011	O	0.882264	-2.854323	-0.918287
H	8.348281	2.217839	0.536907	O	2.630852	1.398752	-1.615300

C	4.246197	-0.866004	2.388445	H	8.040293	0.647921	1.310185
O	3.021673	0.386091	-0.866198	H	1.124071	4.202652	-0.061565
C	6.584144	-0.965674	3.351295	H	-3.067728	-2.487805	-6.262725
C	5.685556	0.868149	-1.289433	H	8.614656	0.719448	-0.368972
O	1.366850	-1.390943	-1.857958	H	2.779945	-2.651541	-3.556843
C	0.540973	-2.409123	-1.972497	H	2.072495	-4.132819	-2.802795
C	1.032672	-3.375046	-3.050252	H	1.075063	-3.069217	-3.833769
O	-0.518301	-2.625426	-1.365628	H	-1.140003	2.356216	-1.175174
C	1.993396	3.081572	-0.407831	H	-2.164370	4.134048	0.429348
H	-2.794879	-0.069549	-4.305167	H	-2.071334	2.543008	1.210948
H	0.376975	1.054437	-6.978393	H	-0.845380	3.789413	1.581667
H	2.995234	0.882303	-4.580610	H	1.083137	3.286852	-1.688377
H	2.559131	1.570931	-6.179149	74			
H	2.469742	2.556794	-4.695263	1a-trans-RPO-in ksi=146			
H	-2.536773	0.082391	-1.989205	C	-1.768706	0.261945	-4.486257
H	-1.216201	0.994339	0.883630	C	-0.916784	0.450744	-3.369887
H	-2.917164	-1.362349	-0.084177	C	0.435655	0.881338	-3.565781
H	-3.442609	0.336715	-0.063020	C	0.883376	1.106628	-4.905101
H	-4.262072	-0.877707	1.971190	C	0.008286	0.892724	-5.960875
H	-3.187453	0.459441	2.389916	C	-1.330239	0.466526	-5.783736
H	-2.424079	-2.513140	2.276668	C	-1.454528	0.235939	-2.059470
H	-2.596907	-1.536904	3.739625	N	-0.750700	0.201462	-0.970373
H	-0.203442	-1.839508	3.083211	Co	1.129679	0.222317	-0.910943
H	-0.648117	-0.122028	3.069193	O	1.150267	2.016749	0.147085
H	-0.595517	-1.954007	0.586397	C	0.565353	3.350351	-0.160182
H	3.860875	-1.313457	3.309388	C	-0.449984	3.477956	-1.256842
H	7.116218	0.135063	0.909022	O	1.278502	1.129130	-2.587545
H	6.779202	0.959157	-1.288258	C	2.303841	1.551375	-5.111954
H	5.247372	1.863289	-1.459944	C	-2.226414	0.234027	-6.974958
H	5.374750	0.251307	-2.145187	C	-1.333749	0.022897	0.366292
H	1.708604	-1.301355	2.565157	C	-0.434787	-0.989626	1.095130
H	-2.276727	1.123766	-7.620606	C	-0.822030	-1.090477	2.568847
H	-1.859050	-0.596840	-7.597389	C	-2.301698	-1.495009	2.680928
H	7.310102	-1.724684	3.019799	C	-3.218712	-0.535053	1.912405
H	7.160860	-0.081041	3.662305	C	-2.798818	-0.400419	0.439581
H	0.315119	3.851319	0.780482	N	0.953748	-0.597875	0.785835
H	2.309405	2.872766	-1.431295	C	1.939164	-0.837271	1.598747
H	-3.248866	-0.012442	-6.659380	C	3.318844	-0.549755	1.360005
H	6.069458	-1.359536	4.237754	C	3.783560	0.036615	0.138323
H	0.576348	-3.070696	-4.003437	C	5.192447	0.272810	-0.000428
H	2.121443	-3.336758	-3.162853	C	6.046356	-0.054938	1.039879
H	0.696408	-4.389934	-2.810003	C	5.601356	-0.627547	2.257938

O	-0.560027	-2.794627	-1.231461
H	-3.668387	0.148373	-2.960430
H	-1.482818	1.661569	-6.337137
H	1.762592	1.171724	-4.960624
H	0.861607	2.070576	-6.225390
H	1.285144	2.840108	-4.672986
H	-2.673356	-0.059642	-0.870844
H	-0.604621	0.480611	1.551167
H	-2.381218	-1.887308	0.761581
H	-2.972244	-0.264939	1.190597
H	-3.106346	-1.803859	3.158156
H	-2.031008	-0.436751	3.462677
H	-1.171158	-3.284625	2.696599
H	-0.972536	-2.526254	4.280958
H	1.149022	-2.508801	2.950049
H	0.617548	-0.857093	3.325947
H	0.063375	-2.337642	0.674305
H	4.963550	-0.866852	2.504801
H	7.299803	1.026228	-0.564224
H	6.370161	1.614819	-2.658280
H	4.656213	2.114722	-2.569103
H	5.056558	0.529133	-3.205635
H	2.760959	-1.392475	2.201934
H	-4.212921	1.835773	-6.029684
H	-3.865691	0.147633	-6.436461
H	8.310472	-0.547567	1.522666
H	7.898675	1.056188	2.150140
H	-0.112982	2.826776	-1.005990
H	0.265705	3.513276	0.688925
H	2.282500	2.661771	-1.551822
H	3.386884	4.520408	-0.124023
H	2.769692	3.715020	1.346473
H	4.005741	2.915025	0.332246
H	-4.851436	0.528140	-5.009566
H	7.270740	-0.397476	2.954862
H	-0.203416	-2.950695	-4.101117
H	1.504784	-3.269732	-3.722376
H	0.212411	-4.380567	-3.119406
74			

1a-trans-RPO-in ksi=154

C	-2.149371	0.138577	-4.129027
C	-1.193183	0.393816	-3.115175

H	-0.571648	4.545149	-1.495617
H	-0.132799	2.943646	-2.156491
H	-1.426998	3.094081	-0.935073
H	2.754453	3.429961	0.291913

74

1a-trans-RPO ksi=211

C	-0.336423	1.000816	-3.185676
C	-1.568224	0.535582	-2.623815
C	-2.741923	0.506588	-3.417991
C	-2.737673	0.900860	-4.744877
C	-1.510361	1.353040	-5.287407
C	-0.333672	1.417038	-4.554206
C	-1.665000	0.127681	-1.254923
N	-0.656947	-0.048172	-0.455227
Co	1.155423	0.049326	-0.966948
O	1.367258	1.761666	0.141539
C	0.604532	2.975035	-0.198887
C	2.042567	2.908227	-0.515370
C	3.110090	3.551305	0.315916
C	-3.981898	0.850539	-5.596889
C	0.960637	1.900189	-5.145887
O	0.785427	1.112489	-2.510096
C	-0.815497	-0.429943	0.958222
C	-2.171359	-0.996432	1.374324
C	-2.143261	-1.359507	2.867708
C	-0.995085	-2.320355	3.200655
C	0.365255	-1.763925	2.748684
C	0.309723	-1.436513	1.259387
N	1.521262	-0.871619	0.645027
C	2.686665	-0.917488	1.216598
C	3.903847	-0.385019	0.684171
C	5.058479	-0.426598	1.507891
C	6.278371	0.075839	1.093260
C	6.344354	0.625950	-0.210640
C	5.255193	0.684256	-1.065779
C	3.983783	0.180446	-0.629672
C	7.500908	0.044519	1.976411
C	5.350329	1.269208	-2.446951
O	2.981675	0.285050	-1.464610
O	1.130522	-1.475913	-2.080088
C	0.300139	-2.495173	-2.074668
C	0.482680	-3.340521	-3.334746

H	-2.696308	-1.527029	0.351132	C	0.097965	0.907971	-3.462130
H	-3.303107	0.140956	0.461797	C	0.380974	1.146041	-4.843078
H	-3.815456	-1.140359	2.555882	C	-0.589457	0.863824	-5.794511
H	-2.772155	0.248969	2.871633	C	-1.869748	0.355033	-5.468153
H	-1.875097	-2.677521	2.621455	C	-1.560828	0.148629	-1.752097
H	-1.922802	-1.724516	4.108988	N	-0.734305	0.159677	-0.751781
H	0.389107	-1.900936	3.169868	Co	1.139790	0.266732	-0.921022
H	-0.136341	-0.207985	3.236133	O	1.278352	2.041213	0.137616
H	-0.296849	-2.007823	0.733523	C	0.509087	3.311309	-0.005143
H	4.430912	-1.212588	2.891084	C	-0.721799	3.350634	-0.861453
H	7.306791	0.342361	0.103925	O	1.026786	1.212943	-2.582931
H	6.662547	1.201116	-2.010575	C	1.742357	1.668988	-5.206566
H	5.075485	2.024866	-1.993336	C	-2.871951	0.045701	-6.552710
H	5.204553	0.421394	-2.697551	C	-1.145681	-0.066260	0.639099
H	2.203704	-1.273918	2.426244	C	-0.118789	-1.043218	1.236466
H	-3.048902	0.918532	-7.199417	C	-0.321836	-1.178618	2.744311
H	-2.520038	-0.771581	-7.201719	C	-1.756643	-1.658195	3.023789
H	7.852721	-1.480798	2.126930	C	-2.805867	-0.740238	2.383464
H	7.682148	0.119224	2.866267	C	-2.568075	-0.566216	0.874567
H	0.421781	3.783547	0.978343	N	1.200783	-0.582898	0.768250
H	1.962262	3.008755	-1.641031	C	2.291181	-0.789828	1.445912
H	-3.836192	-0.259872	-6.125555	C	3.618261	-0.449148	1.037693
H	6.749861	-1.253473	3.501153	C	3.905617	0.158880	-0.228012
H	0.290645	-2.939460	-4.013745	C	5.277792	0.436738	-0.545415
H	1.938722	-3.193852	-3.395878	C	6.267897	0.124082	0.370872
H	0.600635	-4.306770	-2.910159	C	6.000132	-0.470069	1.630020
H	-0.966949	4.405250	-1.058146	C	4.680599	-0.745888	1.933751
H	-0.560059	2.840856	-1.815473	O	3.013016	0.487298	-1.125957
H	-1.580456	2.899119	-0.348100	C	7.127261	-0.788053	2.580852
H	2.723319	3.609429	-0.045819	C	5.582574	1.054536	-1.881373
74				O	1.301515	-1.320549	-1.929743
1a-trans-RPO-in ksi=266				C	0.507626	-2.369025	-1.967386
C	-2.164296	0.336381	-4.457510	C	0.875668	-3.272072	-3.143805
C	-1.153364	0.384069	-3.461422	O	-0.444779	-2.652762	-1.225555
C	0.209058	0.628926	-3.835726	C	1.863729	3.187822	-0.568874
C	0.503333	0.815294	-5.228160	H	-3.124701	-0.258383	-3.834259
C	-0.524883	0.750248	-6.153288	H	-0.345056	1.031929	-6.847990
C	-1.877553	0.510161	-5.798266	H	2.522671	1.061497	-4.727164
C	-1.538239	0.193130	-2.102145	H	1.889201	1.665775	-6.294140
N	-0.723913	0.093911	-1.090104	H	1.884977	2.697169	-4.839490
Co	1.159230	0.048559	-1.222645	H	-2.616180	-0.071100	-1.557971
O	1.355357	2.115044	-0.774406	H	-1.015211	0.901891	1.160135

H	-0.325680	-2.035047	0.456389	C	1.406689	3.068074	0.345647
H	4.113711	-0.400411	3.103821	C	1.222007	2.576756	1.749778
H	7.095671	1.057887	0.374840	O	1.202795	0.729569	-2.994760
H	6.618062	1.425080	-1.926414	C	1.932456	1.062830	-5.619607
H	4.902026	1.787110	-2.303744	C	-2.944815	0.438693	-6.861765
H	5.523650	0.169631	-2.578996	C	-1.212503	-0.122166	0.284287
H	1.997984	-0.968916	2.391156	C	-0.200037	-1.062016	0.958378
H	-2.997420	1.372282	-7.442813	C	-0.491182	-1.207508	2.450036
H	-2.744552	-0.375075	-7.575975	C	-1.924410	-1.730293	2.640398
H	7.612654	-0.201627	2.805209	C	-2.953749	-0.837347	1.937550
H	7.095385	1.458279	3.140008	C	-2.634208	-0.658646	0.444606
H	2.237502	3.764757	0.198205	N	1.127696	-0.560391	0.570051
H	-0.667327	2.715540	-0.364700	C	2.153212	-0.602310	1.369469
H	-3.933943	0.260349	-6.419919	C	3.474340	-0.168156	1.048812
H	6.296570	0.099625	3.959823	C	3.848140	0.200235	-0.286878
H	0.441130	-3.551586	-3.962657	C	5.198437	0.644225	-0.503602
H	1.964448	-3.755056	-3.062151	C	6.076750	0.706041	0.564547
H	0.497767	-4.709058	-2.610130	C	5.722394	0.337059	1.888638
H	1.043586	3.439197	2.409023	C	4.429443	-0.101671	2.099600
H	0.370065	1.892162	1.830040	O	3.060673	0.158451	-1.325587
H	2.125870	2.059334	2.096554	C	6.731738	0.427463	3.006371
H	0.312134	3.853387	-1.450647	C	5.593190	1.032872	-1.900197
74				O	1.299315	-1.685201	-1.947782
1a-trans-RPO-in ksi=66				C	0.393444	-2.635644	-2.032776
C	-1.874903	-0.176776	-4.543122	C	0.873403	-3.744228	-2.970198
C	-1.115288	0.219911	-3.415719	O	-0.717840	-2.707122	-1.486943
C	0.156629	0.856180	-3.592575	C	0.309665	3.116104	-0.645569
C	0.627860	1.052745	-4.929430	H	-3.192948	0.141824	-4.141242
C	-0.151510	0.628596	-5.996139	H	-0.277268	0.883116	-7.211060
C	-1.414255	0.008403	-5.836162	H	2.583750	0.275136	-5.214517
C	-1.660100	0.004971	-2.109169	H	2.041298	1.103069	-6.710848
N	-0.989138	0.128292	-1.006495	H	2.299674	2.007610	-5.190762
Co	0.863427	0.454194	-0.903278	H	-2.613005	0.104097	-1.911890
O	0.354824	2.255102	0.005130	H	-1.147771	0.853665	0.805540
C	0.867676	3.626064	-0.265412	H	-2.703613	-1.618642	-0.089523
C	1.802396	3.857002	-1.413556	H	-3.365253	0.030196	-0.003036
O	0.900283	1.302583	-2.608330	H	-3.962469	-1.260036	2.051351
C	1.974527	1.691621	-5.121969	H	-2.971665	0.152042	2.427190
C	-2.205534	-0.441582	-7.038931	H	-1.988651	-2.750267	2.227828
C	-1.575008	-0.022761	0.330741	H	-2.154496	-1.806120	3.713231
C	-0.579385	-0.842387	1.162779	H	0.217679	-1.907812	2.914625
C	-0.961126	-0.774705	2.640715	H	-0.369488	-0.235042	2.959098

H	-1.655558	-1.197824	-7.620706	C	-2.376592	-1.351505	2.814402
H	7.266603	-2.019737	2.167186	C	-3.402036	-0.647942	1.913434
H	7.199740	-0.574543	3.188153	C	-2.971129	-0.631736	0.435469
H	0.043508	4.338477	-0.161529	N	0.775320	-0.370373	0.801302
H	2.255974	2.446018	0.983910	C	1.812007	-0.742205	1.492772
H	-3.165186	-0.883298	-6.739462	C	3.178853	-0.462075	1.179910
H	6.133138	-1.953408	3.532640	C	3.559728	0.338088	0.053522
H	0.967365	-3.100595	-3.744459	C	4.956972	0.580704	-0.155428
H	2.510614	-3.034555	-2.864885	C	5.884451	0.025222	0.712458
H	1.273713	-4.281643	-2.442482	C	5.524504	-0.775677	1.824532
H	2.319196	4.814635	-1.244835	C	4.176375	-0.997348	2.036789
H	2.533371	3.046014	-1.492609	O	2.718211	0.894524	-0.784124
H	1.247966	3.917470	-2.356770	C	6.583651	-1.360918	2.725471
H	0.793653	3.123838	1.915885	C	5.363339	1.424126	-1.331288
75				O	1.383813	-1.130324	-1.773546
1b-cis-B1-RPO ksi=344				C	0.770059	-2.295561	-1.773118
C	-0.770019	0.949799	2.890774	C	1.440884	-3.247432	-2.763041
C	0.047534	0.600561	1.777816	O	-0.223673	-2.648861	-1.124357
C	1.365415	0.071038	1.997920	C	1.265292	2.900632	0.956859
C	1.808492	-0.086488	3.357929	H	-2.842924	-0.656880	-4.374067
C	0.964460	0.268194	4.393463	H	0.237327	0.772218	-7.009033
C	-0.341150	0.794114	4.192065	H	2.723463	1.198504	-4.486367
C	-0.493122	0.780105	0.475519	H	2.289850	1.635890	-6.171747
N	0.112868	0.525015	-0.654315	H	1.962294	2.749964	-4.818828
Co	1.872394	-0.176108	-0.798201	H	-2.711807	-0.296780	-2.049643
O	2.712717	1.701938	-0.558594	H	-1.599857	0.996959	0.756887
O	2.202597	-0.275529	1.064860	H	-2.949777	-1.653960	0.024699
C	3.187095	-0.637102	3.585799	H	-3.697288	-0.049740	-0.151045
C	-1.208023	1.156721	5.371481	H	-4.383608	-1.134819	2.008121
C	-0.587235	0.663056	-1.947572	H	-3.533706	0.392068	2.257134
C	0.518836	0.863564	-3.008430	H	-2.351949	-2.425546	2.566558
C	-0.062245	0.871954	-4.419745	H	-2.685571	-1.276615	3.867367
C	-1.108712	1.991545	-4.531051	H	-0.253907	-1.346093	3.258419
C	-2.211544	1.831832	-3.476124	H	-0.923490	0.272650	2.986222
C	-1.643362	1.766480	-2.048519	H	-0.641172	-1.878590	0.795672
N	1.492090	-0.172196	-2.668544	H	3.853608	-1.608972	2.884188
C	1.721115	-1.187917	-3.449300	H	6.945935	0.210154	0.520826
C	2.197945	-2.444658	-2.959045	H	6.453243	1.423190	-1.458817
C	1.921250	-2.779512	-1.594094	H	5.030165	2.466214	-1.206655
C	2.289656	-4.073479	-1.124892	H	4.887682	1.057882	-2.252050
C	2.914335	-4.950579	-2.003139	H	1.640493	-1.332745	2.402151
C	3.196344	-4.632400	-3.352766	H	-2.417671	0.397481	-7.719387

C	4.502215	-0.535770	-1.880439
O	5.650886	-1.306938	-1.744218
C	6.640609	-1.052856	-2.757287
O	4.390275	0.287931	-2.802613
H	6.976579	-0.006338	-2.732569
H	7.475416	-1.723788	-2.524601
H	6.244342	-1.270084	-3.759041

75

1b-cis-B1-RPO ksi=140

C	-0.866862	0.669860	2.554152
C	0.074920	0.572892	1.494444
C	1.443776	0.248995	1.784134
C	1.808280	0.035695	3.154387
C	0.840908	0.132257	4.141108
C	-0.515169	0.448728	3.871689
C	-0.385666	0.826074	0.166537
N	0.318622	0.684297	-0.919317
Co	2.063943	-0.058120	-0.968663
O	2.761755	1.832288	-1.306500
O	2.400204	0.165994	0.892905
C	3.239168	-0.309556	3.456393
C	-1.520708	0.526293	4.993485
C	-0.277025	0.907632	-2.254884
C	0.879761	0.823238	-3.276667
C	0.335203	0.808470	-4.700743
C	-0.459000	2.106506	-4.932300
C	-1.573441	2.293793	-3.890355
C	-1.045056	2.216319	-2.446950
N	1.662668	-0.312317	-2.804806
C	1.738925	-1.447379	-3.427389
C	2.104492	-2.668841	-2.773849
C	1.912673	-2.775821	-1.359635
C	2.167557	-4.032057	-0.734951
C	2.597336	-5.097005	-1.516518
C	2.789801	-5.006945	-2.915272
C	2.525013	-3.789215	-3.523333
O	1.445547	-1.796061	-0.606008
C	3.282661	-6.197322	-3.699530
C	1.990008	-4.137204	0.753334
O	3.845913	-0.774300	-1.030227
H	-0.951268	0.054772	-2.460403
H	1.514045	1.713218	-3.149632

C	2.814494	-3.381525	-3.814728
O	1.286671	-1.968366	-0.764509
C	3.913643	-5.620954	-4.237412
C	2.034239	-4.410368	0.316320
O	3.679619	-0.840685	-0.927011
H	-1.057164	-0.313495	-2.170011
H	0.984493	1.844905	-2.823935
H	-0.537807	-0.099628	-4.632721
H	0.739650	1.014921	-5.158850
H	-0.613744	2.968878	-4.401250
H	-1.547023	1.994190	-5.539568
H	-2.775851	0.906442	-3.680748
H	-2.931263	2.660000	-3.548373
H	-1.185980	2.733596	-1.778461
H	-2.462386	1.589707	-1.337479
H	-1.516788	1.172073	0.433839
H	1.321841	0.135152	5.419222
H	-1.769914	1.346325	2.691619
H	3.411749	-0.706485	4.657733
H	3.944091	-0.006550	3.096888
H	3.290235	-1.632657	3.129882
H	1.475568	-1.105234	-4.514100
H	3.223538	-5.928072	-1.620889
H	3.017123	-3.094411	-4.849826
H	2.495269	-5.369365	0.584202
H	0.956077	-4.466539	0.528733
H	2.436531	-3.615320	0.960198
H	-2.177968	1.553595	5.042997
H	-1.401711	0.282079	6.011888
H	3.372381	-6.577458	-4.295388
H	4.025519	-5.232200	-5.258092
H	-0.728316	1.919597	6.004212
H	4.920571	-5.841118	-3.850516
C	2.085073	3.018363	-0.674102
C	3.194384	2.653301	-1.576849
C	4.595508	3.144263	-1.375712
H	1.053500	2.998825	-1.029782
H	2.276854	3.654772	0.192647
H	2.952960	2.319647	-2.587298
H	5.297544	2.384010	-1.738764
H	4.748580	4.066524	-1.956188
H	4.791005	3.354938	-0.316474

75				H	-0.323371	-0.063889	-4.849652
1b-cis-B1-RPO ksi=31				H	1.162270	0.728124	-5.420956
C	-0.381367	0.998494	2.993803	H	0.233911	2.962770	-4.883446
C	0.320057	0.685244	1.797209	H	-0.888657	2.107847	-5.944559
C	1.716023	0.360906	1.853580	H	-2.337047	1.510672	-4.032639
C	2.356844	0.367878	3.139204	H	-2.079891	3.257176	-4.048782
C	1.617978	0.678908	4.267459	H	-0.364424	3.058590	-2.241332
C	0.236263	1.000321	4.228626	H	-1.881160	2.292288	-1.736989
C	-0.403035	0.738929	0.569664	H	-1.426232	1.164637	0.070010
N	0.068075	0.475908	-0.615278	H	1.139638	-0.054274	5.177214
Co	1.853418	-0.060657	-0.968321	H	-1.903202	0.913921	2.302768
O	2.216335	1.948217	-1.082429	H	3.370540	-0.552866	4.518263
O	2.463331	0.070915	0.823879	H	3.909916	0.525265	3.201356
C	3.817823	0.022882	3.200489	H	3.569493	-1.159152	2.842039
C	-0.509358	1.323141	5.499818	H	1.465082	-1.487012	-4.488530
C	-0.773335	0.591940	-1.824825	H	2.811935	-6.047650	-1.018892
C	0.205061	0.779022	-3.007637	H	2.660044	-3.676924	-4.602378
C	-0.531601	0.740671	-4.342131	H	2.313852	-5.119460	1.120343
C	-1.584574	1.860090	-4.363351	H	0.939820	-3.980949	1.041512
C	-2.553604	1.741968	-3.178502	H	2.568416	-3.349732	1.257717
C	-1.822915	1.705529	-1.825004	H	-2.523528	0.757981	4.611357
N	1.226470	-0.230896	-2.750209	H	-1.581866	-0.426105	5.542218
C	1.364290	-1.299205	-3.477618	H	2.616464	-7.064964	-3.576852
C	1.984935	-2.493047	-2.988916	H	3.344002	-5.967713	-4.771575
C	2.004992	-2.725263	-1.575819	H	-1.250362	1.303717	5.724800
C	2.555335	-3.952577	-1.100324	H	4.284887	-6.507946	-3.365437
C	3.058772	-4.863020	-2.019516	C	4.000798	2.242029	-0.632470
C	3.044040	-4.647171	-3.418142	C	2.723309	2.863013	-0.239826
C	2.487411	-3.465476	-3.881317	C	2.294272	4.221393	-0.709056
O	1.491189	-1.889214	-0.691024	H	4.417691	1.458829	0.000886
C	3.645107	-5.665056	-4.354655	H	4.680066	2.763328	-1.307895
C	2.610479	-4.182033	0.382672	H	2.268948	2.481021	0.675399
O	3.716375	-0.532710	-1.302530	H	1.201750	4.266129	-0.817984
H	-1.268249	-0.385730	-1.977921	H	2.586866	4.978789	0.033123
H	0.679025	1.766261	-2.890102	H	2.760407	4.473605	-1.670105
H	-1.028515	-0.235437	-4.469890	C	4.645612	-0.550697	-2.035294
H	0.180943	0.859261	-5.171592	O	5.791116	-1.321664	-1.867915
H	-1.074963	2.837513	-4.325694	C	6.750817	-1.161334	-2.929206
H	-2.141141	1.832848	-5.311104	O	4.511544	0.209719	-3.001299
H	-3.148994	0.820055	-3.289149	H	7.070789	-0.114193	-3.021568
H	-3.267520	2.578322	-3.187876	H	7.599854	-1.797122	-2.653771
H	-1.318414	2.666569	-1.632008	H	6.329493	-1.484603	-3.891356

C	1.068806	1.505239	4.119165	H	-2.555931	1.555810	-1.019940
C	-0.327172	0.150538	0.944525	H	-1.452733	1.046995	0.649119
N	-0.126338	-0.159906	-0.300922	H	2.127326	0.671564	5.236140
Co	1.557291	-0.182267	-1.110228	H	-1.445155	1.241874	2.918509
O	1.310006	1.531990	-2.021313	H	4.177987	0.017724	4.237096
O	2.492786	0.676243	0.284130	H	4.418626	0.739599	2.620052
C	4.256707	1.894315	1.991236	H	4.005086	-0.960904	2.746582
C	0.620491	1.809856	5.526966	H	0.950023	-1.305705	-4.492202
C	-1.233086	-0.570076	-1.189468	H	3.508435	-5.784878	-1.638165
C	-0.689027	-0.462812	-2.632725	H	2.459536	-3.256665	-4.954058
C	-1.680765	-1.047598	-3.629457	H	3.188813	-5.083663	0.620712
C	-2.999364	-0.260887	-3.524471	H	1.601234	-4.289017	0.808016
C	-3.553308	-0.268931	-2.091012	H	3.064679	-3.311268	0.876745
C	-2.527277	0.235324	-1.061271	H	-1.558668	1.570911	5.292047
N	0.642346	-1.058459	-2.523464	H	-0.497436	0.472417	6.198694
C	0.951592	-2.231092	-2.995693	H	3.192320	-6.658301	-4.216188
C	2.033298	-3.018325	-2.485563	H	3.503994	-5.372423	-5.403717
C	2.490981	-2.796395	-1.143012	H	-0.058417	2.179245	6.025097
C	3.488113	-3.680100	-0.620362	H	4.726600	-5.775309	-4.179790
C	3.986649	-4.692729	-1.426761	C	3.244451	2.541521	-1.975415
C	3.541938	-4.923326	-2.752611	C	3.528734	2.385421	-0.538890
C	2.555032	-4.089578	-3.249950	C	3.436085	3.502983	0.454539
O	2.023249	-1.862686	-0.342981	H	3.653998	1.820604	-2.691218
C	4.137320	-6.035905	-3.578752	H	2.931653	3.521540	-2.346318
C	3.972148	-3.449497	0.782982	H	4.134047	1.520109	-0.263798
O	3.360459	-0.302654	-2.003888	H	3.057195	3.121009	1.412766
H	-1.436786	-1.641334	-0.998724	H	4.435746	3.927727	0.627394
H	-0.529223	0.605850	-2.839545	H	2.770228	4.301012	0.100258
H	-1.865589	-2.112848	-3.408724	C	4.287827	-0.642090	-2.465058
H	-1.276184	-0.986620	-4.651059	O	5.244255	-1.641818	-2.413533
H	-2.821594	0.779702	-3.841714	C	5.944175	-1.845695	-3.655687
H	-3.742235	-0.681187	-4.217808	O	4.102628	0.013857	-3.503531
H	-3.851926	-1.297612	-1.825738	H	6.417208	-0.917504	-4.002811
H	-4.463947	0.344874	-2.035601	H	6.702291	-2.607361	-3.442553
H	-2.290466	1.298517	-1.223352	H	5.253025	-2.205850	-4.430539
H	-2.947441	0.143949	-0.049488	75			
H	-1.351848	0.072836	1.327554	1b-cis-B2-RPO ksi=307			
H	3.071284	2.276896	4.417303	C	0.223618	0.934062	3.186847
H	-0.811147	0.708128	3.459865	C	0.648524	0.635273	1.865121
H	4.230553	2.574739	1.127030	C	1.996147	0.917999	1.470429
H	4.802059	0.996935	1.663352	C	2.861878	1.542848	2.426321
H	4.815002	2.372773	2.805782	C	2.389657	1.806943	3.701899

C	0.815852	1.901713	5.357952	H	0.322727	-2.663852	-3.784282
C	-1.299544	-0.640661	-1.219946	H	4.767572	-5.340364	-1.016538
C	-0.799579	-0.633149	-2.682910	H	2.171284	-4.243644	-4.262454
C	-1.825700	-1.277131	-3.605109	H	4.280657	-2.402521	0.914545
C	-3.131667	-0.466959	-3.514118	H	4.812134	-4.112962	1.025197
C	-3.638868	-0.358801	-2.067083	H	3.165485	-3.621062	1.511395
C	-2.572972	0.198947	-1.107543	H	0.752696	2.875127	5.770698
N	0.532085	-1.223038	-2.573597	H	-0.439866	1.561411	5.667516
C	0.843142	-2.413380	-2.987909	H	3.639746	-6.114219	-4.554530
C	1.946822	-3.166793	-2.465258	H	5.210313	-5.868934	-3.762239
C	2.449132	-2.866326	-1.156087	H	1.199802	1.234929	6.266162
C	3.433932	-3.740455	-0.596986	H	4.043730	-7.008555	-3.072400
C	3.892754	-4.814445	-1.347954	C	4.188754	0.906608	-2.182128
C	3.415512	-5.114565	-2.646429	C	3.587275	0.252031	-3.356565
C	2.431775	-4.292188	-3.171598	C	4.340611	-0.663728	-4.273600
O	2.035761	-1.860610	-0.410983	H	3.732007	1.823536	-1.804359
C	3.966393	-6.290183	-3.414542	H	5.234435	0.712468	-1.936821
C	3.935528	-3.456398	0.791473	H	2.685327	0.737431	-3.735793
O	3.160700	-0.355262	-2.384547	H	5.202679	-1.110371	-3.762299
H	-1.517924	-1.693131	-0.955469	H	3.690614	-1.474810	-4.628140
H	-0.641562	0.418132	-2.966687	H	4.697858	-0.099732	-5.147435
H	-2.012091	-2.322287	-3.304251	C	1.354337	2.642260	-1.322648
H	-1.453579	-1.291880	-4.640464	O	0.260591	2.767487	-0.481668
H	-2.951576	0.544113	-3.914336	C	0.343460	3.883756	0.430697
H	-3.902665	-0.926149	-4.149509	O	2.215240	3.519090	-1.405381
H	-3.946410	-1.359076	-1.717035	H	1.216475	3.773331	1.087913
H	-4.536622	0.274996	-2.030054	H	0.415890	4.832527	-0.115075
H	-2.321023	1.242544	-1.352453	H	-0.575983	3.845866	1.024608
H	-2.961259	0.189210	-0.078907	75			
H	-1.320798	0.072558	1.280067	1b-cis-B2-RPO ksi=31			
H	3.212733	2.371752	4.132958	C	0.328767	0.979879	3.052486
H	-0.690733	0.749527	3.374346	C	0.698131	0.661312	1.719565
H	4.231034	2.591737	0.773349	C	2.022715	0.951392	1.260377
H	4.857268	1.057519	1.377609	C	2.922030	1.599970	2.165863
H	4.866045	2.489161	2.441640	C	2.504554	1.882482	3.457481
H	0.195750	-2.897501	-3.730177	C	1.207663	1.576390	3.937735
H	4.661071	-5.458508	-0.909317	C	-0.312881	0.145005	0.853323
H	2.019295	-4.501840	-4.162320	N	-0.159229	-0.200284	-0.388190
H	4.277715	-2.415487	0.882690	Co	1.488876	-0.248520	-1.264050
H	4.757514	-4.132287	1.059538	O	1.188933	1.415317	-2.249629
H	3.129090	-3.571544	1.531201	O	2.466323	0.693431	0.053489
H	0.964138	2.968877	5.582801	C	4.295187	1.957658	1.669876

O	2.558032	-1.515923	-0.488194	H	-0.240006	1.662553	5.541630
C	4.804127	-2.701234	0.586358	H	3.436183	-6.424232	-4.366697
C	5.715250	-4.682391	-3.994250	H	5.035098	-6.154942	-3.643355
C	-0.157729	-0.262652	0.938550	H	1.418666	1.331819	6.082142
C	0.728132	0.230745	1.941139	H	3.874682	-7.224976	-2.841081
C	0.299574	0.156539	3.294326	C	4.484495	-0.417644	-1.746632
C	1.080001	0.611894	4.338576	C	4.068346	0.821499	-2.428105
C	2.339553	1.176431	4.011944	C	4.518627	1.201716	-3.804230
C	2.807738	1.289180	2.713598	H	4.428607	-0.452520	-0.658487
C	2.003953	0.808713	1.625703	H	5.147192	-1.128722	-2.243644
O	2.487926	0.951766	0.419387	H	3.702596	1.632138	-1.795643
C	4.151237	1.880149	2.391471	H	4.790563	0.318896	-4.397340
C	0.634263	0.513981	5.776086	H	3.717899	1.754547	-4.311772
O	0.891397	1.881018	-1.524378	H	5.393487	1.864552	-3.731014
C	1.772058	3.060035	-1.458957	C	1.227207	2.556724	-1.607719
C	1.148368	2.711950	-2.746001	O	0.178162	2.684565	-0.704463
O	5.051708	0.493180	-3.560660	C	0.274271	3.844050	0.149613
C	5.960278	0.176657	-2.481698	O	2.043435	3.463043	-1.781427
H	-0.844980	-2.011830	-1.182229	H	1.183241	3.790250	0.764607
H	-0.463158	0.502506	-2.850960	H	0.290431	4.768566	-0.440893
H	-1.103201	-2.394584	-3.621413	H	-0.611662	3.809444	0.793369
H	-0.772753	-1.077895	-4.767472	75			
H	-2.699209	0.223416	-3.894599	1b-cis-B1-SPO ksi=145			
H	-3.252222	-1.378600	-4.387504	C	3.690646	-3.225880	-3.559406
H	-3.249727	-2.164624	-2.041322	C	2.903432	-2.408342	-2.719316
H	-4.219723	-0.695200	-2.165622	C	3.265846	-2.224855	-1.346656
H	-2.335826	0.671006	-1.241852	C	4.423794	-2.898262	-0.853954
H	-2.724765	-0.670563	-0.152113	C	5.169885	-3.678941	-1.728024
H	-1.143295	-0.597557	1.287924	C	4.835082	-3.854316	-3.091400
H	2.978484	1.535607	4.824677	C	1.663314	-1.855439	-3.182747
H	-0.678681	-0.286800	3.501226	N	1.075142	-0.856576	-2.598999
H	4.048678	2.780094	1.766412	C	-0.352113	-0.581873	-2.702302
H	4.754298	1.171294	1.805339	C	-0.877972	-0.910708	-1.286493
H	4.694119	2.147182	3.306974	C	-2.322033	-0.426763	-1.145269
H	1.168393	-2.335557	-4.034931	C	-3.191932	-1.080033	-2.233908
H	6.071211	-4.165680	-1.342984	C	-2.634882	-0.849558	-3.647471
H	3.396588	-3.337211	-4.605892	C	-1.169493	-1.303452	-3.766863
H	5.781451	-3.151377	0.801549	N	0.100890	-0.346322	-0.333667
H	4.056331	-3.146790	1.259428	Co	1.774425	0.076957	-1.108733
H	4.831417	-1.628776	0.828031	O	3.474787	0.538788	-1.950147
H	0.579121	1.506321	6.250050	C	3.712349	0.597982	-3.233060
H	-0.357785	0.049496	5.852888	O	2.924129	0.763076	-4.174097

C	2.012506	1.539316	3.850014	H	5.269939	-4.791167	-4.991681
C	2.678450	1.345048	2.654090	H	6.705733	-4.217917	-4.119957
C	1.969939	0.805294	1.523499	H	1.335503	-0.090311	6.372252
O	2.644717	0.662723	0.419485	H	5.879247	-5.689767	-3.583119
C	4.133884	1.671517	2.479628	H	1.764239	2.158502	-3.465703
C	-0.020975	1.462207	5.374072	C	-0.065096	3.431489	-3.255653
O	1.522732	1.918116	-1.529572	H	2.815210	2.801280	-1.281653
C	1.067298	2.718661	-2.660334	H	5.700065	-0.785394	-2.022850
C	0.258343	2.659301	-1.425614	H	6.950544	0.117980	-2.947967
O	5.118916	0.624546	-3.649158	H	5.948651	0.958519	-1.711034
C	6.094805	0.028765	-2.764685	H	1.345215	3.858204	-0.847852
H	-0.591602	-2.100818	-1.406374	H	-0.660818	3.849308	-2.433170
H	-0.244111	0.421648	-3.075795	H	0.252948	4.254959	-3.912344
H	-0.757278	-2.484462	-3.899976	H	-0.698928	2.761245	-3.853382
H	-0.440861	-1.134110	-5.009178	75			
H	-2.477997	0.050189	-4.189888	1b-cis-B1-SPO ksi=266			
H	-2.910681	-1.564513	-4.756512	C	3.957091	-3.282308	-3.644653
H	-2.938059	-2.428896	-2.431193	C	3.106549	-2.508576	-2.827667
H	-4.018003	-1.038855	-2.561822	C	3.349977	-2.410951	-1.420534
H	-2.305481	0.447703	-1.533417	C	4.461877	-3.112072	-0.870194
H	-2.621244	-0.947000	-0.489729	C	5.278617	-3.846004	-1.722442
H	-1.261136	-0.293993	0.925745	C	5.057636	-3.943826	-3.116024
H	2.576211	1.948074	4.694252	C	1.910897	-1.909676	-3.346872
H	-1.104452	0.450151	3.062976	N	1.297771	-0.930380	-2.750720
H	4.277644	2.396714	1.665443	C	-0.125660	-0.662589	-2.920590
H	4.700674	0.775229	2.187358	C	-0.707443	-1.007477	-1.528707
H	4.559352	2.078732	3.405676	C	-2.192550	-0.647064	-1.456234
H	1.465083	-2.341955	-4.249772	C	-2.960579	-1.338454	-2.595293
H	6.145688	-4.356794	-1.292641	C	-2.360552	-1.024849	-3.972465
H	3.753583	-3.332580	-4.717213	C	-0.870666	-1.395609	-4.031345
H	5.693501	-3.432967	0.869821	N	0.185146	-0.361210	-0.545509
H	3.939749	-3.491978	1.191603	Co	1.948355	-0.071747	-1.189138
H	4.705217	-1.933904	0.903256	O	3.686824	0.254014	-1.953724
H	0.074399	2.511193	5.693819	C	3.813334	0.667654	-3.186721
H	-1.090936	1.217453	5.336196	O	2.952860	1.081375	-3.971244
H	5.635187	-4.808663	-5.013245	O	2.560023	-1.750490	-0.593995
H	6.997393	-4.229879	-4.033175	C	4.724547	-2.991671	0.604259
H	0.437640	0.842217	6.160090	C	6.012926	-4.721506	-3.986264
H	6.176332	-5.736918	-3.595949	C	-0.216023	-0.084469	0.665199
H	-0.612809	1.998239	-1.446318	C	0.579708	0.479813	1.701475
C	0.245773	3.726369	-0.371222	C	-0.046528	0.709261	2.960325
H	0.790001	2.144138	-3.542624	C	0.638116	1.231187	4.037558

C	0.455608	2.912431	-0.996886	H	5.841088	-1.018157	-2.550240
C	1.667376	3.110280	-1.811246	H	7.046110	0.084177	-3.306255
O	4.958417	0.795150	-3.550306	H	6.161982	0.581775	-1.818937
C	5.896952	0.273513	-2.581773	H	1.714295	3.576826	-2.849883
H	-0.878098	-2.008364	-1.530520	H	1.165022	4.323564	-0.411775
H	-0.269933	0.451603	-3.229512	H	-0.618263	4.391301	-0.516237
H	-0.807473	-2.485631	-3.946566	H	0.166497	3.269213	0.625212
H	-0.350674	-1.210234	-5.098333	75			
H	-2.372403	0.099472	-4.530063	1b-cis-B1-SPO ksi=72			
H	-2.855211	-1.530435	-5.007058	C	3.974942	-3.219175	-3.285614
H	-3.149593	-2.200384	-2.646342	C	3.083565	-2.383967	-2.577707
H	-4.091970	-0.741666	-2.962073	C	3.282743	-2.137431	-1.182489
H	-2.333954	0.670909	-1.873816	C	4.389270	-2.760596	-0.532531
H	-2.852345	-0.620319	-0.775327	C	5.245016	-3.559790	-1.280394
H	-1.391839	-0.728134	0.883298	C	5.069410	-3.802488	-2.663046
H	2.436340	1.189861	4.859515	C	1.892201	-1.881183	-3.201592
H	-1.062194	-0.622396	3.149022	N	1.217958	-0.879431	-2.729267
H	3.597432	2.819366	2.058346	C	-0.186930	-0.625380	-3.020879
H	4.365417	1.248369	1.884483	C	-0.886010	-0.910870	-1.671197
H	4.216964	1.988035	3.511543	C	-2.334005	-0.421019	-1.724477
H	1.508958	-2.405392	-4.084987	C	-3.064864	-1.126112	-2.881873
H	6.103333	-4.011275	-0.773362	C	-2.335245	-0.959267	-4.224645
H	3.800466	-3.386959	-4.351414	C	-0.862901	-1.401767	-4.144300
H	5.538665	-2.934819	1.283379	N	-0.029786	-0.331408	-0.613025
H	3.770625	-2.925484	1.529643	Co	1.709800	0.128140	-1.201255
H	4.588131	-1.420491	1.133515	O	3.453853	0.580990	-1.885819
H	0.011331	0.900280	6.156032	C	3.630921	0.854923	-3.154907
H	-0.894940	-0.497753	5.535702	O	2.798747	1.169343	-4.009515
H	5.727574	-4.815839	-4.456547	O	2.463188	-1.417409	-0.440709
H	7.049338	-4.182878	-3.454589	C	4.592840	-2.501740	0.933727
H	0.772139	-0.698279	6.113646	C	6.055338	-4.655807	-3.421170
H	6.181219	-5.641637	-2.948618	C	-0.395118	-0.338076	0.635528
H	2.615306	2.919693	-1.303342	C	0.403756	0.105190	1.734432
C	1.698222	3.954611	-3.047556	C	-0.095996	-0.120333	3.044807
H	0.559299	2.645422	0.053674	C	0.608543	0.251726	4.173908
H	5.634173	-0.754083	-2.296295	C	1.856729	0.894589	3.979573
H	6.869894	0.288053	-3.086869	C	2.388019	1.160963	2.727120
H	5.928054	0.898584	-1.679832	C	1.669985	0.759778	1.553859
H	-0.481549	3.377240	-1.310805	O	2.204870	1.051067	0.391329
H	0.688435	4.103279	-3.452373	C	3.716320	1.839785	2.546277
H	2.130494	4.937202	-2.806969	C	0.095629	-0.024508	5.565208
H	2.320698	3.461620	-3.805028	O	0.886904	1.855072	-1.930762

H	-1.039699	0.426296	-4.862252
H	-2.111545	2.393944	-3.795145
H	-3.358998	1.332110	-4.457275
H	-3.821963	0.384846	-2.221273
H	-3.948229	2.143918	-2.148702
H	-1.668625	2.301805	-1.112248
H	-2.705530	1.203210	-0.185011
H	-1.315428	0.422604	1.207272
H	3.260460	0.563683	4.819097
H	-0.805472	0.436536	3.438833
H	4.788747	-0.586777	1.904704
H	5.095599	0.466344	3.315356
H	4.753840	1.164901	1.703994
H	-0.009334	-1.738077	-4.274927
H	3.293928	-5.984975	-1.907297
H	1.379885	-3.664480	-4.978453
H	3.513977	-5.177927	0.320846
H	2.035125	-4.323490	0.844325
H	3.486582	-3.393663	0.507006
H	1.028007	-0.223880	6.345191
H	1.079461	1.541097	6.206770
H	3.787919	-6.192986	-4.656253
H	2.264282	-7.005346	-4.265319
H	-0.407718	0.661804	5.789864
H	2.314867	-5.795777	-5.566019
H	4.279548	1.162764	-1.253294
C	5.805711	-0.449337	-1.451772
H	3.243569	0.954031	-3.455525
H	1.775684	4.666943	0.805040
H	0.467283	3.797155	1.693761
H	2.162505	3.212388	1.777156
H	4.342057	-0.496538	-3.908606
H	6.665267	0.217216	-1.614893
H	5.784960	-0.721734	-0.388608
H	5.940689	-1.358459	-2.051833
75			
1b-cis-B2-SPO ksi=318			
C	1.776377	-3.367980	-4.215973
C	1.500686	-2.418654	-3.203988
C	1.918035	-2.664063	-1.854538
C	2.586178	-3.897596	-1.571487
C	2.850216	-4.781137	-2.609125

75			
1b-cis-B2-SPO ksi=242			
C	1.703144	-3.800011	-3.942476
C	1.432126	-2.769124	-3.010842
C	1.819009	-2.915692	-1.636239
C	2.492692	-4.118561	-1.254328
C	2.757014	-5.082884	-2.216268
C	2.375782	-4.953266	-3.574741
C	0.643716	-1.637936	-3.398446
N	0.613971	-0.526047	-2.723635
C	-0.497969	0.422721	-2.763910
C	-1.165800	0.231942	-1.383409
C	-2.197667	1.336790	-1.150851
C	-3.236026	1.317510	-2.286372
C	-2.588160	1.407033	-3.676662
C	-1.526279	0.311753	-3.881940
N	-0.066671	0.153619	-0.398004
Co	1.610584	-0.187379	-1.145318
O	3.374029	-0.633421	-2.012705
C	3.905168	0.146345	-3.141852
C	4.543093	0.266876	-1.820824
O	1.556864	-2.037101	-0.691952
C	2.911049	-4.271701	0.180501
C	2.700937	-6.041331	-4.567894
C	-0.280220	0.273414	0.877220
C	0.710053	0.273060	1.904883
C	0.271213	0.405501	3.248624
C	1.156324	0.499960	4.305884
C	2.540114	0.478643	3.999719
C	3.029526	0.357740	2.709047
C	2.112469	0.232669	1.615576
O	2.624993	0.116744	0.416653
C	4.500144	0.352159	2.400864
C	0.688446	0.626893	5.734175
O	1.889881	1.665396	-1.714137
C	2.177375	2.569833	-0.807246
O	3.248443	3.166260	-0.689280
O	1.094541	2.840661	0.013919
C	1.406055	3.689610	1.139667
H	-1.669053	-0.753996	-1.399875
H	-0.042847	1.424584	-2.766691
H	-2.008457	-0.680774	-3.865284

H	-1.290423	0.196939	1.295844	C	2.467076	-4.539474	-3.950569
H	3.343908	0.235527	4.832166	C	0.663312	-1.287899	-3.489029
H	-0.728914	-0.063631	3.502429	N	0.593199	-0.239396	-2.726558
H	4.918413	-0.417736	1.817878	C	-0.554641	0.662874	-2.671320
H	5.134534	0.540634	3.306558	C	-1.184942	0.330062	-1.300333
H	4.691386	1.330012	1.762797	C	-2.242231	1.378217	-0.950846
H	0.000102	-1.348013	-4.361431	C	-3.307309	1.415345	-2.061390
H	3.384470	-5.706814	-2.374071	C	-2.698861	1.636037	-3.455343
H	1.437352	-3.156144	-5.233811	C	-1.603228	0.602349	-3.774100
H	3.564231	-5.110876	-0.081539	N	-0.062145	0.197240	-0.346900
H	2.127678	-4.227567	0.510232	Co	1.612470	0.027389	-1.154058
H	3.621562	-3.349640	0.237613	O	3.309745	-0.144775	-2.232542
H	1.175146	-0.985934	6.248806	C	4.435913	0.762450	-1.943841
H	1.174005	0.780167	6.384008	C	4.551977	-0.668461	-1.612542
H	3.892691	-5.634071	-5.162183	O	1.699717	-1.848987	-0.844046
H	2.409330	-6.532459	-4.804455	C	3.002931	-4.170832	-0.153521
H	-0.295857	-0.070593	5.859466	C	2.803667	-5.531467	-5.036073
H	2.384042	-5.218633	-6.001273	C	-0.255346	0.151270	0.935309
H	4.377269	-0.925417	-0.565477	C	0.757575	0.089530	1.940097
C	5.302227	-1.650490	-2.461726	C	0.342048	0.015757	3.295197
H	4.225735	1.498912	-1.167755	C	1.241956	0.046052	4.344101
H	1.469468	4.658651	1.265585	C	2.613817	0.184692	4.018662
H	0.295314	3.579150	2.109206	C	3.079794	0.267696	2.715650
H	2.043505	3.170282	2.079031	C	2.151667	0.191096	1.628628
H	4.895735	1.136769	-2.860597	O	2.643239	0.252940	0.414233
H	6.311472	-1.795739	-2.049006	C	4.537119	0.440744	2.391677
H	4.790932	-2.622399	-2.470340	C	0.799628	-0.061623	5.782025
H	5.393746	-1.288913	-3.493881	O	1.782950	1.933720	-1.538761
75				C	2.017699	2.763541	-0.550999
1b-trans-SPO ksi=142				O	3.032340	3.444466	-0.398156
C	4.019906	1.259191	-0.053864	O	0.942805	2.852765	0.324792
C	3.709690	0.808535	1.269364	C	1.215329	3.620703	1.515451
C	4.587595	1.113363	2.342923	H	-1.660689	-0.665155	-1.394083
C	5.743951	1.849982	2.162891	H	-0.137593	1.678499	-2.599639
C	6.038322	2.285825	0.847214	H	-2.046916	-0.406644	-3.830157
C	5.226635	2.011792	-0.242033	H	-1.144268	0.816945	-4.750616
C	2.533563	0.048701	1.565124	H	-2.260365	2.646129	-3.506804
N	1.589026	-0.252928	0.726270	H	-3.487352	1.594080	-4.220754
C	0.417131	-1.061907	1.094933	H	-3.862351	0.461648	-2.057081
C	-0.770519	-0.463537	0.315789	H	-4.041285	2.204383	-1.842590
C	-2.011154	-1.340909	0.461355	H	-1.741698	2.353054	-0.844356
C	-2.357284	-1.502842	1.949658	H	-2.720285	1.149140	0.012289

H	6.950012	2.867583	0.678577	C	-1.171010	-2.050830	2.752758
H	6.504965	3.039267	-1.641474	C	0.087210	-1.183707	2.579433
H	4.764682	3.115942	-2.040009	N	-0.282680	-0.225570	-1.051207
H	5.645869	1.623445	-2.319577	Co	1.513470	0.346956	-1.066386
H	2.430247	-0.292863	2.601761	O	2.172122	-1.245904	-1.856092
H	-2.580174	-1.838141	-6.598968	C	1.612732	-2.431056	-1.882606
H	-2.047472	-0.541781	-7.692627	O	0.746738	-2.928773	-1.158423
H	7.680883	1.793012	3.136106	C	6.667306	2.186618	3.307308
H	6.761758	3.275408	3.441737	C	5.562396	2.477418	-1.631501
H	-0.260539	2.535627	-2.024410	O	3.282085	1.042019	-1.115222
C	-1.069824	3.659601	-0.278817	C	-0.966462	-0.516367	-2.115970
H	2.113813	3.132302	-1.772237	C	-0.522714	-0.293150	-3.460770
H	-1.084274	-2.020355	-7.537471	C	0.639857	0.491670	-3.748134
H	6.298107	1.763586	4.251042	C	1.002925	0.686481	-5.116629
H	2.520601	-1.753542	-4.334002	C	0.231945	0.103774	-6.113520
H	3.930084	-2.242341	-3.344750	C	-0.917982	-0.676706	-5.846498
H	3.256228	-3.380060	-4.566692	C	-1.278281	-0.851526	-4.520555
H	1.753061	4.105994	-0.218284	O	1.374876	1.078026	-2.828781
H	-1.882379	2.948341	-0.076909	C	-1.699865	-1.301106	-6.975410
H	-0.684711	4.041581	0.675193	C	2.226920	1.505784	-5.417279
H	-1.494172	4.499016	-0.848825	O	0.925548	2.135132	-0.292205
75				C	1.440301	3.353865	-0.944585
1b-trans-SPO ksi=262				C	0.016511	3.009457	-1.081174
C	3.925181	1.194866	-0.079473	O	2.123447	-3.229244	-2.889192
C	3.461588	0.950351	1.256396	C	3.016462	-2.598249	-3.837263
C	4.122195	1.549442	2.361768	H	-2.155748	-1.453638	-4.270358
C	5.193640	2.407941	2.196367	H	0.538202	0.248111	-7.154144
C	5.635461	2.649761	0.870162	H	2.485903	1.451445	-6.482281
C	5.050340	2.072025	-0.244655	H	2.071773	2.563006	-5.151121
C	2.323375	0.125134	1.515862	H	3.077820	1.160421	-4.813236
N	1.487237	-0.297428	0.612494	H	-1.949964	-0.982469	-1.993930
C	0.326068	-1.139830	0.917196	H	-0.976105	0.533447	0.749719
C	-0.834355	-0.564357	0.082025	H	-1.802470	-2.321537	0.005217
C	-2.050953	-1.486681	0.150764	H	-2.865859	-0.896776	-0.070768
C	-2.461203	-1.697629	1.617036	H	-3.227038	-2.167365	2.055912
C	-1.298443	-2.218398	2.471071	H	-2.656560	-0.523951	2.362184
C	-0.070439	-1.297770	2.380335	H	-0.946629	-3.075214	2.414082
N	-0.280128	-0.285453	-1.257532	H	-1.432369	-2.118515	3.818865
Co	1.559084	0.162880	-1.222833	H	0.923989	-1.645222	3.123523
O	2.142871	-1.534597	-1.839040	H	-0.075430	-0.181714	3.014005
C	1.500462	-2.673124	-1.915914	H	0.589384	-2.057115	0.651338
O	0.498890	-3.075594	-1.316258	H	4.325641	0.750923	3.341131

H	6.943056	2.814222	3.412502	C	5.874996	3.076169	3.365059
H	5.815924	4.173421	3.291430	C	5.525275	2.347372	-1.642527
H	0.338329	2.066720	1.074775	O	3.402438	0.674389	-1.157625
C	1.508488	3.938750	0.881943	C	-0.958583	-0.500077	-2.349289
H	-0.862469	2.180150	-1.122020	C	-0.490187	-0.271292	-3.677648
H	-1.355671	-1.603436	-7.868723	C	0.779633	0.340083	-3.944383
H	5.413883	2.778652	4.316172	C	1.155563	0.546452	-5.312973
H	2.841060	-2.157927	-4.196902	C	0.291865	0.152645	-6.321640
H	4.027369	-2.727209	-2.987200	C	-0.967458	-0.451624	-6.075130
H	3.459465	-3.847982	-4.277705	C	-1.332662	-0.649248	-4.756902
H	0.038664	3.741161	-1.563189	O	1.612876	0.755852	-3.026936
H	2.399133	3.556899	1.399412	C	-1.854322	-0.864393	-7.222849
H	1.828578	4.603367	0.069956	C	2.489668	1.179986	-5.589907
H	0.909452	4.516891	1.600711	O	1.272044	2.151518	-0.849943
75				C	-0.014310	2.842740	-0.946062
1b-trans-SPO-in ksi=207				C	0.696674	2.797835	0.346623
C	4.056072	1.030384	-0.294581	O	2.093311	-3.547485	-2.806407
C	3.860800	0.568536	1.048574	C	3.176426	-3.024641	-3.612612
C	4.909844	0.697285	1.996767	H	-2.291627	-1.119717	-4.522998
C	6.132765	1.254282	1.671589	H	0.603603	0.309081	-7.358953
C	6.319128	1.679379	0.332422	H	2.703291	1.195445	-6.666236
C	5.337871	1.575850	-0.640302	H	2.523123	2.211712	-5.207826
C	2.649898	-0.062461	1.475721	H	3.290220	0.639157	-5.064921
N	1.585412	-0.250613	0.751208	H	-1.973763	-0.900259	-2.256169
C	0.409954	-0.997169	1.240088	H	-1.108358	0.412870	0.528656
C	-0.825936	-0.330841	0.602890	H	-1.781820	-2.442906	-0.322723
C	-2.078926	-1.161745	0.864807	H	-2.897849	-1.057927	-0.405062
C	-2.272082	-1.335588	2.380140	H	-3.308223	-2.397346	1.663445
C	-1.031315	-1.941245	3.048306	H	-2.820930	-0.741724	2.036687
C	0.237525	-1.124766	2.750800	H	-1.013782	-3.224087	2.122629
N	-0.477034	-0.078022	-0.808967	H	-1.612253	-2.320708	3.520056
Co	1.346667	0.400763	-1.015672	H	0.759589	-1.730713	2.957695
O	1.812267	-1.185349	-1.969043	H	-0.300988	-0.312703	2.825217
C	1.219152	-2.357318	-1.915519	H	0.535626	-2.127283	0.471830
O	0.454580	-2.832018	-1.075003	H	3.748223	1.334452	3.367102
C	7.242835	1.398907	2.682677	H	6.476029	3.333496	0.715466
C	5.569400	2.002107	-2.063620	H	6.322145	3.102075	-1.648397
O	3.149969	1.000452	-1.238381	H	4.689690	2.688715	-2.270741
C	-1.287814	-0.308217	-1.798126	H	5.901842	1.428591	-2.116463
C	-0.978864	-0.073305	-3.181110	H	2.134465	-0.138774	2.563429
C	0.164380	0.695085	-3.577208	H	-2.788651	-1.312881	-6.860162
C	0.404238	0.883933	-4.972985	H	-2.116960	-0.004330	-7.858112

H	1.780133	-1.685711	-4.478266	C	-0.463422	0.311474	-5.894285
H	3.303726	-2.208611	-3.696004	C	-1.596258	-0.448597	-5.520038
H	2.440027	-3.327618	-4.810763	C	-1.838239	-0.616256	-4.165112
H	-0.294750	2.919339	-1.696968	O	0.991418	1.261255	-2.724176
H	3.267079	3.769690	-0.786525	C	-2.487476	-1.063415	-6.570175
H	2.192090	3.231821	-2.105016	C	1.612770	1.676513	-5.386112
H	2.249787	4.963133	-1.631178	O	0.769928	2.348807	0.071318
75				C	-0.146546	3.229056	-0.660434
1b-trans-SPO-in ksi=131				C	1.183775	3.729984	-0.273453
C	3.887098	1.129726	-0.261821	O	1.556718	-3.155650	-2.990836
C	3.642617	0.501419	1.004550	C	2.322459	-2.542086	-4.056189
C	4.687865	0.416170	1.961172	H	-2.697934	-1.206172	-3.836639
C	5.950040	0.927532	1.720132	H	-0.249431	0.445066	-6.959118
C	6.172622	1.550697	0.467097	H	1.789726	1.592576	-6.465900
C	5.193890	1.665325	-0.507636	H	1.492386	2.742233	-5.136831
C	2.361920	-0.020472	1.371925	H	2.501073	1.331724	-4.838577
N	1.292594	-0.030701	0.629519	H	-2.272360	-0.734807	-1.579006
C	0.055822	-0.710376	1.083785	H	-0.939074	0.664594	1.070240
C	-1.079467	-0.215125	0.176778	H	-1.960894	-2.141902	0.376031
C	-2.335854	-1.054790	0.396738	H	-2.966424	-0.674264	0.434052
C	-2.752252	-0.962126	1.875222	H	-3.151669	-1.967859	2.569883
C	-1.610546	-1.345165	2.826853	H	-2.487180	-0.352383	2.832462
C	-0.332194	-0.534691	2.550617	H	-0.885652	-2.969388	2.679471
N	-0.539179	-0.143019	-1.192355	H	-1.182204	-2.011797	4.135390
Co	1.246956	0.467546	-1.202921	H	1.105896	-1.631449	3.196194
O	2.027001	-1.144656	-1.831531	H	0.168248	-0.123071	3.209656
C	1.583553	-2.366090	-1.621552	H	0.485178	-1.993989	0.774685
O	0.667803	-2.774757	-0.909467	H	4.732534	0.334730	3.013320
C	7.059865	0.833814	2.737211	H	7.286603	2.103505	0.046299
C	5.447146	2.338859	-1.827229	H	6.595911	2.363753	-2.203415
O	2.985575	1.293526	-1.199813	H	4.869988	2.795860	-2.364005
C	-1.222367	-0.459715	-2.250031	H	5.387426	1.163402	-2.751576
C	-0.782469	-0.267455	-3.599854	H	2.636370	-0.420840	2.511673
C	0.375289	0.520423	-3.909940	H	-3.315531	-1.619352	-6.111685
C	0.699659	0.731439	-5.288658	H	-2.919348	-0.296588	-7.231300
C	-0.098686	0.163064	-6.269739	H	8.152087	0.868992	2.359948
C	-1.241941	-0.620797	-5.979562	H	7.518899	2.454776	2.828964
C	-1.564687	-0.813179	-4.646891	H	1.235837	4.334559	0.637559
O	1.140772	1.096505	-3.014035	C	2.291145	3.926131	-1.263801
C	-2.064379	-1.217347	-7.094120	H	-1.032059	3.507938	-0.085385
C	1.905804	1.567683	-5.612917	H	-1.927053	-1.763551	-7.208673
O	0.228673	2.504981	-0.734750	H	6.945530	0.991872	3.658044

75				C	0.894871	3.630234	-1.389306
1b-trans-SPO ksi=66				C	0.647881	3.675018	0.064357
C	3.791596	1.430936	-0.119293	O	2.303627	-3.301756	-2.338842
C	3.654567	0.754146	1.136216	C	3.327229	-2.804273	-3.233405
C	4.719457	0.789594	2.075895	H	-2.442470	-1.408453	-4.381397
C	5.900770	1.462574	1.825046	H	0.173615	0.326321	-7.317077
C	6.017266	2.130963	0.580748	H	2.121246	1.549476	-6.688895
C	5.013846	2.134870	-0.375377	H	1.754393	2.613643	-5.304342
C	2.469944	0.036731	1.497473	H	2.783958	1.210865	-5.056508
N	1.407170	-0.110471	0.762781	H	-2.217872	-0.896266	-2.114001
C	0.286492	-0.974653	1.189898	H	-1.295579	0.832844	0.457397
C	-0.930624	-0.568408	0.343577	H	-2.122048	-2.098194	0.115641
C	-2.070389	-1.565114	0.537747	H	-3.160988	-0.697755	-0.236636
C	-2.448078	-1.616323	2.027875	H	-3.625210	-1.606570	2.054664
C	-1.239762	-1.931501	2.919949	H	-3.074267	0.070857	2.091160
C	-0.072076	-0.960689	2.674470	H	-1.380861	-2.416475	2.706423
N	-0.439502	-0.360023	-1.023562	H	-1.925331	-1.203241	3.871099
Co	1.229309	0.505411	-1.016688	H	0.470166	-0.882909	3.216155
O	2.158868	-0.945402	-1.795601	H	-0.497162	0.534729	2.767964
C	1.892246	-2.225490	-1.688055	H	0.203466	-1.775832	0.847897
O	1.155534	-2.829968	-0.907277	H	4.473429	-0.069929	2.917097
C	7.034029	1.491248	2.820453	H	7.164508	1.960807	0.254379
C	5.158726	2.846077	-1.691811	H	6.504913	2.610091	-1.934757
O	2.865431	1.482861	-1.046013	H	4.840276	3.252274	-1.927247
C	-1.040739	-0.782029	-2.092147	H	5.151174	1.685405	-2.659837
C	-0.599063	-0.516080	-3.430546	H	2.289651	-0.439041	2.383442
C	0.403507	0.470558	-3.700746	H	-2.933067	-1.760278	-6.699410
C	0.769268	0.706379	-5.062631	H	-2.434722	-0.440016	-7.780143
C	0.153882	-0.025699	-6.068575	H	7.905426	0.240890	2.355663
C	-0.841275	-1.000064	-5.818274	H	7.453053	1.829130	2.994476
C	-1.203945	-1.220233	-4.499250	H	-0.234911	4.231469	0.397409
O	0.985908	1.198898	-2.776903	C	1.727074	3.494731	1.089919
C	-1.461767	-1.770762	-6.957010	H	0.248425	4.177523	-2.077687
C	1.832746	1.730677	-5.343627	H	-1.471851	-1.924441	-7.695306
O	0.247970	2.163615	-0.363226	H	6.710035	0.359899	3.663673
C	0.915087	3.189650	0.459510	H	2.894969	-2.127873	-3.981989
C	0.661536	3.454073	-0.967746	H	4.110825	-2.273018	-2.678069
O	2.588588	-2.979660	-2.614961	H	3.740591	-3.695977	-3.717693
C	3.347814	-2.254275	-3.610712	H	1.897626	3.379319	-1.742152
H	-1.965238	-1.968800	-4.263704	H	1.351732	2.934314	1.956958
H	0.463087	0.155191	-7.102705	H	2.591165	2.966411	0.677355
H	2.120844	1.720234	-6.402772	H	2.054504	4.483541	1.444016

C	1.811952	1.412142	-4.913039	H	1.486139	2.744001	-5.086765
C	-0.759219	-0.085244	-2.569381	H	2.718539	1.543841	-4.719101
N	-0.271716	-0.081347	-1.361000	H	-1.944321	-1.391100	-1.977704
Co	1.554550	0.245024	-0.957922	H	-1.262945	0.426776	0.693936
O	1.291940	2.137076	-0.243353	H	-1.742344	-2.556587	0.186756
C	0.414747	2.602916	0.833431	H	-2.948678	-1.271313	-0.055770
C	0.099739	2.938547	-0.570096	H	-3.238772	-2.364303	2.184491
C	0.389627	4.271756	-1.189036	H	-2.874163	-0.642188	2.323083
C	-0.839694	0.445082	-7.508739	H	-0.894484	-2.957944	2.714930
C	3.169220	2.054451	-4.851318	H	-1.533225	-1.901227	3.979637
O	1.898448	1.174600	-2.585142	H	0.786563	-1.265068	3.289269
C	-1.049557	-0.553070	-0.198474	H	-0.348436	0.062883	2.982351
C	-2.289643	-1.399320	-0.485476	H	0.563193	-1.990293	0.863412
C	-2.945198	-1.820712	0.840069	H	4.588294	0.258711	3.023185
C	-1.958875	-2.543488	1.766265	H	6.945287	2.666332	0.357568
C	-0.699485	-1.700455	2.027596	H	6.155306	3.296336	-1.788348
C	-0.062415	-1.328554	0.693068	H	4.402067	3.639085	-1.800723
N	1.168274	-0.530064	0.722872	H	4.992392	2.151216	-2.528760
C	1.883652	-0.356779	1.796858	H	2.477974	-0.428005	2.491294
C	3.120315	0.354348	1.859720	H	-2.243438	-2.451481	-6.595125
C	3.685950	0.601622	3.139282	H	-1.917356	-1.096439	-7.698095
C	4.887336	1.266280	3.293439	H	7.946727	1.037653	2.403677
C	5.557187	1.682311	2.113932	H	7.288802	2.522454	3.110030
C	5.064897	1.456721	0.839093	H	1.511099	3.305673	-1.637136
C	3.807222	0.783138	0.674997	C	-0.472052	4.298048	-1.463231
C	5.477631	1.548961	4.652604	H	1.921242	2.921028	0.779774
C	5.788134	1.905140	-0.398878	H	-0.710088	-2.375590	-7.487631
O	3.384559	0.594512	-0.546780	H	6.772880	0.940278	3.733572
O	2.151988	-1.338999	-1.813857	H	2.692560	-1.591595	-4.192207
H	-1.707459	-0.286158	-5.007071	H	4.141806	-1.656882	-3.144153
H	1.599632	1.567682	-7.029662	H	3.781341	-3.025380	-4.257500
H	3.880421	1.405778	-4.320078	H	0.247094	3.607156	1.215831
H	3.550381	2.267584	-5.857964	H	-0.853679	3.889420	-2.408233
H	3.136002	2.994419	-4.279743	H	-1.291356	4.340076	-0.733399
H	-1.779822	-0.454338	-2.715340	H	-0.114978	5.321127	-1.652116
H	-1.366960	0.348901	0.361932	75			
H	-1.978051	-2.280368	-1.066475	1b-trans-RPO ksi=330			
H	-3.017596	-0.834436	-1.086529	C	1.222498	0.964727	-3.684718
H	-3.811148	-2.465834	0.632272	C	-0.073187	0.351904	-3.742559
H	-3.337051	-0.925287	1.353380	C	-0.725845	0.195650	-4.993867
H	-1.657102	-3.496382	1.302970	C	-0.152153	0.619582	-6.177783
H	-2.445843	-2.792541	2.720347	C	1.125200	1.230814	-6.102740

C	-0.298103	3.601246	1.619092	H	0.007975	-2.275903	2.642300
C	0.260551	-0.714398	-7.760455	H	-0.962992	-0.789900	2.595619
C	3.170017	2.238893	-4.841065	H	0.181295	-2.241086	0.122499
O	1.563650	1.540746	-2.708729	H	3.139642	0.254421	4.021202
C	-1.343220	-0.278136	-0.533443	H	6.510134	2.211739	2.211926
C	-2.583547	-1.124361	-0.808002	H	5.126524	2.513624	-1.032748
C	-3.389737	-1.275368	0.493783	H	6.084176	1.041795	-1.013551
C	-2.538650	-1.835921	1.641691	H	6.685252	2.483656	-0.144046
C	-1.257509	-1.014143	1.866956	H	1.513966	-0.780194	2.738574
C	-0.479894	-0.936441	0.554558	H	-1.812185	-0.050515	-7.389997
N	0.806408	-0.208233	0.577454	H	-1.012724	1.414443	-8.001493
C	1.628412	-0.318170	1.578766	H	6.476530	1.098947	4.760134
C	2.941281	0.246089	1.660020	H	5.590853	2.630588	4.826101
C	3.692020	0.003180	2.841352	H	-0.138425	1.812403	1.340885
C	4.964631	0.511998	3.022366	H	0.901725	3.340675	1.473804
C	5.505333	1.298991	1.975521	H	-0.669727	2.332058	-1.053031
C	4.822927	1.571603	0.800373	H	1.200678	4.784927	-0.657471
C	3.505591	1.040057	0.608852	H	0.681132	4.136950	-2.238618
C	5.767582	0.242754	4.270920	H	-0.511807	4.900725	-1.157403
C	5.417366	2.402985	-0.301714	H	-0.233925	-0.164189	-8.197208
O	2.892101	1.348061	-0.508775	H	4.841134	1.146509	5.451843
O	2.170527	-0.849976	-1.783936	C	1.484882	-2.403371	-2.183184
H	-1.053755	-1.101017	-5.378710	O	2.148281	-3.121551	-3.159638
H	2.272337	1.005209	-7.102384	C	3.335401	-2.513978	-3.723474
H	3.803858	1.900558	-4.009026	O	0.407300	-2.857713	-1.786433
H	3.766927	2.288367	-5.760587	H	3.101747	-1.529922	-4.150388
H	2.842548	3.258018	-4.583179	H	4.118606	-2.398354	-2.963941
H	-1.688884	-0.731779	-3.135792	H	3.662928	-3.203440	-4.509686
H	-1.662026	0.710431	-0.153585	75			
H	-2.268133	-2.110677	-1.184230	1b-trans-RPO ksi=134			
H	-3.211687	-0.654990	-1.579487	C	1.221434	0.990743	-3.850698
H	-4.259594	-1.924777	0.317653	C	0.105777	0.105783	-4.011861
H	-3.788154	-0.288367	0.784240	C	-0.201666	-0.421791	-5.288783
H	-2.253547	-2.874866	1.408827	C	0.560264	-0.121471	-6.406263
H	-3.129487	-1.869508	2.568620	C	1.653861	0.759863	-6.233447
H	-0.655568	-1.488931	2.654369	C	1.993723	1.318313	-5.008849
H	-1.506935	0.003656	2.214549	C	-0.740845	-0.233385	-2.905002
H	-0.233257	-1.944957	0.186282	N	-0.451753	0.004564	-1.663441
H	3.237757	-0.613105	3.622289	Co	1.222328	0.623912	-1.070665
H	6.513499	1.707710	2.094348	O	0.268600	2.310502	-0.453170
H	4.831103	3.320015	-0.467473	C	0.960012	3.591676	-0.675439
H	5.398029	1.853798	-1.253911	C	0.773912	3.097487	0.700319

C	-3.352683	-1.662181	0.112852	H	6.451507	2.686235	-0.068145
C	-2.490105	-1.336758	-1.116985	H	1.301743	-0.894952	2.452937
N	0.761369	-0.453415	0.564242	H	-0.635859	-1.347214	-7.726643
C	1.350152	-0.319258	1.714779	H	0.093529	0.069125	-8.515277
C	2.565209	0.393866	1.962026	H	6.692320	-0.308756	4.040885
C	3.338866	0.983167	0.910289	H	6.064793	1.178934	4.767830
C	4.555581	1.654749	1.266928	H	1.930621	3.466993	-1.154860
C	4.930200	1.729573	2.598947	H	0.291155	4.357842	-1.071332
C	4.171690	1.160084	3.651641	H	1.643069	2.627315	1.162199
C	3.008254	0.497077	3.307487	H	-1.148026	4.004245	1.053913
O	3.024506	0.957734	-0.361087	H	-0.654693	2.792836	2.272109
C	4.635371	1.281408	5.082163	H	0.108409	4.397056	2.260030
C	5.381464	2.256970	0.164814	H	1.095798	-1.336164	-8.118276
O	2.229807	-1.129098	-1.753834	H	5.192943	-0.353267	4.992143
C	1.738020	-2.289605	-2.113690	C	1.742319	-2.080784	-1.935139
O	2.600033	-2.988338	-2.938477	O	2.537775	-2.807635	-2.801790
C	3.778708	-2.287457	-3.401979	C	3.563467	-2.079707	-3.518165
O	0.671634	-2.837906	-1.824489	O	0.782740	-2.664630	-1.428700
C	1.265388	3.371069	-0.589088	H	3.119874	-1.278401	-4.123912
H	-0.839361	-0.934745	-5.544073	H	4.297169	-1.646257	-2.826941
H	2.693042	1.031645	-7.001941	H	4.042794	-2.823616	-4.164284
H	4.155635	1.609879	-3.793440	75			
H	4.225047	2.104453	-5.517179	1b-trans-RPO-in ksi=154			
H	3.321663	3.066629	-4.319509	C	0.052165	-0.323983	-5.378584
H	-1.509641	-0.732405	-3.316342	C	0.343205	0.094773	-4.057087
H	-1.642987	0.441747	-0.231721	C	1.513975	0.879131	-3.799695
H	-2.124379	-2.263572	-1.586637	C	2.354792	1.224554	-4.902439
H	-3.094170	-0.796787	-1.861671	C	2.024566	0.776594	-6.173908
H	-4.200879	-2.294048	-0.187867	C	0.877244	-0.006440	-6.444768
H	-3.782510	-0.727214	0.512045	C	-0.563786	-0.274310	-3.008863
H	-2.204832	-3.341525	0.849799	N	-0.334552	-0.115476	-1.741216
H	-3.170971	-2.538870	2.094103	Co	1.339122	0.382329	-1.033104
H	-0.719772	-2.095558	2.358685	O	0.654485	2.105227	-0.162549
H	-1.614659	-0.585392	2.093665	C	-0.190992	3.199774	-0.719032
H	-0.141787	-2.185514	-0.099520	C	-0.868456	3.020236	-2.044662
H	2.397219	0.034023	4.087683	O	1.846737	1.332415	-2.611320
H	5.859253	2.253077	2.845433	C	3.585625	2.042723	-4.627633
H	4.800914	2.998442	-0.404684	C	0.591278	-0.483250	-7.846716
H	5.681641	1.487783	-0.562074	C	-1.286724	-0.501720	-0.689522
H	6.281400	2.740601	0.565865	C	-0.462673	-1.244799	0.379017
H	0.883936	-0.788258	2.589581	C	-1.305515	-1.532550	1.617594
H	-0.337205	-1.067448	-7.885503	C	-2.539130	-2.356008	1.212625

C	4.680850	1.981589	2.580268	H	0.490454	0.360896	-8.545951
C	3.864785	1.426196	3.599778	H	5.623771	0.818122	5.226142
C	2.749276	0.715257	3.201799	H	4.726132	2.335618	5.387037
O	3.049946	0.992081	-0.473663	H	-0.811939	3.606906	0.084623
C	4.220504	1.615823	5.052964	H	1.879110	3.255283	-1.484371
C	5.295017	2.427360	0.164792	H	1.405120	-1.121138	-8.224107
O	2.299540	-1.255925	-1.649206	H	3.932766	0.792489	5.769824
C	1.790310	-2.388240	-2.075310	H	3.497728	-1.384750	-3.960578
O	2.749336	-3.201060	-2.648366	H	4.427207	-2.005574	-2.563023
C	4.062089	-2.624284	-2.851011	H	4.292056	-2.997414	-4.059893
O	0.639637	-2.827882	-2.016117	H	-1.195601	4.009881	-2.398251
C	-0.390254	3.042052	-1.415480	H	-0.189513	2.585958	-2.784161
H	-0.730384	-0.775722	-5.892524	H	-1.759838	2.386611	-1.953752
H	3.033521	0.785719	-7.257151	H	1.687825	3.932879	0.245225
H	4.552338	1.051734	-4.063344	75			
H	4.645468	1.671869	-5.743626	1b-trans-RPO-in ksi=278			
H	3.862015	2.619248	-4.446298	C	0.229615	-0.288529	-5.700529
H	-1.365270	-0.634894	-3.682750	C	0.552934	0.052814	-4.360773
H	-1.677038	0.514983	-0.688250	C	1.807804	0.681687	-4.066747
H	-1.989327	-2.249142	-1.953503	C	2.701982	0.946512	-5.157104
H	-2.965015	-0.817853	-2.363780	C	2.331562	0.585580	-6.441741
H	-4.171908	-2.263328	-0.721692	C	1.095356	-0.038518	-6.748558
H	-3.842340	-0.657853	-0.065040	C	-0.404274	-0.234471	-3.342969
H	-2.247669	-3.216127	0.524835	N	-0.220708	-0.080511	-2.062632
H	-3.329411	-2.380586	1.646498	Co	1.432770	0.381394	-1.269689
H	-0.920158	-1.865661	2.088859	O	0.875795	2.398987	-1.094774
H	-1.821384	-0.393373	1.679478	C	0.257077	3.316463	-0.116800
H	-0.147596	-2.063976	-0.305104	C	-0.271758	2.778414	1.178105
H	2.092067	0.268579	3.953650	O	2.187778	1.062391	-2.876795
H	5.567727	2.552087	2.872949	C	4.016137	1.606044	-4.847178
H	4.710241	3.058365	-0.520462	C	0.763212	-0.415151	-8.170839
H	5.735385	1.635664	-0.459535	C	-1.254986	-0.435315	-1.072321
H	6.103485	3.022968	0.607424	C	-0.515142	-1.103909	0.095532
H	0.694872	-0.628536	2.368467	C	-1.452043	-1.352724	1.274711
H	-0.220459	-0.898965	-8.233574	C	-2.631162	-2.223638	0.811344
H	0.747960	0.468396	-8.827453	C	-3.362785	-1.599932	-0.383127
H	5.206031	1.184010	5.285431	C	-2.408952	-1.312899	-1.553936
H	4.264936	2.683174	5.320180	N	0.677299	-0.275685	0.340373
H	0.856909	4.228012	-0.042631	C	1.213592	-0.165087	1.520707
H	-1.251359	2.371232	-1.435849	C	2.409042	0.549405	1.831347
H	1.507572	-1.112702	-8.584623	C	3.251688	1.103297	0.811195
H	3.481212	1.135974	5.707911	C	4.413655	1.838160	1.229424

C	1.891131	-2.142311	-1.879487	H	3.994894	-1.710568	-3.455250
O	2.922543	-2.814476	-2.508482	H	4.540926	-2.386220	-1.892601
C	4.068540	-2.030047	-2.916877	H	4.632787	-3.394132	-3.382363
O	0.864977	-2.780139	-1.639285	H	-0.892502	3.551607	1.654422
C	0.006900	2.944743	0.478720	H	-0.884073	1.883110	1.021997
H	-0.198231	-1.340173	-5.837862	H	0.551329	2.529146	1.860227
H	3.370621	0.841968	-6.824987	H	-0.315593	3.749629	-2.243466
H	4.143955	1.822322	-3.477336	75			
H	4.505590	2.175143	-5.199744	1b-trans-RPO-in ksi=66			
H	3.319121	3.145716	-4.289652	C	0.592381	-0.631563	-5.576740
H	-1.294511	-1.006143	-3.775581	C	0.598571	-0.081772	-4.273024
H	-1.976405	0.424452	-0.871533	C	1.620271	0.846322	-3.890187
H	-2.170329	-2.420109	-1.994971	C	2.624667	1.178043	-4.852520
H	-3.102533	-1.023926	-2.584890	C	2.579282	0.593824	-6.110778
H	-4.444363	-2.371167	-0.947141	C	1.571564	-0.318207	-6.505524
H	-4.177046	-0.717192	-0.388303	C	-0.444387	-0.452397	-3.362673
H	-2.643821	-3.215566	0.529031	N	-0.434168	-0.191501	-2.092277
H	-3.805748	-2.291479	1.488160	Co	1.042152	0.526664	-1.168478
H	-1.437746	-1.753191	2.088659	O	-0.179841	2.130150	-0.727834
H	-2.276725	-0.310460	1.487844	C	0.089816	3.592921	-0.843859
H	-0.471745	-2.131045	-0.233294	C	1.382791	4.070672	-1.430498
H	1.993644	-0.470766	3.913520	O	1.677576	1.432853	-2.718147
H	5.401665	2.009181	3.084445	C	3.713662	2.129316	-4.441246
H	4.299917	3.459999	0.174575	C	1.589751	-0.930225	-7.884087
H	5.061835	2.002827	-0.449826	C	-1.523343	-0.538010	-1.171561
H	5.812948	2.882424	0.918774	C	-0.863873	-1.148537	0.075498
H	0.421928	-0.937812	2.331303	C	-1.892158	-1.302777	1.194728
H	0.740003	-1.610707	-8.026432	C	-3.039995	-2.201973	0.703667
H	1.540318	-0.158771	-8.667988	C	-3.669675	-1.675515	-0.592910
H	5.225838	0.086588	5.121685	C	-2.620845	-1.459911	-1.696988
H	4.346335	1.545371	5.606476	N	0.330451	-0.328454	0.368501
H	-0.817656	4.089167	-1.200486	C	0.902664	-0.355378	1.535514
H	0.935946	2.737271	1.009847	C	2.119668	0.304336	1.898058
H	2.512740	-1.506251	-8.053580	C	2.866077	1.104642	0.973317
H	3.546092	-0.039539	5.685646	C	4.071558	1.724454	1.441481
H	3.766179	-1.227716	-3.602951	C	4.473569	1.532482	2.754071
H	4.576867	-1.591629	-2.048412	C	3.745629	0.747013	3.681889
H	4.730777	-2.738085	-3.427377	C	2.583113	0.149204	3.231821
H	1.543334	5.108247	-1.098641	O	2.512686	1.340794	-0.267056
H	2.216276	3.440352	-1.103993	C	4.239480	0.575355	5.096742
H	1.342484	4.052585	-2.525110	C	4.861784	2.562258	0.475035
H	-0.899025	3.022089	1.082729	O	2.203207	-0.893217	-1.622987

H	4.487418	1.568786	-3.340840
H	4.827621	2.056094	-5.035343
H	3.794916	3.054058	-3.979400
H	-1.258075	-0.577515	-3.694210
H	-1.759367	0.550141	-0.629345
H	-2.155091	-2.112287	-2.093383
H	-3.025115	-0.603567	-2.459853
H	-4.394638	-2.091259	-0.980558
H	-4.023562	-0.550446	-0.200884
H	-2.593665	-3.224443	0.292367
H	-3.686957	-2.404698	1.413720
H	-1.281760	-2.059186	2.008868
H	-2.075119	-0.510666	1.656897
H	-0.381100	-2.133061	-0.352094
H	1.768723	-0.286104	4.158542
H	5.384548	1.923046	3.448623
H	4.658888	2.998147	0.214299
H	5.497509	1.475171	-0.031547
H	6.040607	2.579774	1.268433
H	0.373577	-0.904502	2.461785
H	0.498383	-0.868606	-8.073071
H	1.524282	0.490640	-8.583823
H	4.900999	0.296946	5.651929
H	4.003311	1.806015	5.879035
H	-0.948854	3.708612	-0.256079
H	2.014676	3.262904	-1.174810
H	2.262147	-1.059849	-8.149161
H	3.166620	0.246136	6.032678
H	3.877791	-1.396171	-3.580768
H	4.531258	-2.042304	-2.045195
H	4.627686	-3.032683	-3.546084
H	-0.771607	4.244793	-2.728361
H	0.260864	2.805134	-2.970216
H	-1.456554	2.620981	-2.513516
H	1.454367	3.861619	0.500930

75

1b-trans-RPO ksi=206

C	1.251991	1.001834	-3.732359
C	0.012644	0.309925	-3.918972
C	-0.454402	0.040195	-5.228850
C	0.263707	0.414540	-6.352855
C	1.486810	1.096616	-6.150123

75

1b-trans-RPO-in ksi=146

C	0.585849	-0.203684	-5.515993
C	0.707922	0.188606	-4.160798
C	1.856952	0.928161	-3.732067
C	2.855818	1.248512	-4.702404
C	2.689757	0.824539	-6.014076
C	1.562176	0.091410	-6.453365
C	-0.346299	-0.160353	-3.253305
N	-0.283520	-0.032632	-1.963637
Co	1.286637	0.414049	-1.025116
O	0.451723	2.128817	-0.260206
C	-0.180450	3.304430	-0.922631
C	-0.552009	3.226900	-2.372851
O	2.031933	1.366838	-2.504700
C	4.063156	2.020338	-4.248826
C	1.453397	-0.359583	-7.888529
C	-1.379107	-0.398580	-1.054480
C	-0.729260	-1.187942	0.097593
C	-1.740284	-1.462085	1.207625
C	-2.938073	-2.232352	0.626957
C	-3.574417	-1.493557	-0.557216
C	-2.544908	-1.179948	-1.654717
N	0.490421	-0.447702	0.460923
C	0.951186	-0.405241	1.674729
C	2.153995	0.242339	2.097432
C	3.041950	0.889531	1.179384
C	4.227152	1.500921	1.708053
C	4.472827	1.450047	3.070534
C	3.605100	0.812532	3.992008
C	2.464157	0.220624	3.483310
O	2.856246	0.977510	-0.114349
C	3.933939	0.788239	5.464128
C	5.163363	2.177158	0.746355
O	2.256978	-1.099777	-1.623073
C	1.800401	-2.248221	-2.061428
O	2.768298	-2.969950	-2.735108
C	4.029687	-2.306041	-2.984774
O	0.687114	-2.767802	-1.953559
C	1.212750	3.371341	-0.443042
H	-0.297328	-0.775294	-5.813030
H	3.476755	1.059864	-6.737175

H	-0.480423	-2.278406	2.444877	C	1.987927	1.398924	-4.891120
H	-1.366938	-0.742683	2.340668	C	-0.794351	-0.102198	-2.807298
H	-0.127253	-2.241797	-0.059463	N	-0.418122	-0.077535	-1.564347
H	2.685350	-0.006875	4.044351	Co	1.338955	0.295319	-0.998941
H	6.125594	2.095192	2.559799	O	0.695212	1.989339	-0.072515
H	4.935827	2.751508	-0.654012	C	0.193350	3.133145	-0.857745
H	5.758204	1.209629	-0.815171	C	1.530948	3.208258	-0.248489
H	6.456185	2.472623	0.243458	C	1.829854	3.939052	1.024256
H	1.100157	-0.889754	2.635470	C	-0.213732	0.100868	-7.749001
H	-1.188605	-0.403793	-7.731633	C	3.294046	2.116369	-4.692657
H	-0.315674	1.014630	-8.354180	O	1.739460	1.327504	-2.555316
H	5.973146	0.784608	5.006219	C	-1.279053	-0.503134	-0.448343
H	5.086969	2.310715	5.147495	C	-2.535760	-1.290539	-0.812031
H	0.122510	2.925853	-1.925417	C	-3.292637	-1.676553	0.468826
H	-0.655411	3.619879	-0.372758	C	-2.399513	-2.446215	1.450335
H	2.364223	2.999040	-0.922142	C	-1.117955	-1.666670	1.789538
H	0.931140	4.042634	1.645721	C	-0.380859	-1.324595	0.498860
H	2.599851	3.400425	1.593636	N	0.876370	-0.573366	0.615237
H	2.216630	4.941707	0.790356	C	1.525527	-0.437847	1.731500
H	0.495074	-0.557778	-8.274019	C	2.762118	0.265691	1.901363
H	4.307316	0.786581	5.622881	C	3.267412	0.413568	3.219323
C	1.499625	-2.308885	-2.267956	C	4.455201	1.071450	3.484315
O	2.217474	-2.970865	-3.246769	C	5.176841	1.581061	2.376942
C	3.356219	-2.273958	-3.805966	C	4.739879	1.460201	1.066849
O	0.449758	-2.835211	-1.888746	C	3.493188	0.804748	0.794612
H	3.046138	-1.318380	-4.249585	C	4.980706	1.245962	4.887462
H	4.120158	-2.085752	-3.041342	C	5.522101	2.006357	-0.094759
H	3.748381	-2.942492	-4.580683	O	3.105248	0.757378	-0.455771
82				O	2.089397	-1.204335	-1.882513
1a'-trans-RPO C1 dE=5.26 TS				H	-1.400301	-0.496264	-5.341949
C	4.110900	-0.326155	-0.420165	H	2.073831	1.392638	-7.024940
C	3.935374	-0.294624	1.004545	H	3.920967	1.578188	-3.967765
C	5.061807	-0.183983	1.856995	H	3.835491	2.219614	-5.641644
C	6.351690	-0.079130	1.365875	H	3.134444	3.121942	-4.273163
C	6.514860	-0.103649	-0.041952	H	-1.795655	-0.479028	-3.040968
C	5.454251	-0.228352	-0.924237	H	-1.567047	0.419699	0.090130
C	2.640824	-0.392813	1.607597	H	-2.233692	-2.190947	-1.369631
N	1.510347	-0.362469	0.970928	H	-3.193739	-0.694811	-1.462575
C	0.211752	-0.505711	1.646690	H	-4.175548	-2.277742	0.207827
C	-0.721769	0.518200	0.979920	H	-3.668134	-0.761078	0.957563
C	-2.162141	0.308874	1.444940	H	-2.118698	-3.413487	1.003263
C	-2.221025	0.433670	2.977143	H	-2.954189	-2.670798	2.373033

H	7.524551	-0.009608	-0.456291	C	-1.254775	-0.540113	3.664064
H	6.691399	-0.082005	-2.685037	C	0.187709	-0.347546	3.165440
H	5.017438	0.540020	-2.881814	N	-0.465273	0.424543	-0.469857
H	5.295208	-1.192067	-2.846646	Co	1.328172	-0.013196	-0.878670
H	2.617079	-0.489413	2.699619	O	0.919882	-1.834768	-1.366603
H	-3.587903	1.591449	-6.459697	C	-0.111124	-2.594378	-1.118073
H	-3.665787	-0.178640	-6.481295	O	-1.054572	-2.411576	-0.325000
H	8.301278	-0.705177	2.093964	C	7.544312	0.073897	2.278203
H	8.042057	1.047487	2.136976	C	5.638013	-0.239098	-2.415187
H	1.544029	2.287682	1.512128	O	3.151479	-0.455774	-1.289086
H	2.956723	3.273411	0.767682	C	-1.411469	0.559949	-1.347419
H	0.159964	2.738042	-0.502660	C	-1.242277	0.535691	-2.769036
H	1.045342	4.988290	-1.247392	C	0.053766	0.472640	-3.381783
H	2.620499	4.229509	-1.616565	C	0.114827	0.508733	-4.818320
H	1.171754	3.767714	-2.554694	C	-1.055587	0.581003	-5.555923
H	-4.488118	0.728050	-5.194005	C	-2.341209	0.630175	-4.961343
H	7.244244	0.005723	3.333138	C	-2.403009	0.613661	-3.578669
H	-0.757064	-3.703283	-2.835992	O	1.183727	0.413209	-2.739283
H	0.920369	-4.074036	-2.357975	C	-3.583172	0.696609	-5.816436
H	-0.471504	-4.710142	-1.397176	C	1.473695	0.453081	-5.457502
O	1.295985	4.599013	1.842915	O	2.062424	1.794458	-0.690604
C	0.348506	4.235328	2.607817	C	1.229534	2.969555	-0.561082
O	-0.274170	5.345836	3.232049	C	1.537590	4.056237	-1.559921
C	-1.356307	4.990025	4.103634	C	1.947470	2.882890	0.704454
O	-0.087122	3.086226	2.868915	C	-0.086043	-3.863778	-1.979288
H	-1.741216	5.936792	4.506287	H	-3.375775	0.655213	-3.078738
H	-2.154367	4.461755	3.560030	H	-0.979390	0.593674	-6.648569
H	-1.016689	4.342657	4.926438	H	2.024548	-0.435553	-5.115752
82				H	1.395106	0.437627	-6.553144
1a'-cis-B1-RPO C1 dE=20.33 TS				H	2.084741	1.316676	-5.153329
C	0.396138	-2.427898	-0.592541	H	-2.435219	0.704356	-0.985339
C	-0.011150	-2.635550	-1.951995	H	-0.402100	1.522210	1.312676
C	-0.438874	-3.909037	-2.383157	H	-2.503144	-0.683634	1.109033
C	-0.460246	-4.999301	-1.524278	H	-2.823442	1.067507	0.999623
C	-0.075641	-4.780881	-0.180106	H	-3.250676	0.253301	3.323647
C	0.331189	-3.543538	0.301484	H	-1.947660	1.463326	3.257080
C	-0.106582	-1.494256	-2.819622	H	-1.570033	-1.578316	3.462169
N	0.568186	-0.406464	-2.625606	H	-1.290284	-0.399557	4.755526
C	0.207896	0.888874	-3.182045	H	0.842799	-1.093479	3.641275
C	-0.201561	1.710273	-1.935820	H	0.544905	0.657812	3.441767
C	-0.367903	3.182089	-2.317033	H	-0.172764	-1.497220	1.354882
C	-1.406474	3.308521	-3.445299	H	4.889750	-0.166023	2.937925

H	-0.083245	-5.628644	0.513427	C	-1.069244	2.425225	-4.656798
H	-0.738575	-4.033340	-3.427965	C	-0.871745	0.954078	-4.253727
H	0.081737	-2.624838	2.239206	N	0.787189	1.407980	-0.882181
H	1.753151	-2.860475	1.755168	Co	1.838243	-0.143322	-1.243967
H	0.774884	-4.272445	2.283565	O	2.869920	-1.704078	-1.662157
H	2.159972	3.085294	5.579476	C	3.121633	-2.111250	-2.883459
H	3.399814	4.120627	4.847172	O	2.862923	-1.542666	-3.954913
H	-1.718305	-6.769286	-1.422124	C	-0.863877	-6.375363	-1.995652
H	-1.149622	-6.359774	-3.056506	C	0.757278	-3.326203	1.726066
H	1.685088	4.397630	4.478207	O	0.772649	-1.268031	-0.109636
H	-0.039749	-7.098461	-1.884232	C	0.894976	2.151572	0.177219
H	3.312428	3.230251	-2.296180	C	1.792010	1.926458	1.265790
H	3.546283	2.288890	-0.710060	C	2.778597	0.884443	1.250418
H	4.602741	1.454328	-3.530317	C	3.631401	0.758171	2.399312
H	6.232528	0.846535	-1.673069	C	3.486531	1.633319	3.461647
H	4.893937	0.013184	-0.823602	C	2.531808	2.680764	3.477782
H	5.443889	-0.581300	-2.414350	C	1.710545	2.806818	2.374661
H	3.007722	-4.246738	-2.688589	O	2.992526	0.059774	0.260233
H	4.265369	-3.689389	-3.834958	C	2.438553	3.618371	4.655693
H	4.516727	-3.567533	-2.050466	C	4.671029	-0.326826	2.387049
O	5.300103	3.729803	-1.122246	O	2.881824	1.014174	-2.446060
C	4.698487	4.470488	-0.276955	C	4.322447	1.255726	-2.487057
O	5.592407	4.942848	0.731268	C	5.278656	0.314394	-1.802333
C	4.937504	5.683255	1.768203	C	3.719527	2.376330	-1.772087
O	3.495151	4.803900	-0.207740	C	3.788317	-3.492200	-2.867932
H	5.724133	5.960548	2.484533	H	-1.176020	1.306620	-1.596023
H	4.449745	6.590580	1.377658	H	1.143466	1.317534	-3.571007
H	4.169935	5.072566	2.269449	H	-1.821089	0.540825	-3.869912
82				H	-0.574856	0.350868	-5.124536
1a'-cis-B2-RPO C1 dE=16.90 TS				H	-0.141237	2.791747	-5.126115
C	1.362446	-2.485718	-1.470012	H	-1.862208	2.506648	-5.415936
C	0.245384	-2.380259	-2.364680	H	-2.396665	3.016826	-3.053530
C	-0.024600	-3.411711	-3.290978	H	-1.489814	4.360760	-3.756503
C	0.783321	-4.534330	-3.384968	H	0.609715	3.576966	-2.634266
C	1.869879	-4.638040	-2.483505	H	-0.687461	3.780541	-1.452350
C	2.166874	-3.667948	-1.536652	H	0.253933	3.037852	0.263463
C	-0.674205	-1.293214	-2.190986	H	4.151482	1.514708	4.323468
N	-0.359629	-0.173274	-1.609468	H	0.976259	3.615766	2.333354
C	-1.330872	0.674050	-0.924751	H	5.168659	-0.405235	3.363085
C	-0.928039	0.510752	0.564274	H	5.433921	-0.126954	1.619470
C	-1.751953	1.442650	1.454135	H	4.219869	-1.294605	2.125236
C	-3.253956	1.212970	1.219103	H	-0.823109	-1.531926	-3.649604

H	2.520839	-5.516060	-2.543067	C	-3.634931	1.343154	-0.262074
H	-0.883612	-3.301645	-3.959869	C	-2.810996	0.379464	-1.130640
H	4.073518	-2.988059	-0.802697	N	0.536725	0.683407	0.604352
H	3.842320	-4.754696	-0.728301	Co	1.389930	0.263487	-1.030178
H	3.029643	-3.666458	0.441007	O	2.051491	-0.122240	-2.826879
H	5.593556	2.093712	5.028701	C	3.258441	0.564835	-3.305007
H	5.347591	3.721860	4.374938	C	3.163774	1.071823	-4.716169
H	-0.362266	-5.387968	-5.007281	C	0.537935	-5.607638	-4.416708
H	1.384445	-5.690574	-5.117074	C	3.341534	-3.785287	-0.606620
H	4.026178	2.905942	5.238027	O	1.665368	-1.581136	-0.567998
H	0.404573	-6.597824	-3.952444	C	1.144911	1.158792	1.648307
H	3.895522	-1.082079	-2.009943	C	2.552097	1.371624	1.781246
H	3.429283	-1.596488	-3.755813	C	3.485407	1.051782	0.739884
H	3.628219	1.293649	-2.583176	C	4.884336	1.273653	0.993255
H	2.742947	0.305445	-5.381893	C	5.275975	1.811134	2.208171
H	2.529794	1.968664	-4.755780	C	4.363521	2.153166	3.239545
H	4.181155	1.325019	-5.044371	C	3.021992	1.920612	3.004168
H	1.054013	5.340165	-1.653324	O	3.162670	0.561976	-0.423567
H	2.549015	4.605964	-1.011112	C	4.856692	2.748019	4.535822
H	2.083529	4.274150	-2.689368	C	5.868816	0.903075	-0.077685
O	5.700369	-1.244566	-3.451769	O	1.402229	2.116088	-1.640568
C	6.456265	-0.230878	-3.350473	C	0.917171	3.229602	-1.169119
O	7.782129	-0.614858	-2.950924	O	-0.044952	3.387683	-0.388740
C	8.683366	0.487856	-2.818002	C	3.585923	-0.824345	-3.012985
O	6.230003	0.985845	-3.529865	C	1.690549	4.447813	-1.680835
H	9.642020	0.059551	-2.489936	H	-1.133524	-0.545110	0.829445
H	8.819689	1.020851	-3.772929	H	-1.110495	1.720816	-1.179926
H	8.325995	1.217488	-2.074383	H	-3.039860	-0.662328	-0.844268
82				H	-3.074285	0.493585	-2.193543
1a'-trans-SPO C1 dE=8.19 TS				H	-3.449059	2.376798	-0.595859
C	-2.001360	-0.772798	-3.969996	H	-4.709884	1.147616	-0.397307
C	-1.049991	-0.290976	-3.036952	H	-3.531372	0.203994	1.572667
C	0.054650	0.505624	-3.485776	H	-3.832998	1.928223	1.823171
C	0.134353	0.800906	-4.890870	H	-1.467682	2.475616	1.205540
C	-0.823160	0.297226	-5.756195	H	-1.521715	1.268339	2.515945
C	-1.909436	-0.504152	-5.324778	H	0.537393	1.445067	2.514767
C	-1.251236	-0.595022	-1.652491	H	6.345273	1.976748	2.376155
N	-0.425363	-0.319747	-0.691434	H	2.284435	2.162958	3.775695
Co	1.310311	0.382765	-0.938377	H	5.809093	-0.168908	-0.318142
O	0.855186	2.228810	-0.414826	H	6.895259	1.129860	0.239277
C	0.475962	2.646804	0.928347	H	5.669123	1.423288	-1.025951
C	1.221847	3.855842	1.428479	H	-1.717182	-1.454180	-2.492883

H	6.560937	3.519577	0.222907	O	0.978700	1.005033	-2.716793
H	5.890990	3.536976	-2.062971	C	1.284621	1.646641	-5.358238
H	4.133479	3.267000	-2.317856	C	-2.913927	-1.041280	-6.315081
H	5.256961	1.951165	-2.605176	C	-0.721266	-0.634907	0.716529
H	2.665771	-0.128340	2.616854	C	0.602167	-1.113706	1.333267
H	-3.684302	-1.638650	-5.808056	C	0.464110	-1.259704	2.847355
H	-3.424201	-0.231076	-6.861172	C	-0.669677	-2.251985	3.158716
H	6.477650	4.064438	2.988654	C	-1.989426	-1.826146	2.502689
H	6.306249	2.541309	3.885809	C	-1.835358	-1.645182	0.983204
H	0.431713	1.831172	1.653649	N	1.635300	-0.187034	0.836240
H	-1.364987	1.935745	-0.051132	C	2.626335	0.211588	1.574986
H	-2.435078	-1.686593	-7.069488	C	3.673861	1.092452	1.158195
H	7.595127	2.725300	2.676058	C	3.827226	1.495574	-0.211572
H	3.243763	-2.895774	-3.070251	C	4.915185	2.385408	-0.522140
H	2.284238	-4.333683	-2.540585	C	5.753341	2.828201	0.486766
H	1.629023	-3.199037	-3.750673	C	5.608409	2.437148	1.842410
H	-0.855176	3.678778	-0.494746	C	4.574754	1.568696	2.144704
H	0.717880	4.245820	2.324271	O	3.069598	1.111237	-1.194179
H	2.255511	3.584590	1.684546	C	6.543849	2.967623	2.901391
H	1.240180	4.642318	0.662308	C	5.068555	2.817144	-1.952424
O	-2.243945	3.573072	1.406068	O	1.999434	-1.220034	-1.753234
C	-2.489289	2.748855	2.337765	C	1.564166	-2.451081	-1.743846
O	-3.453143	3.258821	3.250894	C	2.242986	-3.279853	-2.841434
C	-3.779334	2.356560	4.315359	O	0.706970	-2.979668	-1.011138
O	-2.022173	1.602557	2.557076	C	-0.701730	2.777207	0.086761
H	-4.516485	2.880423	4.939318	H	-2.828808	-1.381421	-3.592655
H	-4.213299	1.419540	3.932662	H	-0.729285	0.527665	-6.822954
H	-2.893173	2.100087	4.915820	H	1.251143	2.643575	-4.892467
82				H	2.240774	1.202781	-5.043926
1a'-cis-B1-SPO C1 dE=19.59 TS				H	1.273731	1.761000	-6.450819
C	1.741803	1.969870	3.214008	H	-2.182912	-1.112550	-1.399674
C	1.810360	1.263802	1.983294	H	-1.011294	0.307984	1.217089
C	3.067861	0.730411	1.531651	H	-1.587200	-2.598239	0.488265
C	4.216930	0.941212	2.376598	H	-2.787282	-1.279257	0.570539
C	4.085152	1.641047	3.562328	H	-2.772527	-2.571971	2.710606
C	2.849703	2.175865	4.013374	H	-2.318228	-0.867320	2.933890
C	0.600210	1.118032	1.238533	H	-0.380176	-3.251412	2.790977
N	0.486572	0.558288	0.069855	H	-0.797645	-2.336546	4.249018
Co	1.947420	-0.104273	-0.956954	H	1.402678	-1.626637	3.290489
O	2.545812	1.713445	-1.402271	H	0.235099	-0.279006	3.296852
C	1.763822	2.927922	-1.332058	H	0.821715	-2.088351	0.865986
C	2.397635	4.014590	-0.498345	H	4.425314	1.241799	3.178560

H	3.265602	-5.936865	-1.662745	O	3.258591	0.075750	0.428722
H	1.010937	-3.649268	-4.527649	C	5.532853	0.395949	1.899820
H	3.782331	-3.258290	0.616815	C	2.770222	2.944643	5.309327
H	3.802190	-5.051666	0.492122	C	-0.820656	0.455287	-0.612488
H	2.403872	-4.185480	1.192863	C	-0.518702	0.484993	-2.130081
H	3.400041	3.848874	5.285141	C	-1.780738	0.193998	-2.938501
H	1.738843	3.263581	5.514577	C	-2.858646	1.233992	-2.594384
H	1.820841	-5.807458	-5.170286	C	-3.152959	1.250437	-1.088492
H	3.418021	-6.164168	-4.482188	C	-1.881756	1.499077	-0.258387
H	3.109925	2.338522	6.164725	N	0.594808	-0.454360	-2.249642
H	1.984201	-7.000315	-3.861453	C	0.482999	-1.581856	-2.881552
H	0.708986	2.776734	-1.087793	C	1.307889	-2.724143	-2.601269
H	1.496539	2.151029	-3.390962	C	1.867223	-2.841184	-1.287036
H	4.961316	-0.855225	-4.899102	C	2.562175	-4.045552	-0.958620
H	5.566329	-1.211621	-3.234612	C	2.695862	-5.038029	-1.921911
H	4.439138	-2.329853	-4.029889	C	2.151124	-4.929723	-3.222653
H	3.044801	3.135756	-3.106481	C	1.448324	-3.772195	-3.532685
H	3.457327	4.130880	-0.761855	O	1.733824	-1.919226	-0.360687
H	1.880058	4.966974	-0.682532	C	2.352136	-6.031185	-4.234951
H	2.326189	3.763680	0.569383	C	3.176519	-4.152376	0.408841
O	1.223064	4.540796	-3.683543	O	3.405246	-0.720598	-2.044930
C	-0.038310	4.500361	-3.551564	C	3.494028	-0.532006	-3.338660
O	-0.661743	5.628178	-4.153167	C	4.708352	-1.268960	-3.916103
C	-2.089151	5.633736	-4.031107	O	2.726697	0.095595	-4.085395
O	-0.769808	3.648586	-2.989552	C	2.080638	2.793692	-2.746634
H	-2.429914	6.555778	-4.521464	H	-1.211245	-0.556996	-0.392366
H	-2.541129	4.759269	-4.524531	H	-0.176221	1.496232	-2.395319
H	-2.405415	5.631388	-2.976649	H	-2.148582	-0.821980	-2.708571
82				H	-1.547294	0.229457	-4.013098
1a'-cis-B2-SPO C1 dE=16.83 TS				H	-2.500803	2.226657	-2.906926
C	0.789391	0.106403	3.452749	H	-3.779753	1.011926	-3.155526
C	1.090732	0.167829	2.066871	H	-3.597781	0.285651	-0.784855
C	2.432836	0.442369	1.639728	H	-3.896777	2.028116	-0.857335
C	3.428023	0.672874	2.651560	H	-1.486751	2.503435	-0.479010
C	3.070553	0.587368	3.987745	H	-2.129916	1.457817	0.812835
C	1.752826	0.299204	4.425046	H	-0.299714	1.538155	1.705325
C	0.014966	-0.018490	1.144087	H	4.979738	1.795376	4.175332
N	0.116168	-0.039025	-0.148779	H	0.769658	2.367142	3.523158
Co	1.754363	0.006532	-1.093902	H	6.343741	0.656130	2.593806
O	1.675611	1.886817	-1.577929	H	5.767567	0.784231	0.897858
C	0.902618	2.848158	-1.151747	H	5.487230	-0.698255	1.791657
C	1.564540	4.219054	-1.315129	H	-0.323873	-1.697802	-3.613873

H	4.292691	-5.524103	-1.885032	O	2.821066	0.513969	0.395495
H	1.876456	-3.550945	-4.845425	C	4.828432	0.991227	2.214819
H	2.999337	-3.848317	0.935226	C	1.430628	0.215475	5.897289
H	4.408529	-2.930305	0.425353	C	-1.059687	-0.279707	-1.008373
H	4.450851	-4.715745	0.342494	C	-0.615538	0.074581	-2.448095
H	1.646413	1.163742	6.415860	C	-1.694926	-0.297847	-3.456771
H	0.368298	-0.017781	6.055358	C	-2.977619	0.475024	-3.107255
H	4.654637	-5.615283	-4.723235	C	-3.437318	0.173123	-1.672502
H	3.381907	-6.710442	-4.157274	C	-2.340311	0.469123	-0.637089
H	2.023288	-0.567074	6.398323	N	0.689705	-0.575778	-2.542921
H	3.043009	-5.554137	-5.465743	C	0.898886	-1.666230	-3.218534
H	4.550083	-0.773716	-0.722569	C	1.919761	-2.621980	-2.895970
H	4.245970	1.658746	-1.049148	C	2.430413	-2.674801	-1.555446
H	2.196329	4.248661	-2.210965	C	3.280394	-3.773858	-1.202793
H	0.802956	5.007517	-1.342886	C	3.616080	-4.711264	-2.168148
H	2.217188	4.385887	-0.445322	C	3.141702	-4.654008	-3.501317
H	4.888566	1.515211	-2.805692	C	2.282854	-3.617696	-3.831682
H	5.011693	-2.255086	-2.757947	O	2.142356	-1.807169	-0.617310
H	5.469401	-0.793973	-3.680130	C	3.575028	-5.686210	-4.513422
H	6.449969	-1.304207	-2.267350	C	3.817318	-3.830266	0.199820
O	6.586170	1.839554	-1.226526	O	3.307156	-0.010011	-2.277280
C	7.182055	1.121796	-0.362445	C	4.612795	-0.392733	-1.744326
O	8.123468	1.902297	0.383254	C	5.433329	-1.244409	-2.678279
C	8.829414	1.152281	1.376954	C	4.649297	1.059206	-1.852609
O	7.072289	-0.090987	-0.082808	O	-0.239557	2.758022	-0.661253
H	9.493121	1.868517	1.881960	H	-1.249747	-1.371946	-1.002686
H	8.141731	0.700009	2.107913	H	-0.441324	1.158921	-2.470233
H	9.425534	0.341595	0.928974	H	-1.897633	-1.382532	-3.421362
83				H	-1.360107	-0.058378	-4.477855
1b'-trans-RPO C1 dE=4.10 TS				H	-2.782381	1.555352	-3.206023
C	3.845197	1.518078	0.628669	H	-3.775635	0.225831	-3.823574
C	3.206987	1.260026	1.887875	H	-3.727565	-0.890866	-1.608146
C	3.731196	1.820723	3.078305	H	-4.337593	0.759721	-1.433869
C	4.847075	2.640823	3.077935	H	-2.094839	1.539799	-0.601979
C	5.469503	2.890614	1.829865	H	-2.687719	0.168590	0.362733
C	5.011043	2.357707	0.635410	H	-0.982344	-0.139907	1.586428
C	2.046519	0.425420	1.986253	H	3.849855	0.752237	4.738997
N	1.360114	-0.024589	0.981588	H	-0.244267	-0.103112	3.745917
C	0.195678	-0.907228	1.132809	H	5.257187	0.201723	1.580380
C	-0.858970	-0.383462	0.140323	H	5.484517	1.138445	3.083008
C	-2.035483	-1.353261	0.049007	H	4.855093	1.902853	1.599572
C	-2.645604	-1.538401	1.448609	H	0.203951	-1.922629	-4.029161

H	3.218090	1.603236	4.020235	C	-1.598493	-2.012054	2.465187
H	6.347792	3.544522	1.801702	C	-0.401806	-1.047928	2.529833
H	4.931009	3.055412	-1.394130	N	-0.132911	-0.094963	-1.109759
H	6.050779	1.726113	-1.146358	Co	1.643094	0.485918	-0.814754
H	6.495369	3.360511	-0.566235	O	2.367496	-1.210915	-1.417239
H	1.714495	0.164740	2.998303	C	1.818230	-2.376076	-1.570557
H	-1.769370	-1.238870	-6.994291	O	0.860819	-2.911428	-0.997893
H	-1.025435	0.075921	-7.931294	C	5.378426	3.266959	4.344214
H	6.433848	3.002684	4.518779	C	5.667005	2.648812	-0.684797
H	5.323345	4.367290	4.306581	O	3.458237	1.030973	-0.516552
H	-0.211748	2.181082	1.342512	C	-0.630054	-0.354670	-2.280237
H	0.685528	3.821047	1.167532	C	0.000515	-0.072941	-3.535821
H	-0.776762	2.221225	-1.075337	C	1.231440	0.658564	-3.623884
H	0.824965	4.857380	-1.206122	C	1.750576	0.936792	-4.934727
H	0.246725	3.920744	-2.614259	C	1.074441	0.479218	-6.054398
H	-0.928533	4.718153	-1.518805	C	-0.133457	-0.257020	-5.978804
H	-0.191405	-1.479942	-7.772124	C	-0.646959	-0.509285	-4.718152
H	4.801094	2.936486	5.218646	O	1.909785	1.108026	-2.606977
H	3.028779	-1.617046	-3.860178	C	-0.815052	-0.749023	-7.231920
H	4.288735	-2.104641	-2.693525	C	3.031961	1.716605	-5.022331
H	3.834750	-3.217771	-4.036727	O	1.250452	2.350907	-0.419664
O	-1.694032	3.992415	1.385181	C	-0.039716	2.948899	-0.720492
C	-2.533530	3.083870	1.664339	C	0.033758	4.189069	-1.570678
O	-3.862035	3.582158	1.693699	C	0.131619	3.000757	0.724870
C	-4.849059	2.591372	2.010478	O	2.465502	-3.152265	-2.537939
O	-2.354283	1.861290	1.901124	C	3.466363	-2.469884	-3.322784
H	-5.814431	3.115463	2.001341	H	-1.579874	-1.071694	-4.615770
H	-4.857458	1.778071	1.268429	H	1.499617	0.694565	-7.040409
H	-4.672651	2.147094	3.001901	H	3.820520	1.231931	-4.427929
83				H	3.364761	1.816139	-6.064229
1b'-cis-B1-RPO C1 dE=15.03 TS				H	2.908641	2.720986	-4.588872
C	1.750474	-3.516322	-3.536115	H	-1.614970	-0.831896	-2.329410
C	1.467532	-2.449628	-2.658071	H	-1.241354	0.575394	0.534845
C	1.368720	-2.677223	-1.245822	H	-1.677853	-2.311502	-0.361226
C	1.563161	-4.008852	-0.766138	H	-2.806875	-0.954985	-0.627730
C	1.862902	-5.019099	-1.670467	H	-3.476735	-2.259002	1.396605
C	1.968342	-4.803380	-3.064837	H	-3.058821	-0.573221	1.782026
C	1.115199	-1.149291	-3.150874	H	-1.236466	-3.015430	2.183638
N	1.184299	-0.071320	-2.428079	H	-2.054773	-2.102658	3.463044
C	0.292297	1.069042	-2.661725	H	0.350355	-1.441548	3.231019
C	-0.568675	1.078376	-1.376854	H	-0.736429	-0.062863	2.895090
C	-1.516765	2.277796	-1.364482	H	0.513481	-1.889543	0.741944

H	3.826778	-1.413786	3.207653	C	-2.395861	2.253826	-2.627103
H	0.681411	-1.082478	-4.155095	C	-1.550016	2.223590	-3.907430
H	2.047355	-6.025142	-1.279253	C	-0.590754	1.023566	-3.906851
H	1.822985	-3.306874	-4.607224	N	0.383265	0.955163	-0.254755
H	1.792944	-5.266630	0.970595	Co	1.937187	-0.046298	-0.671421
H	0.491814	-4.047947	1.111169	O	3.542454	-1.061103	-1.078877
H	2.168444	-3.528642	1.230080	C	4.182381	-1.027374	-2.198513
H	0.049882	3.549694	5.380095	O	4.022170	-0.330258	-3.210099
H	0.677997	2.277039	6.450150	O	1.064856	-1.734997	-0.380684
H	1.681815	-6.809050	-3.849640	C	1.502229	-4.237772	0.717769
H	2.269691	-5.627525	-5.041670	C	2.339913	-5.936837	-3.989578
H	1.741020	3.593112	5.922977	C	0.162973	1.526100	0.893280
H	3.372757	-6.278436	-3.812007	C	0.986191	1.422084	2.054548
H	1.518894	3.211349	-1.074898	C	0.611579	2.171100	3.201105
H	3.086109	3.731505	-0.188176	C	1.327281	2.120437	4.382318
H	2.902184	1.992852	-2.791324	C	2.467994	1.276426	4.417881
H	5.339705	1.712017	-2.486421	C	2.881567	0.518879	3.336942
H	4.995102	3.450714	-2.755910	C	2.143419	0.572186	2.101151
H	5.330415	2.858903	-1.104568	O	2.576300	-0.161846	1.122865
H	6.431833	-1.091284	-3.616304	C	4.098328	-0.361070	3.379238
H	6.739702	-2.815572	-3.194285	C	0.928325	2.925337	5.594419
H	5.329617	-2.357975	-4.216186	O	3.055671	1.564866	-0.705718
O	2.526868	5.123291	-1.967322	C	3.389404	2.354529	-1.881131
C	1.507907	5.164502	-2.716127	C	4.862501	2.605287	-2.065212
O	1.520108	6.296974	-3.575597	C	2.597160	3.196450	-0.993699
C	0.381789	6.382685	-4.441581	O	5.212406	-1.983296	-2.154092
O	0.531328	4.374364	-2.798126	C	5.966597	-2.057163	-3.371157
H	0.512808	7.305838	-5.022448	H	-1.154794	0.139469	-1.388828
H	0.326315	5.519294	-5.122718	H	0.871607	2.003242	-2.680779
H	-0.558731	6.428544	-3.871598	H	-1.169057	0.082770	-3.916041
83				H	0.037242	1.033734	-4.810621
1b'-cis-B2-RPO C1 dE=12.45 TS				H	-0.964128	3.152645	-3.966132
C	2.489009	-3.725022	-3.799040	H	-2.203188	2.173180	-4.792540
C	2.010479	-2.756708	-2.885424	H	-3.055861	1.368100	-2.596159
C	2.697119	-2.531726	-1.643898	H	-3.049940	3.138454	-2.629726
C	3.856590	-3.326920	-1.360315	H	-0.924198	3.205669	-1.353005
C	4.288199	-4.246979	-2.304283	H	-2.159111	2.255337	-0.471379
C	3.632241	-4.462933	-3.541700	H	-0.731286	2.152331	0.993646
C	0.762185	-2.094053	-3.126275	H	3.056343	1.226812	5.340352
N	0.405161	-1.000251	-2.523730	H	-0.274304	2.809875	3.130718
C	-0.972762	-0.559935	-2.358523	H	4.614622	-0.275737	4.345122
C	-1.236812	-0.759294	-0.847461	H	4.791330	-0.098377	2.566600

H	5.185872	0.974788	1.032994	C	-2.534712	-0.045906	-0.461134
H	5.283904	2.210188	2.318627	C	-3.695035	-0.596267	-1.308949
H	0.048999	-2.574922	-3.809649	C	-3.408147	-0.523703	-2.818050
H	5.192148	-4.823195	-2.082004	C	-2.077105	-1.205104	-3.185475
H	1.944870	-3.871050	-4.737284	N	-0.019843	-0.315344	-0.146086
H	5.141919	-2.139789	-0.089918	Co	1.474496	-0.049060	-1.275717
H	5.316309	-3.899515	0.113208	O	2.836205	0.148831	-2.636959
H	3.889842	-3.038556	0.774572	C	3.744183	1.281243	-2.556300
H	2.019431	1.669636	6.103820	C	3.898335	2.033090	-3.852296
H	0.879679	0.311670	5.965075	O	2.300944	-1.682286	-0.726835
H	3.517279	-5.557764	-5.403753	C	4.590738	-3.095271	-0.069608
H	5.171097	-5.132837	-4.915004	C	4.185905	-5.451926	-4.538011
H	2.622122	0.004295	6.123113	C	0.018078	-0.208727	1.147249
H	4.320222	-6.449296	-4.090028	C	1.135015	0.240274	1.913155
H	4.624155	-0.231669	-1.217571	C	1.004785	0.237068	3.327760
H	4.959283	-0.491805	-3.046953	C	2.005455	0.699023	4.159978
H	3.524650	1.923199	-1.697334	C	3.181442	1.202649	3.546213
H	4.066494	1.337700	-4.686331	C	3.369053	1.241977	2.174823
H	2.992794	2.622666	-4.048761	C	2.338042	0.740840	1.305170
H	4.763481	2.707475	-3.777623	O	2.564853	0.795833	0.023341
H	0.715045	4.493711	0.609439	C	4.629023	1.770620	1.554213
H	-1.024536	4.153408	0.404161	C	1.873894	0.670334	5.663152
H	-0.121796	3.422411	1.787518	O	0.795115	1.652205	-1.990967
O	6.597610	0.887927	-2.047834	C	0.404758	2.720971	-1.365505
C	7.099842	0.474811	-0.955808	O	0.144485	3.807477	-1.894802
O	8.366462	1.079423	-0.709970	C	4.567052	0.118775	-2.241854
C	8.969631	0.667312	0.523073	O	0.260290	2.537994	0.009274
O	6.658207	-0.338577	-0.111263	C	-0.065460	3.730901	0.736623
H	9.924479	1.207747	0.586026	H	-1.349865	-1.848521	-0.678041
H	8.336674	0.921757	1.386891	H	-0.960632	0.524125	-2.549245
H	9.149929	-0.418687	0.543103	H	-2.137133	-2.287445	-2.977200
83				H	-1.868519	-1.085221	-4.259314
1b'-trans-SPO C1 dE=5.10 TS				H	-3.358720	0.533883	-3.125769
C	-1.077384	-1.507071	-4.183342	H	-4.236275	-0.980095	-3.381409
C	-0.268610	-0.813017	-3.248737	H	-3.873841	-1.648758	-1.027681
C	0.942190	-0.178763	-3.684682	H	-4.620348	-0.047834	-1.075814
C	1.279972	-0.272293	-5.079613	H	-2.399708	1.033893	-0.630371
C	0.451716	-0.969718	-5.943360	H	-2.754602	-0.181467	0.607950
C	-0.742463	-1.605492	-5.522529	H	-0.886603	-0.463731	1.717092
C	-0.716958	-0.749437	-1.889874	H	3.987893	1.577608	4.184966
N	-0.064011	-0.220760	-0.900524	H	0.074852	-0.149147	3.757699
Co	1.712985	0.407471	-1.012279	H	4.402325	2.535832	0.797586

H	1.025618	-0.388979	3.535743	O	1.270674	2.292753	-1.136786
H	-0.110364	0.875670	3.002227	C	0.566204	3.053563	-0.130515
H	0.869843	-1.472463	1.249951	C	1.201874	4.394822	0.150904
H	3.908405	2.699206	3.124425	O	1.757683	0.487170	-2.920981
H	6.545804	4.120595	0.040563	C	2.546543	0.396912	-5.532882
H	6.344625	3.369941	-2.214365	C	-1.598066	-2.362287	-6.508535
H	4.713309	2.774204	-2.677314	C	-0.608183	-0.161681	0.467397
H	5.976862	1.619805	-2.289012	C	0.581702	-0.418156	1.409035
H	2.346613	1.031277	2.717515	C	0.180779	-0.179335	2.861802
H	-2.495315	-2.768033	-6.020998	C	-1.000074	-1.098520	3.217029
H	-1.929897	-1.717859	-7.338500	C	-2.180845	-0.896458	2.258798
H	7.061881	4.292236	2.744635	C	-1.764618	-1.104555	0.793460
H	5.818663	5.509798	2.409973	N	1.691497	0.384741	0.876610
H	0.348365	2.495368	0.784868	C	2.513309	1.045591	1.633696
H	-1.078477	2.052105	-1.198915	C	3.612420	1.835685	1.166001
H	-1.049731	-3.207862	-6.954831	C	4.046802	1.786350	-0.201307
H	5.566787	4.322017	3.705546	C	5.143056	2.636580	-0.579560
H	2.673462	-2.398177	-3.564799	C	5.729403	3.465344	0.363169
H	4.116489	-2.624784	-2.538832	C	5.311954	3.515141	1.716939
H	3.462291	-4.014226	-3.482316	C	4.266532	2.687707	2.090187
H	-0.443350	3.614891	-2.005077	O	3.531872	1.019953	-1.118046
H	2.141993	4.258941	0.702295	C	5.973544	4.455873	2.693647
H	1.416901	4.920561	-0.789223	C	5.577379	2.608752	-2.017358
H	0.511681	5.006244	0.749480	O	2.415758	-1.400749	-1.209991
O	-2.202788	4.068608	-0.434102	C	1.867231	-2.555915	-0.995165
C	-2.647291	3.498087	0.617838	O	2.360118	-3.557418	-1.838456
O	-3.756186	4.201535	1.145353	C	3.206509	-3.108336	-2.918012
C	-4.313332	3.600779	2.323370	O	1.022359	-2.918128	-0.165235
O	-2.258018	2.465003	1.207572	C	-0.474693	2.948530	-1.149306
H	-5.158350	4.239171	2.612927	H	-1.991992	-1.983101	-3.817286
H	-4.665837	2.577722	2.124872	H	0.739567	-1.035155	-6.998165
H	-3.577345	3.556759	3.140020	H	2.736090	0.205240	-6.597763
83				H	2.494857	1.483994	-5.367363
1b'-cis-B1-SPO C1 dE=16.31 TS				H	3.403026	0.046722	-4.937995
C	1.215196	0.716792	1.559419	H	-1.695920	-1.195052	-1.682352
C	-0.174903	0.543552	1.229787	H	-0.967184	0.869971	0.635226
C	-1.174096	0.824548	2.199408	H	-1.444889	-2.143177	0.611821
C	-0.868307	1.272639	3.469659	H	-2.626054	-0.887504	0.144655
C	0.505345	1.442759	3.785583	H	-2.997149	-1.589893	2.514263
C	1.525581	1.180943	2.888546	H	-2.570834	0.128013	2.368282
C	-0.613758	0.103806	-0.055572	H	-0.661873	-2.147261	3.167090
N	0.148850	-0.144612	-1.079410	H	-1.316247	-0.911758	4.255053

H	-2.220807	0.683853	1.911732	Co	2.033290	0.067326	-1.097999
H	3.449788	2.063376	2.515459	O	1.916997	2.012839	-1.279037
H	3.527911	0.429568	3.149207	C	0.730323	2.781031	-1.580884
H	3.090224	1.773563	4.249771	C	0.373611	3.804858	-0.531340
H	2.459294	-1.749304	-4.449178	C	-1.938278	1.582660	4.487261
H	5.834541	-4.588202	-0.553793	C	2.974731	1.377346	3.231868
H	4.776404	-2.796281	-4.319789	O	2.213357	0.494649	0.761310
H	4.669539	-4.038456	1.461981	C	-0.416825	-0.610640	-2.365546
H	2.912067	-3.872411	1.180614	C	0.577750	-0.157026	-3.459718
H	3.872222	-2.428124	1.462273	C	0.198290	-0.744500	-4.815873
H	-1.907029	2.639031	4.800063	C	-1.225875	-0.296004	-5.181065
H	-2.938792	1.386724	4.077421	C	-2.231065	-0.701999	-4.094537
H	6.597860	-4.369047	-4.255740	C	-1.834381	-0.151582	-2.713280
H	7.578716	-4.051512	-2.811933	N	1.867628	-0.538616	-2.889424
H	-1.824229	0.972693	5.398080	C	2.611381	-1.471336	-3.400152
H	6.637655	-5.549786	-2.925581	C	3.558556	-2.232524	-2.630380
H	-0.129168	2.180749	-1.892066	C	4.608171	-2.940494	-3.249099
H	1.737584	2.462685	-3.526707	C	5.446293	-3.777794	-2.523107
H	6.115021	-1.058741	-1.015020	C	5.182200	-3.934555	-1.142906
H	7.548979	0.023002	-1.130684	C	4.147866	-3.276499	-0.488632
H	6.146093	0.470763	-0.093375	C	3.316853	-2.377007	-1.224651
H	2.416257	3.855416	-2.504118	O	2.346760	-1.760780	-0.589845
H	1.259896	4.387062	-0.246258	C	3.896572	-3.419548	0.986483
H	-0.386384	4.490330	-0.932692	C	6.622827	-4.474367	-3.162559
H	-0.025302	3.306791	0.363512	O	3.946474	0.296259	-1.212837
O	0.548172	4.543842	-3.826879	C	4.541549	0.769591	-2.271165
C	-0.508301	3.985549	-4.254357	O	5.940515	0.684747	-2.179343
O	-1.409710	4.934160	-4.807301	C	6.456130	-0.013630	-1.029551
C	-2.610034	4.356858	-5.335750	O	4.087476	1.254040	-3.307248
O	-0.849459	2.776309	-4.250070	C	1.653183	3.100942	-2.659578
H	-3.209107	5.198123	-5.709694	H	-0.378805	-1.716897	-2.343947
H	-2.394200	3.657480	-6.158401	H	0.519061	0.938693	-3.532862
H	-3.171486	3.810300	-4.562579	H	0.249097	-1.847204	-4.774335
83				H	0.914113	-0.406590	-5.580152
1b'-cis-B2-SPO C1 dE=16.56 TS				H	-1.236485	0.799099	-5.286802
C	2.750815	0.625578	1.418286	H	-1.516595	-0.735505	-6.147773
C	1.660388	1.537634	1.632934	H	-2.296669	-1.803814	-4.040390
C	1.433266	2.081517	2.926550	H	-3.235722	-0.336727	-4.355326
C	2.220479	1.749453	4.010588	H	-1.860391	0.949225	-2.737187
C	3.280778	0.832140	3.788811	H	-2.556313	-0.499730	-1.959430
C	3.563256	0.274472	2.553305	H	-1.697995	-0.010543	-0.176737
C	0.799273	1.965414	0.581212	H	0.773339	1.804892	4.783904

H	3.910445	0.543272	4.636685	N	0.828840	1.545794	-0.650003
H	0.602444	2.783112	3.051132	Co	2.016773	0.222588	-1.292557
H	4.288826	-1.657156	1.960616	O	3.081806	1.642380	-2.144540
H	5.192318	-0.911378	3.305420	C	3.268550	2.820625	-1.626038
H	5.431515	-0.368410	1.626484	O	3.752584	2.770015	-0.331663
H	-0.382870	-0.674280	-4.173252	C	3.864070	4.042779	0.323443
H	0.328399	-5.635520	-1.101058	C	1.975125	2.322835	5.384578
H	-0.204787	-3.126832	-4.553627	C	4.679740	-0.706401	2.356320
H	1.015021	-4.746685	0.995246	O	3.068008	0.093693	0.273089
H	0.316443	-3.131933	1.322495	C	-0.116012	2.059447	-1.664917
H	2.011384	-3.261714	0.884605	C	0.428988	1.615263	-3.043170
H	1.784077	1.530171	6.125982	C	-0.588768	1.897081	-4.139777
H	2.842677	2.898183	5.745754	C	-0.845380	3.414479	-4.172647
H	0.589324	-6.416110	-3.840668	C	-1.314168	3.942255	-2.807137
H	-1.099014	-6.349530	-3.307430	C	-0.342098	3.573971	-1.672691
H	1.105482	2.994762	5.382288	N	0.861648	0.242486	-2.806404
H	-0.595388	-5.482116	-4.776540	C	0.284138	-0.803724	-3.310377
H	3.862906	-1.945419	-0.415925	C	0.396066	-2.118359	-2.740701
H	4.996294	0.000236	-1.428950	C	0.042699	-3.258486	-3.496053
H	2.897646	4.567759	0.325344	C	0.024888	-4.527705	-2.937594
H	4.170226	3.814450	1.350571	C	0.334185	-4.642102	-1.561379
H	4.610719	4.678527	-0.171401	C	0.665076	-3.554312	-0.765974
H	5.216022	-0.935304	-3.037642	C	0.722899	-2.248999	-1.350758
H	4.997632	-3.858218	-1.679207	O	1.031522	-1.244223	-0.564974
H	3.208449	-3.941967	-1.860148	C	1.018856	-3.692697	0.687619
H	4.220911	-3.296726	-3.186885	C	-0.288465	-5.755153	-3.757429
O	6.922431	-1.431425	-1.659807	O	3.186566	-1.029719	-2.220618
C	7.099257	-1.733959	-0.447150	C	4.041487	-1.988075	-1.493584
O	6.920571	-3.166503	-0.230802	C	4.110183	-3.360803	-2.096389
C	7.090551	-3.569493	1.129605	C	4.806686	-0.875358	-2.037719
O	7.374635	-1.041671	0.553100	O	3.069816	3.903580	-2.198980
H	6.924812	-4.657493	1.154153	H	-1.081003	1.536392	-1.512722
H	8.102839	-3.339424	1.499047	H	1.345914	2.193417	-3.232985
H	6.371138	-3.069887	1.797233	H	-1.533074	1.358302	-3.945078
82				H	-0.204515	1.552431	-5.111961
1a'-trans-RPO C2 dE=5.26 TS				H	0.090131	3.923906	-4.453848
C	4.304088	0.428174	-0.276256	H	-1.589894	3.655513	-4.946836
C	4.033558	0.201548	1.117412	H	-2.310860	3.523516	-2.581667
C	5.016901	0.505600	2.092245	H	-1.434273	5.035314	-2.849109
C	6.247493	1.042452	1.757033	H	0.633310	4.064273	-1.819527
C	6.505902	1.266061	0.380416	H	-0.751929	3.915797	-0.710643
C	5.592011	0.974220	-0.618377	H	0.051690	2.724309	0.848731

H	-0.924862	-3.112837	2.672353	C	2.798350	-0.371429	1.557444
H	-1.109494	-2.193042	4.175108	N	1.753039	-0.560303	0.810780
H	1.198086	-1.980686	3.218618	C	0.531030	-1.217884	1.295117
H	0.382223	-0.396312	3.292623	C	-0.631652	-0.406585	0.713636
H	0.497643	-2.202096	0.799128	C	-1.959917	-1.124328	0.954445
H	4.776715	0.314876	3.143248	C	-2.147609	-1.334229	2.466500
H	7.469925	1.698131	0.090219	C	-0.966379	-2.091605	3.088070
H	6.850905	1.706575	-2.210159	C	0.370303	-1.385043	2.804208
H	5.085767	1.861045	-2.507746	N	-0.277814	-0.107916	-0.689459
H	5.847996	0.287770	-2.645959	Co	1.581623	-0.003872	-0.983910
H	2.740978	-0.661512	2.613586	O	1.796383	-1.804136	-1.671003
H	-3.199898	3.008446	-5.994496	C	0.954123	-2.796729	-1.719455
H	-3.200428	1.397783	-6.733850	O	-0.136452	-2.930562	-1.129672
H	8.234317	0.873256	2.623849	C	7.278564	1.392646	2.802104
H	7.496874	2.473470	2.812486	C	5.872013	1.226868	-2.072581
H	1.211287	1.845322	1.497528	O	3.487948	0.158238	-1.249265
H	2.109854	3.292833	0.894338	C	-1.188491	0.196000	-1.561841
H	-0.694875	2.292956	0.012395	C	-0.957382	0.679148	-2.889059
H	-0.786751	4.731429	-0.767538	C	0.363686	0.862494	-3.419017
H	1.000240	4.736318	-0.896064	C	0.478624	1.420688	-4.741154
H	0.016586	3.702598	-1.977707	C	-0.662121	1.745984	-5.455387
H	-4.109366	1.685230	-5.234587	C	-1.971595	1.552356	-4.948009
H	6.929695	1.115965	3.806859	C	-2.086881	1.021459	-3.675265
H	1.002326	-3.717983	-3.657551	O	1.468960	0.571938	-2.802263
H	2.534443	-3.887289	-2.768084	C	-3.180617	1.929441	-5.768655
H	1.093391	-4.878232	-2.308638	C	1.863236	1.641384	-5.280756
O	-0.850818	4.111303	1.650860	O	1.660145	1.894869	-0.601571
C	-1.257299	3.318193	2.567495	C	0.129153	2.999982	0.024630
O	-1.880448	4.038609	3.612657	C	0.100096	4.113257	-0.960882
C	-2.381408	3.205503	4.668525	C	1.365223	2.519819	0.647342
O	-1.182486	2.073372	2.653679	C	1.442863	-3.901536	-2.666130
H	-2.821111	3.890291	5.405344	H	-3.079599	0.865320	-3.241587
H	-3.148483	2.507981	4.299327	H	-0.541671	2.176140	-6.455537
H	-1.576935	2.616139	5.132847	H	2.418407	0.692899	-5.335171
82				H	1.830750	2.100558	-6.278307
1a'-cis-B1-RPO C2 dE=19.09 TS				H	2.442316	2.285067	-4.601747
C	1.916754	-2.791672	-1.874783	H	-2.238832	0.105394	-1.260942
C	0.752102	-2.845023	-2.710526	H	-0.666641	0.559022	1.252237
C	0.481435	-3.996970	-3.482018	H	-1.947522	-2.079876	0.408367
C	1.330236	-5.094118	-3.478652	H	-2.798404	-0.522347	0.575483
C	2.471311	-5.035680	-2.642469	H	-3.085937	-1.879853	2.652583
C	2.773558	-3.939369	-1.847079	H	-2.237358	-0.347670	2.948937

H	6.672839	0.571620	2.144811	C	-0.214586	-1.787182	-2.618712
H	2.593016	0.491993	3.493071	N	0.071077	-0.600649	-2.184991
H	7.226804	0.556480	-0.167998	C	-0.913910	0.329743	-1.654847
H	6.080644	1.637088	-1.018850	C	-0.591445	0.364086	-0.142417
H	5.996610	-0.107801	-1.297709	C	-1.347070	1.520605	0.514680
H	-1.256120	-2.018545	-2.876162	C	-2.857081	1.346330	0.273997
H	3.154949	-5.891209	-2.625242	C	-3.200146	1.190881	-1.217353
H	-0.419132	-4.007525	-4.103293	C	-2.395680	0.058113	-1.880107
H	3.714198	-3.775131	0.089140	N	0.877418	0.386143	-0.021508
H	4.592021	-2.990867	-1.211855	Co	1.789366	-0.008837	-1.642719
H	4.609248	-4.782366	-1.088049	O	2.646972	-0.422819	-3.311392
H	5.800368	-0.386634	4.635493	C	2.072419	-0.259328	-4.480613
H	5.786014	1.385662	4.651249	O	0.988278	0.289641	-4.731907
H	1.013667	-7.229469	-3.728547	C	1.064223	-6.309739	-4.333242
H	0.112554	-6.211002	-4.873712	C	3.992825	-3.880783	-0.970312
H	4.332832	0.482873	5.135162	O	2.216907	-1.787838	-1.089056
H	1.858111	-6.460323	-5.082740	C	1.464814	0.502528	1.133441
H	3.381720	2.036992	-2.994668	C	2.873595	0.486936	1.347512
H	2.077516	3.062391	-3.791640	C	3.816677	0.501843	0.262305
H	2.846661	2.889835	-0.761344	C	5.213528	0.554997	0.595101
H	1.643887	5.201905	-1.219500	C	5.601480	0.541262	1.920998
H	0.459620	4.291458	-2.209334	C	4.682026	0.507229	3.001803
H	0.577642	4.000287	-0.445596	C	3.337981	0.498905	2.690872
H	2.693530	-1.969766	-5.616975	O	3.508973	0.492813	-1.005807
H	2.633900	-0.454314	-6.565472	C	5.174278	0.496834	4.428134
H	3.982189	-0.768193	-5.405661	C	6.195689	0.656231	-0.533010
O	3.877504	4.807654	-1.777737	O	1.403447	1.822127	-2.203116
C	4.765162	4.499694	-0.928871	C	2.210274	3.205711	-1.586625
O	5.982089	5.231983	-1.138195	C	1.148655	4.232577	-1.356171
C	7.012507	4.904640	-0.199768	C	2.443465	2.582665	-2.878552
O	4.733758	3.683443	0.021691	C	2.909189	-0.890768	-5.598419
H	7.877816	5.528450	-0.467307	H	-0.950378	-0.593414	0.285668
H	6.702454	5.115952	0.835925	H	-0.655320	1.312262	-2.076831
H	7.288887	3.839824	-0.254111	H	-2.682330	-0.912332	-1.439043
82				H	-2.611046	0.010635	-2.957842
1a'-cis-B2-RPO C2 dE=17.05 TS				H	-2.976423	2.135414	-1.740310
C	2.244233	-2.463144	-1.781544	H	-4.279037	1.009723	-1.338127
C	2.466423	-1.922396	-3.089961	H	-3.203249	0.450186	0.817686
C	3.065856	-2.707144	-4.094043	H	-3.404541	2.201717	0.698070
C	3.478680	-4.011220	-3.851870	H	-0.990214	2.464958	0.074662
C	3.244399	-4.541913	-2.562662	H	-1.138227	1.564485	1.593687
C	2.638416	-3.816515	-1.543570	H	0.837265	0.620680	2.029045

H	1.552555	-0.775738	5.528921
H	-1.648149	0.547489	2.982400
H	3.748152	-1.780377	2.952690
H	3.710056	-1.255763	4.667334
H	4.177415	-0.126710	3.360589
H	1.708005	-0.381983	-4.436652
H	3.566731	-5.566663	-2.348235
H	3.228308	-2.256612	-5.077211
H	2.849429	-3.710647	0.590993
H	2.866468	-5.379489	-0.072457
H	1.345218	-4.450274	0.068202
H	-1.227427	-1.087948	6.030141
H	-0.704073	0.565122	6.395936
H	4.181606	-4.304240	-5.874163
H	5.225551	-5.034215	-4.638700
H	-2.089669	0.291922	5.317830
H	3.686715	-5.806523	-5.060890
H	4.742381	0.188334	0.815050
H	5.411776	-1.428427	0.219873
H	5.332851	1.324409	-1.225540
H	7.161471	-0.807271	-1.542547
H	5.901164	-1.334797	-2.691487
H	6.746949	0.198219	-2.976415
H	4.211319	4.013570	-0.777999
H	3.075439	5.018617	0.210851
H	4.054158	3.711197	0.963243
O	4.480170	0.791948	-3.005379
C	4.412714	2.043091	-3.185156
O	3.326751	2.402514	-4.061508
C	3.116905	3.816150	-4.164184
O	5.118463	2.960302	-2.714639
H	2.332602	3.956504	-4.922045
H	2.779513	4.242350	-3.205760
H	4.033341	4.341550	-4.468987

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1a'-trans-SPO C2 dE=8.61 TS

C	-2.356183	-1.033030	-3.553011
C	-1.304083	-0.490751	-2.773790
C	-0.230659	0.216106	-3.412811
C	-0.285926	0.359287	-4.842753
C	-1.337942	-0.197720	-5.551077
C	-2.394469	-0.911134	-4.931412

C	1.949655	-0.616138	-3.393912
N	1.684166	0.261880	-2.483947
C	0.736720	1.352354	-2.656797
C	-0.374992	0.990092	-1.648784
C	-1.395040	2.124865	-1.543230
C	-1.955817	2.453294	-2.938030
C	-0.845930	2.749415	-3.958512
C	0.158471	1.590182	-4.044155
N	0.315789	0.596958	-0.399383
Co	2.107228	0.073376	-0.655934
O	3.990136	-0.500530	-1.058076
C	5.275755	0.249655	-1.390646
C	6.346364	-0.459404	-2.197473
C	4.176354	-4.831142	-4.909851
C	2.418602	-4.380716	-0.167441
O	1.670801	-1.800724	-0.799455
C	-0.308082	0.586866	0.736784
C	0.243354	0.203642	2.000093
C	1.615292	-0.188379	2.151132
C	2.064561	-0.541351	3.470567
C	1.181119	-0.497872	4.536642
C	-0.174559	-0.109610	4.399329
C	-0.609581	0.235960	3.131716
O	2.487086	-0.245965	1.186551
C	-1.094882	-0.083502	5.595356
C	3.500854	-0.951550	3.632747
O	2.883257	1.823071	-0.439720
C	2.390841	3.012856	-0.227253
O	1.195491	3.366331	-0.270527
C	5.021339	-0.435337	-0.036314
C	3.503427	4.020339	0.063991
H	-0.865816	0.075828	-2.036253
H	1.216065	2.271052	-2.295825
H	-0.353224	0.681066	-4.406897
H	0.976296	1.821498	-4.739949
H	-0.309232	3.663847	-3.658044
H	-1.284213	2.945160	-4.949500
H	-2.555893	1.599747	-3.301308
H	-2.642597	3.310809	-2.863966
H	-0.878252	2.990731	-1.105229
H	-2.224858	1.847138	-0.875686
H	-1.354881	0.913681	0.751166

H	0.008522	-3.078605	3.060197	C	-1.366790	-0.656516	-1.352748
H	-0.230852	-2.115096	4.528455	N	-0.437356	-0.322251	-0.511146
H	1.840242	-1.435070	3.291743	Co	1.281545	0.287431	-1.006018
H	0.666485	-0.089895	3.387115	O	1.011741	2.169726	-0.615727
H	0.968843	-1.998335	0.981002	C	0.484444	2.984733	1.048429
H	4.545258	1.841690	2.731585	C	1.426013	4.125850	1.211189
H	6.268772	3.883284	-0.638171	O	0.777892	0.759103	-2.795921
H	5.445613	3.542875	-2.851717	C	0.834698	1.107093	-5.508613
H	3.753840	2.942447	-2.958678	C	-3.504095	-1.516158	-5.756436
H	5.084862	1.814292	-3.145873	C	-0.573910	-0.541375	0.940678
H	2.899109	0.220148	2.465925	C	0.811999	-1.002942	1.429782
H	-4.254160	-1.997260	-5.113601	C	0.852386	-1.085391	2.952987
H	-4.021193	-0.756802	-6.365021	C	-0.232636	-2.066814	3.428441
H	6.236167	4.808481	2.024131	C	-1.621138	-1.652930	2.923281
H	6.290365	3.424391	3.134865	C	-1.654813	-1.523414	1.391285
H	0.538275	2.154578	1.747697	N	1.773818	-0.108249	0.774316
H	-1.071313	2.026646	-0.142442	C	2.777331	0.429947	1.396486
H	-3.122077	-2.281461	-6.452044	C	3.731482	1.317510	0.800818
H	7.499367	3.579145	1.840884	C	3.786656	1.518214	-0.620001
H	2.743643	-3.281667	-3.111399	C	4.744641	2.467756	-1.117443
H	1.662639	-4.581705	-2.470180	C	5.568994	3.144760	-0.232224
H	1.042976	-3.360300	-3.617002	C	5.531886	2.940749	1.169590
H	-0.507511	3.614965	-0.798761	C	4.616889	2.020064	1.653986
H	1.302627	4.540978	2.219812	O	3.041542	0.897430	-1.487281
H	2.462135	3.772012	1.108081	C	6.435686	3.726179	2.088372
H	1.239673	4.913783	0.470447	C	4.768063	2.715596	-2.598991
O	-1.152818	3.776802	2.321378	O	1.798371	-1.425115	-1.747870
C	-1.582377	2.822347	3.046281	C	1.288844	-2.618781	-1.623175
O	-2.771999	3.182429	3.724386	C	1.730089	-3.530509	-2.774786
C	-3.315529	2.134496	4.538811	O	0.521338	-3.061106	-0.745275
O	-1.116637	1.671723	3.227714	C	-0.233787	2.731954	-0.201779
H	-4.210660	2.558057	5.014086	H	-3.153646	-1.573657	-3.033644
H	-3.595083	1.258411	3.933614	H	-1.345939	-0.085861	-6.640773
H	-2.599839	1.806002	5.307560	H	0.871342	2.150668	-5.160090
82				H	1.804881	0.667241	-5.234671
1a'-cis-B1-SPO C2 dE=19.27 TS				H	0.721715	1.098740	-6.601420
C	1.897451	1.966250	3.128912	H	-2.276701	-1.124195	-0.960858
C	1.902070	1.238531	1.909995	H	-0.778127	0.434745	1.414185
C	3.114535	0.617007	1.450959	H	-1.474445	-2.495429	0.904944
C	4.287918	0.766180	2.273811	H	-2.649099	-1.164798	1.083736
C	4.220319	1.493274	3.449154	H	-2.376814	-2.385510	3.248343
C	3.029142	2.112233	3.908914	H	-1.883164	-0.679334	3.365971

H	5.132588	1.599621	4.046004	C	0.671155	1.149370	1.188816
H	0.958026	2.430680	3.444689	N	0.508151	0.582858	0.030746
H	6.394682	0.346186	2.466720	Co	1.919641	-0.134598	-1.024131
H	5.803696	0.486130	0.776690	O	2.628544	1.653386	-1.400843
H	5.440686	-0.961428	1.698243	C	1.939700	3.236328	-1.263106
H	-0.435574	-1.508854	-3.725387	C	2.885018	3.990265	-0.383142
H	2.871456	-6.013821	-1.869114	O	3.242073	-0.072441	0.358785
H	0.792865	-3.517651	-4.692202	C	5.558569	0.129146	1.787891
H	3.524830	-3.428414	0.488326	C	3.018230	2.902346	5.194281
H	3.446080	-5.215999	0.312694	C	-0.812075	0.520283	-0.625674
H	2.090798	-4.293000	1.024720	C	-0.526590	0.619486	-2.144403
H	3.711009	3.758407	5.150346	C	-1.803537	0.413176	-2.954621
H	2.014670	3.297491	5.403916	C	-2.856006	1.450326	-2.534306
H	1.491902	-5.702722	-5.387774	C	-3.138806	1.366257	-1.028492
H	3.043354	-6.188355	-4.673906	C	-1.856844	1.550961	-0.198117
H	3.322588	2.285187	6.055130	N	0.549404	-0.358581	-2.323539
H	1.540146	-6.934759	-4.106639	C	0.376104	-1.460049	-2.990848
H	0.914152	3.087069	-0.942672	C	1.127226	-2.659641	-2.739425
H	1.565029	2.229106	-3.182443	C	1.665050	-2.847799	-1.423911
H	4.859033	-1.100868	-4.987055	C	2.280127	-4.101462	-1.120351
H	5.398091	-1.608164	-3.338931	C	2.362004	-5.074149	-2.108377
H	4.117593	-2.512322	-4.172267	C	1.838611	-4.897789	-3.410813
H	3.247276	2.885884	-3.008457	C	1.211878	-3.691264	-3.697032
H	3.887947	4.030035	-0.826938	O	1.581744	-1.944023	-0.474816
H	2.509588	5.011691	-0.251660	C	1.983990	-5.985522	-4.447202
H	2.952071	3.504467	0.600233	C	2.872671	-4.281034	0.249097
O	1.090783	5.077986	-2.166454	O	3.334334	-0.839112	-2.123391
C	-0.091279	4.847951	-2.542895	C	3.452521	-0.621929	-3.408862
O	-0.577947	5.838402	-3.442992	C	4.543147	-1.508743	-4.019762
C	-1.913390	5.603285	-3.904752	O	2.785076	0.142746	-4.124750
O	-0.864797	3.897919	-2.243525	C	2.340483	2.557507	-2.488381
H	-2.160773	6.450427	-4.559357	H	-1.199965	-0.501308	-0.448122
H	-1.984371	4.662323	-4.472699	H	-0.145533	1.632039	-2.341311
H	-2.628598	5.553051	-3.069216	H	-2.193070	-0.605715	-2.780573
82				H	-1.580087	0.502955	-4.028601
1a'-cis-B2-SPO C2 dE=16.14 TS				H	-2.479298	2.457439	-2.767339
C	0.609221	-0.004107	3.485621	H	-3.784083	1.287592	-3.104406
C	0.951858	0.076423	2.109375	H	-3.592399	0.387401	-0.788363
C	2.284501	0.448288	1.726169	H	-3.870991	2.135483	-0.739932
C	3.236742	0.714028	2.770992	H	-1.455578	2.561690	-0.370969
C	2.839992	0.608034	4.093972	H	-2.093663	1.440486	0.871159
C	1.524566	0.251234	4.487982	H	-0.198936	1.616650	1.666273

H	3.585467	0.807539	4.870684	C	-0.071927	-0.217094	1.157863
H	-0.417182	-0.283415	3.743987	N	0.067121	-0.242977	-0.132082
H	5.114860	0.262007	1.802834	Co	1.688735	0.098035	-1.033261
H	5.251983	1.286542	3.262794	O	1.361439	2.002999	-1.288282
H	4.653217	1.955132	1.719043	C	0.410293	2.797483	-0.884537
H	0.455981	-1.718275	-4.187440	C	0.885808	4.249688	-0.776726
H	5.134398	-4.761567	-2.395503	O	2.700069	0.574598	0.496234
H	2.369845	-2.954045	-5.151016	C	4.639097	1.073634	2.376693
H	3.621139	-3.438459	0.608518	C	1.157768	0.152972	5.948627
H	5.031785	-2.513700	0.072165	C	-1.050082	-0.605569	-1.027991
H	5.052241	-4.291096	-0.056695	C	-0.668554	-0.054351	-2.423613
H	1.322571	1.107648	6.474023	C	-1.670101	-0.496577	-3.483176
H	0.099713	-0.117809	6.071643	C	-3.063179	0.018840	-3.087122
H	5.488323	-4.542750	-5.168941	C	-3.470288	-0.498162	-1.699128
H	4.358002	-5.859328	-4.811661	C	-2.443492	-0.126890	-0.615858
H	1.761234	-0.608918	6.468180	N	0.721352	-0.480177	-2.557443
H	3.909276	-4.595711	-5.980886	C	1.099883	-1.447916	-3.340153
H	4.828656	-0.405947	-0.918354	C	2.260063	-2.256431	-3.107441
H	3.996358	1.917512	-0.857646	C	2.782763	-2.363802	-1.774703
H	1.661400	4.470452	-1.520070	C	3.830993	-3.312395	-1.532096
H	0.036147	4.935311	-0.878913	C	4.313323	-4.065019	-2.592764
H	1.329204	4.385567	0.221012	C	3.819298	-3.955187	-3.916643
H	4.403368	2.173631	-2.638340	C	2.786251	-3.061851	-4.144952
H	5.090823	-1.459159	-3.242660	O	2.335292	-1.675575	-0.752576
H	5.200913	0.173036	-3.962306	C	4.421971	-4.780612	-5.026677
H	6.524541	-0.442127	-2.924690	C	4.414418	-3.401569	-0.150740
O	6.844766	0.850966	-0.991302	O	3.212962	0.456517	-2.219129
C	7.128021	0.149202	0.015949	C	4.807377	0.150346	-1.851870
O	8.243265	0.675945	0.748495	C	5.439267	-0.431916	-3.077060
C	8.580758	-0.081304	1.915287	C	4.190639	1.465600	-1.830681
O	6.590644	-0.900097	0.459082	O	-0.767213	2.506656	-0.594652
H	9.439027	0.431987	2.373107	H	-1.044037	-1.710083	-1.118402
H	7.744167	-0.119870	2.630297	H	-0.675161	1.040793	-2.336479
H	8.855215	-1.117978	1.663109	H	-1.692928	-1.597750	-3.558098
83				H	-1.374946	-0.105603	-4.469135
1b'-trans-RPO C2 dE=6.69 TS				H	-3.048341	1.120926	-3.074603
C	4.011339	1.188814	0.447722	H	-3.806662	-0.284899	-3.840332
C	3.415000	0.927976	1.728675	H	-3.577614	-1.596537	-1.745498
C	4.009420	1.438476	2.909142	H	-4.457282	-0.097469	-1.422169
C	5.154989	2.215313	2.881188	H	-2.388845	0.961482	-0.474155
C	5.734921	2.471822	1.613277	H	-2.742995	-0.582675	0.339635
C	5.209052	1.984987	0.427283	H	-1.063867	-0.433610	1.572945

H	-2.886139	-0.805491	1.882370	C	2.238159	0.121946	1.855317
H	-1.081420	-3.290190	2.034344	N	1.489837	-0.264907	0.868423
H	-1.811212	-2.450962	3.413199	C	0.323842	-1.142257	1.035108
H	0.589869	-1.806947	3.086029	C	-0.770647	-0.544722	0.141702
H	-0.486261	-0.397608	2.899889	C	-1.968480	-1.489954	0.053413
H	0.599755	-2.106802	0.576151	C	-2.502731	-1.753373	1.471038
H	3.528951	1.215058	3.866995	C	-1.410416	-2.302393	2.398578
H	6.635795	3.093010	1.563729	C	-0.193835	-1.362824	2.453111
H	5.075003	2.727283	-1.582767	N	-0.115988	-0.176960	-1.130166
H	6.154650	1.355361	-1.406587	Co	1.708093	0.264099	-0.929326
H	6.680763	2.960345	-0.811939	O	2.365387	-1.480815	-1.482756
H	1.953138	-0.176977	2.871461	C	1.723028	-2.577645	-1.734489
H	-2.809855	0.740384	-6.645175	O	0.617800	-2.983097	-1.353486
H	-1.984749	2.195926	-7.241713	C	5.764607	2.783788	4.139453
H	6.804497	2.446644	4.278869	C	5.823309	2.280829	-0.911572
H	5.782898	3.885796	4.120064	O	3.564074	0.738741	-0.687846
H	0.281915	1.996627	1.250110	C	-0.787289	-0.081657	-2.235944
H	1.111465	3.572836	0.910790	C	-0.294276	0.426012	-3.480054
H	-1.019202	2.124331	-0.829547	C	1.058863	0.873064	-3.646484
H	0.548108	4.774010	-1.266367	C	1.424342	1.426575	-4.923448
H	-0.019770	3.670357	-2.557690	C	0.485852	1.498021	-5.939337
H	-1.202552	4.597591	-1.601139	C	-0.848853	1.044857	-5.790422
H	-1.484525	0.596744	-7.819270	C	-1.206107	0.517743	-4.562167
H	5.192484	2.477389	5.026106	O	1.985295	0.825228	-2.735353
H	3.518632	-1.990683	-3.630671	C	-1.831233	1.149604	-6.931335
H	4.409789	-2.733305	-2.279025	C	2.834341	1.919195	-5.088398
H	4.067724	-3.705275	-3.757042	O	1.380295	2.138816	-0.599742
O	-2.097752	3.840945	0.525330	C	-0.364847	2.953568	-0.582461
C	-2.641869	2.999660	1.313538	C	-0.240391	4.069497	-1.557665
O	-3.779277	3.557681	1.946717	C	0.610084	2.696387	0.474960
C	-4.443273	2.656466	2.844228	O	2.447952	-3.449876	-2.557140
O	-2.324929	1.818736	1.584480	C	3.686053	-2.927707	-3.082696
H	-5.299268	3.213854	3.247368	H	-2.228853	0.163625	-4.401025
H	-4.794750	1.754106	2.321354	H	0.792524	1.929721	-6.898183
H	-3.779940	2.340944	3.663773	H	3.555835	1.108123	-4.908614
83				H	2.994765	2.329941	-6.094428
1b'-cis-B1-RPO C2 dE=17.09 TS				H	3.064181	2.692185	-4.339486
C	1.943330	-4.399914	-2.524972	H	-1.840637	-0.384644	-2.224778
C	1.749423	-3.102280	-2.002517	H	-1.118146	0.396174	0.609364
C	2.019817	-2.828139	-0.620006	H	-1.648609	-2.420469	-0.439665
C	2.486541	-3.909920	0.194127	H	-2.770938	-1.037212	-0.546758
C	2.683365	-5.159064	-0.376940	H	-3.347331	-2.458274	1.423928

H	-1.916564	2.136074	-1.150402	C	2.422575	-5.437805	-1.740160
H	-0.915678	1.446226	0.673680	C	1.142740	-2.080904	-2.806946
H	3.254702	2.160598	4.674159	N	1.215207	-0.820591	-2.519880
H	-0.649961	1.910060	2.902498	C	0.288874	0.186634	-3.012723
H	5.217776	1.568011	3.467765	C	-0.508587	0.580400	-1.747839
H	5.037373	2.185731	1.804385	C	-1.333168	1.837082	-2.032991
H	5.032990	0.438483	2.080674	C	-2.273105	1.572225	-3.222374
H	0.548191	-2.391682	-3.675409	C	-1.519162	1.071145	-4.465570
H	3.071704	-5.962248	0.258318	C	-0.653561	-0.163347	-4.156512
H	1.723191	-4.573031	-3.582768	N	0.468473	0.675211	-0.646731
H	3.221513	-4.499037	2.134186	Co	2.157231	-0.078259	-1.053800
H	1.880104	-3.315784	2.179572	O	3.885230	-0.832501	-1.479535
H	3.484355	-2.772699	1.713750	C	4.329499	-0.978838	-2.688061
H	-0.473386	2.657043	5.169979	O	3.815381	-0.732858	-3.784066
H	0.807775	1.835536	6.089242	O	1.814161	-1.669513	-0.042119
H	2.197103	-7.598331	-1.715222	C	2.788060	-3.620390	1.637203
H	2.320505	-6.888680	-3.341244	C	2.687740	-6.810540	-2.308416
H	1.040293	3.507976	5.548166	C	0.124915	1.126066	0.525383
H	3.765968	-7.040382	-2.322152	C	0.992657	1.280374	1.644787
H	4.379245	1.714610	-0.972758	C	0.432254	1.755045	2.860420
H	4.335604	2.561527	-2.590462	C	1.209871	2.038165	3.964128
H	2.301572	2.911560	-0.234086	C	2.614475	1.890421	3.828460
H	1.045119	4.293485	-1.814902	C	3.222863	1.453163	2.666248
H	2.597271	5.142038	-1.810560	C	2.410333	1.076471	1.542495
H	2.252369	3.962133	-3.112215	O	3.028872	0.616114	0.490231
H	6.290392	-0.776931	-4.465036	C	4.714614	1.400222	2.506301
H	7.239137	-2.101810	-3.695793	C	0.614795	2.533910	5.258319
H	5.662868	-2.445690	-4.496839	O	2.578192	1.506443	-2.104645
O	4.018960	4.472564	0.180040	C	2.746025	3.138729	-1.194923
C	3.214100	4.747700	1.130959	C	2.112364	4.184481	-2.045732
O	3.916763	5.175015	2.295369	C	3.764243	2.232003	-1.712633
C	3.053279	5.478639	3.398080	O	5.629135	-1.516206	-2.612978
O	1.966385	4.692342	1.174379	C	6.231120	-1.717809	-3.898124
H	3.714885	5.715515	4.243443	H	-1.191993	-0.262143	-1.521116
H	2.403485	6.341215	3.178797	H	0.907385	1.049728	-3.300934
H	2.411228	4.621015	3.645884	H	-1.299881	-1.013654	-3.877561
83				H	-0.075494	-0.462445	-5.043225
1b'-cis-B2-RPO C2 dE=15.02 TS				H	-0.866275	1.876463	-4.840956
C	1.748488	-3.607865	-4.138491	H	-2.232854	0.841277	-5.271493
C	1.514450	-2.582012	-3.196053	H	-3.019708	0.814821	-2.925709
C	1.968587	-2.727084	-1.843084	H	-2.834105	2.487119	-3.466187
C	2.659291	-3.931275	-1.492342	H	-0.641218	2.663551	-2.258898

H	-1.521504	2.513752	-1.226122	C	2.882252	-4.895588	-2.465933
H	-2.522099	1.454190	-0.203157	C	2.442931	-4.761061	-3.804581
H	-1.110618	0.585315	1.152651	C	0.687805	-1.458444	-3.537731
H	3.582933	0.413841	4.609494	N	0.664935	-0.355331	-2.856080
H	-0.525149	0.517266	3.348336	C	-0.449668	0.585952	-2.863786
H	5.036439	1.127979	1.507277	C	-1.052133	0.432314	-1.447301
H	5.004850	-0.616783	1.597456	C	-2.062602	1.554881	-1.197743
H	5.364671	0.328074	3.068822	C	-3.155223	1.513556	-2.280207
H	-0.009040	-1.573201	-4.378925	C	-2.569835	1.561302	-3.701096
H	3.436958	-5.795650	-2.181828	C	-1.532202	0.447063	-3.925872
H	1.380763	-3.470772	-5.159942	N	0.088218	0.362466	-0.510359
H	3.849313	-3.276924	0.177961	Co	1.760480	0.008605	-1.342349
H	3.654770	-5.049281	0.057750	O	3.312090	-0.301334	-2.434029
H	2.317024	-4.008918	0.636423	C	4.875688	0.654305	-1.894305
H	1.486702	1.378246	6.127797	C	5.394165	1.281939	-3.140769
H	-0.053806	0.603941	5.693576	O	1.747633	-1.849378	-0.891605
H	2.269021	-5.606617	-5.787533	C	3.148607	-4.084584	-0.079461
H	3.822973	-5.939553	-4.995223	C	2.739675	-5.836240	-4.821492
H	1.347016	-0.387146	6.153875	C	-0.088051	0.445078	0.775844
H	2.370637	-6.820642	-4.492093	C	0.939809	0.387312	1.762490
H	4.390825	-1.158874	-0.795232	C	0.545275	0.460632	3.125788
H	5.075720	-1.456572	-2.449461	C	1.461494	0.461627	4.158194
H	4.444758	1.290358	-1.127344	C	2.836417	0.405372	3.808335
H	5.785828	0.531342	-3.839288	C	3.288672	0.340799	2.501595
H	4.591147	1.851532	-3.628900	C	2.335282	0.314066	1.422675
H	6.198436	1.976695	-2.870053	O	2.811617	0.240242	0.214825
H	1.455450	4.892771	0.611619	C	4.748411	0.292181	2.161185
H	0.167724	3.712269	0.985860	C	1.038302	0.517790	5.605512
H	1.690387	3.692842	1.941067	O	1.867239	1.902012	-1.916375
O	6.786966	0.987890	-0.735280	C	1.384460	2.877141	-1.209558
C	7.192127	-0.019552	-0.067138	O	0.580522	3.738842	-1.602834
O	8.191647	0.377859	0.874395	C	4.523736	-0.762516	-1.803148
C	8.676823	-0.702034	1.679770	O	1.878667	2.903578	0.087091
O	6.861094	-1.220331	-0.112161	C	1.256212	3.866450	0.949871
H	9.435240	-0.265171	2.344570	H	-1.567411	-0.548616	-1.418638
H	7.870418	-1.153269	2.278647	H	-0.001613	1.589350	-2.923818
H	9.127077	-1.497141	1.065706	H	-2.020718	-0.541296	-3.859116
83				H	-1.090954	0.530837	-4.930892
1b'-trans-SPO C2 dE=5.37 TS				H	-2.080179	2.536068	-3.856439
C	-0.866091	-1.074661	-4.572554	H	-3.377194	1.482165	-4.445300
C	-0.126590	-0.483077	-3.518496	H	-3.745983	0.587262	-2.165531
C	1.095663	0.211122	-3.805452	H	-3.852990	2.351979	-2.133729

H	-1.555454	-2.224017	0.065535	C	1.511676	0.290987	-5.178813
H	-2.703514	-0.908663	-0.305310	C	0.746980	-0.309843	-6.165612
H	-3.212764	-1.900387	1.931522	C	-0.453548	-1.010031	-5.892437
H	-2.760895	-0.180960	2.038622	C	-0.660575	-0.571268	-2.191372
H	-0.918691	-2.562874	2.645060	N	-0.074449	-0.154110	-1.111033
H	-1.634978	-1.464273	3.837922	Co	1.719524	0.439404	-1.040571
H	0.745635	-0.872338	3.328605	O	1.356600	2.348275	-0.900361
H	-0.366677	0.455979	2.880690	C	0.385063	3.230010	0.248419
H	0.714312	-1.674055	0.924166	C	1.213271	4.405542	0.651141
H	3.573138	2.315811	3.437531	O	1.851626	0.792608	-2.918559
H	6.384028	4.067585	0.696173	C	2.786445	1.028397	-5.478392
H	6.349520	3.537786	-1.626553	C	-1.233715	-1.662104	-7.007527
H	4.779849	2.927481	-2.254711	C	-0.700771	-0.253018	0.219901
H	6.065337	1.790050	-1.886819	C	0.426755	-0.643023	1.194057
H	2.069031	0.679525	2.764691	C	-0.059565	-0.574473	2.638967
H	-2.157773	-2.118962	-6.627254	C	-1.256975	-1.525030	2.805611
H	-1.514022	-0.935199	-7.786737	C	-2.379624	-1.189618	1.815317
H	6.699022	3.979714	3.458272	C	-1.880801	-1.212999	0.359884
H	5.482057	5.217805	3.101818	N	1.573072	0.198037	0.828552
H	0.072177	2.508544	0.997198	C	2.322449	0.792358	1.704088
H	-0.749762	2.214783	-1.321841	C	3.445809	1.627108	1.394985
H	-0.648356	-2.454883	-7.501210	C	3.980317	1.707605	0.066168
H	5.121929	3.936297	4.276885	C	5.074607	2.611311	-0.153916
H	2.739913	-2.079360	-3.898107	C	5.569397	3.364300	0.899849
H	4.129375	-2.429451	-2.831783	C	5.056309	3.281811	2.217392
H	3.511349	-3.704832	-3.945163	C	4.008417	2.402837	2.437215
H	0.086739	3.740874	-1.876392	O	3.550364	1.013941	-0.950641
H	2.099329	4.073665	1.208652	C	5.618709	4.145973	3.319538
H	1.541021	4.977591	-0.225832	C	5.605085	2.733114	-1.554070
H	0.604857	5.051118	1.296748	O	2.387907	-1.335637	-1.450549
O	-1.590587	4.155319	0.838515	C	1.812926	-2.498002	-1.391633
C	-2.280627	3.282197	1.436689	O	2.332492	-3.406781	-2.318657
O	-3.633823	3.683546	1.609819	C	3.235169	-2.858850	-3.302858
C	-4.452550	2.710412	2.271661	O	0.923950	-2.934253	-0.650095
O	-1.944632	2.149657	1.877971	C	0.055030	2.931103	-1.137971
H	-5.449771	3.163238	2.358120	H	-1.789278	-1.603624	-4.317936
H	-4.517780	1.776065	1.692538	H	1.093737	-0.242279	-7.202332
H	-4.063329	2.465250	3.271368	H	3.047116	0.950322	-6.542563
83				H	2.695823	2.092427	-5.210364
1b'-cis-B1-SPO C2 dE=17.80 TS				H	3.612223	0.636326	-4.866734
C	2.092293	0.561280	1.556899	H	-1.648364	-1.035511	-2.096429
C	0.709314	0.178493	1.643011	H	-1.045922	0.757264	0.505739

H	-2.182248	-2.898709	-2.892958	C	-0.013055	0.391216	2.845801
H	-3.596750	-1.867910	-2.626706	C	0.562441	0.971056	3.961078
H	-2.230404	-0.232626	-1.358124	C	1.929505	1.338681	3.869778
H	-2.075662	-1.867083	-0.645317	C	2.689770	1.147353	2.728884
H	-1.017006	-0.740275	0.749685	C	0.009100	-0.411862	0.546370
H	2.405809	1.809494	4.736578	N	0.477183	-0.566723	-0.655960
H	-1.067450	0.098746	2.870188	Co	2.138482	0.132178	-1.245396
H	4.274550	2.238993	1.777623	O	1.530456	1.957759	-0.994009
H	4.780233	0.698000	2.449052	C	-0.188401	2.696230	-0.868232
H	4.456356	2.067462	3.556059	C	-0.145533	3.487879	0.393816
H	1.763838	-1.167237	-4.837692	C	-0.223179	1.225189	5.224084
H	6.880725	-3.241626	-2.817991	C	4.129277	1.565848	2.635350
H	4.148262	-1.498605	-5.648448	O	2.848044	0.416358	0.510890
H	6.428811	-3.211136	-0.466984	C	-0.326136	-1.173005	-1.734064
H	4.709805	-3.574825	-0.139056	C	0.017696	-0.361537	-3.008218
H	5.291499	-1.930840	0.078519	C	-0.638971	-0.976535	-4.241622
H	-0.245022	2.297166	5.478099	C	-2.159637	-1.052073	-4.037391
H	-1.263296	0.889155	5.113286	C	-2.506206	-1.849129	-2.772993
H	6.194631	-2.439313	-6.461302	C	-1.838141	-1.248019	-1.524037
H	7.539369	-2.098008	-5.354922	N	1.482728	-0.335446	-2.970329
H	0.210144	0.696936	6.088750	C	2.205209	-0.951068	-3.858222
H	6.914826	-3.751111	-5.500412	C	3.516556	-1.470862	-3.585307
H	-0.840888	1.830338	-0.930951	C	4.413265	-1.784178	-4.626573
H	0.609422	2.368491	-2.887112	C	5.627699	-2.409766	-4.375876
H	6.145562	0.147117	-2.677869	C	5.922446	-2.758484	-3.036868
H	7.180624	1.587813	-2.981880	C	5.063706	-2.493350	-1.977091
H	6.161269	1.488910	-1.499289	C	3.829821	-1.817111	-2.228628
H	1.329868	3.778385	-2.033916	O	3.028003	-1.577928	-1.217707
H	0.595553	4.294195	0.334109	C	5.403522	-2.825520	-0.551053
H	-1.138188	3.922626	0.566133	C	6.618216	-2.690330	-5.479355
H	0.101796	2.836902	1.244054	O	3.801267	0.877209	-1.906610
O	-1.868706	3.833073	-1.769658	C	3.880545	1.623648	-2.968725
C	-2.536893	3.042614	-2.503233	O	5.206037	1.912584	-3.328364
O	-3.494069	3.735808	-3.286159	C	6.225873	1.237728	-2.566919
C	-4.268813	2.889915	-4.145637	O	3.001623	2.098261	-3.689469
O	-2.467055	1.792819	-2.617541	C	0.831185	2.808018	-1.911334
H	-4.979406	3.552337	-4.657844	H	0.080816	-2.189758	-1.892490
H	-3.634891	2.380227	-4.887664	H	-0.378120	0.654635	-2.867295
H	-4.814157	2.122856	-3.574886	H	-0.233879	-1.990037	-4.410202
83				H	-0.398714	-0.372926	-5.129928
1b'-cis-B2-SPO C2 dE=15.70 TS				H	-2.558645	-0.032146	-3.933022
C	2.190722	-0.157242	1.623174	H	-2.628405	-1.515811	-4.919561

H	-3.466925	2.463499	-3.822832	C	0.791934	-0.395341	1.850390
H	-3.763741	0.787221	-2.024615	C	0.359248	-0.936617	3.092595
H	-4.102348	2.402078	-1.389353	C	1.246804	-1.244476	4.103619
H	-1.828166	2.497122	-0.331269	C	2.623178	-0.978312	3.871597
H	-2.703160	1.038008	0.192151	C	3.111444	-0.445041	2.691176
H	-1.246124	-0.199648	1.201809	C	-0.202725	-0.060049	0.887732
H	3.341875	-1.204011	4.666089	N	0.014653	0.402825	-0.309945
H	-0.711907	-1.110635	3.234973	Co	1.730231	0.567686	-1.077497
H	4.980048	-0.683716	1.598660	O	1.628491	2.528071	-0.921537
H	5.158155	-0.431353	3.357593	C	1.007663	3.123789	0.053380
H	4.717677	0.917207	2.275751	O	1.414775	2.688689	1.306234
H	0.260433	-0.018631	-4.593494	C	0.639813	3.198709	2.401780
H	3.922050	-4.511799	-3.696166	C	0.793500	-1.841630	5.413061
H	1.882152	-1.412045	-5.869927	C	4.566936	-0.155338	2.475144
H	3.833753	-4.635853	-1.319708	O	2.692910	0.324721	0.525198
H	2.602560	-3.667168	-0.447327	C	-1.095546	0.694594	-1.238862
H	4.216211	-3.004234	-0.719381	C	-0.478155	1.415060	-2.461535
H	1.219260	-2.846338	5.567873	C	-1.509885	1.540828	-3.575416
H	1.106878	-1.224978	6.270654	C	-2.693492	2.370297	-3.045152
H	4.510293	-3.625502	-6.333613	C	-3.297752	1.756086	-1.771922
H	3.121585	-4.724623	-6.298448	C	-2.242553	1.536009	-0.674243
H	-0.301057	-1.934185	5.447496	N	0.747412	0.658919	-2.706821
H	2.985595	-3.145272	-7.106715	C	0.910321	-0.141561	-3.716582
H	4.243221	-0.850046	-1.039835	C	1.820959	-1.251258	-3.715117
H	4.363499	1.479693	-0.219942	C	2.194306	-1.873771	-4.928531
H	-0.427472	2.971529	2.264364	C	2.954786	-3.031908	-4.947093
H	1.020024	2.683751	3.291587	C	3.316271	-3.600334	-3.701466
H	0.757362	4.286784	2.501485	C	2.970524	-3.041388	-2.479640
H	5.184505	2.022973	-1.787045	C	2.214587	-1.824231	-2.461458
H	6.479413	-0.589966	-2.668516	O	1.892893	-1.322797	-1.291388
H	5.054396	-1.440237	-3.355006	C	3.426895	-3.626688	-1.172157
H	5.307152	0.295902	-3.697344	C	3.413394	-3.664379	-6.237956
O	6.132657	-1.193891	-0.260287	O	3.411681	0.876902	-2.058624
C	7.325776	-0.791131	-0.147333	C	4.669565	-0.115432	-1.702053
O	7.791320	-0.888729	1.215744	C	5.417191	-0.492771	-2.939492
C	9.128251	-0.422558	1.408548	C	4.584174	1.271746	-1.266057
O	8.117044	-0.331458	-1.002154	O	0.147546	4.010647	-0.066092
H	9.351476	-0.564159	2.476519	H	-1.488938	-0.276163	-1.600936
H	9.850471	-0.988663	0.798529	H	-0.163042	2.416711	-2.133062
H	9.230510	0.642962	1.146077	H	-1.862326	0.543319	-3.892077
82				H	-1.064118	2.028838	-4.455720
1a'-trans-RPO C1, C2 dE=0.00 pre-reactive				H	-2.337560	3.388323	-2.819847

H	-2.257777	0.925230	-0.559059	C	4.272086	-0.240616	-0.714471
H	-0.241333	1.011628	1.595028	C	4.196042	-0.482408	0.699351
H	-2.194165	-1.279217	1.107289	C	5.380093	-0.510916	1.478961
H	-2.607315	0.448637	1.338361	C	6.632210	-0.298897	0.928923
H	-2.845422	-0.804633	3.494646	C	6.696693	-0.056486	-0.466767
H	-1.640745	0.496358	3.566793	C	5.577842	-0.027265	-1.281935
H	-1.042103	-2.499948	3.223287	C	2.949175	-0.737323	1.355894
H	-0.752661	-1.541418	4.684178	N	1.774260	-0.652380	0.809574
H	1.338630	-1.877846	3.347616	C	0.535061	-1.000861	1.525052
H	0.924829	-0.148039	3.476211	C	-0.497153	0.050056	1.108971
H	0.199271	-1.957214	1.091549	C	-1.891163	-0.341223	1.598182
H	5.284828	-0.705150	2.552011	C	-1.855919	-0.490890	3.128264
H	7.675963	0.120553	-0.924823	C	-0.784321	-1.489608	3.584428
H	6.691817	0.439465	-3.069516	C	0.606607	-1.112340	3.045507
H	5.018902	1.091887	-3.031014	N	-0.335733	0.253245	-0.343455
H	5.269161	-0.617592	-3.331835	Co	1.430930	-0.028228	-0.941548
H	3.007040	-1.026310	2.412395	O	1.150746	-1.756620	-1.678398
H	-3.538220	3.635557	-5.333157	C	0.151095	-2.587860	-1.522535
H	-3.943552	2.007652	-5.904473	O	-0.781813	-2.553756	-0.704706
H	8.587867	-1.103598	1.429557	C	7.888416	-0.320317	1.764970
H	8.429264	0.638583	1.712089	C	5.657351	0.238202	-2.758594
H	1.669679	2.039951	1.652746	O	3.256660	-0.210537	-1.524637
H	3.021969	3.085977	0.915152	C	-1.301958	0.741700	-1.055199
H	0.056551	2.747180	-0.027795	C	-1.217968	1.123868	-2.433473
H	0.833507	5.066279	-0.721353	C	0.008978	1.078070	-3.167247
H	2.401146	4.390708	-1.270117	C	-0.008976	1.527947	-4.530559
H	0.884345	3.977824	-2.125998	C	-1.191216	1.994406	-5.085218
H	-4.508790	2.554813	-4.311746	C	-2.408975	2.052270	-4.366331
H	7.654642	-0.512510	2.821327	C	-2.392534	1.616056	-3.051954
H	-0.399422	-3.429072	-3.415122	O	1.159383	0.689378	-2.685537
H	1.248094	-3.877521	-2.911353	C	-3.663167	2.588790	-5.011575
H	-0.189558	-4.637676	-2.122702	C	1.282116	1.488418	-5.298154
O	-1.784797	2.931022	0.924375	O	2.001672	1.858487	-0.496572
C	-1.501791	3.086059	2.138858	C	1.101824	3.015621	-0.229623
O	-2.535034	3.771452	2.862261	C	1.330691	4.180484	-1.142586
C	-2.257187	3.952091	4.254041	C	2.065648	2.573033	0.788918
O	-0.484516	2.730045	2.798172	C	0.223795	-3.718820	-2.556471
H	-3.106262	4.517473	4.664229	H	-3.304603	1.661100	-2.450932
H	-2.165789	2.988390	4.780808	H	-1.174156	2.338023	-6.125215
H	-1.322415	4.511022	4.413956	H	1.690635	0.467193	-5.322258
82				H	1.140097	1.847533	-6.326529
1a'-cis-B1-RPO C1 dE=9.31 pre-reactive				H	2.049392	2.103905	-4.804958

H	-2.944111	2.415121	-3.665123	C	1.909157	-2.518789	-1.584278
H	-3.323433	1.439235	-1.404705	C	1.501279	-2.186977	-2.915038
H	-3.239057	3.206608	-1.292895	C	1.696198	-3.101566	-3.967901
H	-0.884955	3.107788	-0.509483	C	2.309824	-4.331729	-3.759163
H	-1.931259	2.089869	0.529365	C	2.703021	-4.651324	-2.440494
H	-0.620924	1.024962	1.765754	C	2.514183	-3.791986	-1.363564
H	3.937338	-0.507259	5.093687	C	0.800265	-0.946175	-3.130438
H	-0.055896	0.583256	3.936448	N	0.914691	0.067998	-2.337691
H	5.648616	-0.851923	3.483570	C	-0.061708	1.154631	-2.256096
H	5.541207	0.338383	2.154461	C	-0.646071	0.983053	-0.836828
H	5.091394	-1.330278	1.845771	C	-1.506106	2.194428	-0.481265
H	0.100712	-0.879915	-3.971815	C	-2.644656	2.306633	-1.511751
H	3.198291	-5.610599	-2.256478	C	-2.107808	2.379844	-2.949114
H	1.377426	-2.815214	-4.974112	C	-1.187722	1.191656	-3.282872
H	2.122689	-4.215708	0.720009	N	0.486590	0.671196	0.069802
H	3.593314	-3.300979	0.420117	Co	2.066888	0.114501	-0.830752
H	3.547368	-5.058060	0.045597	O	3.644956	-0.440844	-1.772251
H	1.621583	-1.003338	6.584675	C	3.930479	-0.073642	-3.001460
H	2.041023	0.710100	6.752518	O	3.395473	0.819672	-3.669765
H	2.136466	-6.278764	-4.709322	C	2.577481	-5.287064	-4.896854
H	2.158724	-4.904958	-5.838074	C	2.974091	-4.121314	0.028931
H	0.399332	0.244240	6.259048	O	1.717271	-1.729393	-0.544961
H	3.658023	-5.437995	-5.051483	C	0.348282	0.709235	1.357534
H	1.852993	3.799989	0.031108	C	1.357198	0.367887	2.318577
H	2.898902	2.515597	0.925705	C	2.711397	0.072132	1.945651
H	3.449982	3.680193	-1.923232	C	3.639575	-0.236065	2.997652
H	5.613478	3.065057	-0.570871	C	3.210071	-0.254688	4.314760
H	4.874172	1.455217	-0.280063	C	1.876571	0.034153	4.694851
H	5.303734	1.965049	-1.938128	C	0.983184	0.347908	3.685733
H	4.642526	-1.929260	-3.812593	O	3.178886	0.093313	0.725499
H	5.446037	-0.479126	-4.496776	C	1.463275	-0.005156	6.145483
H	5.858536	-1.077853	-2.844418	C	5.059555	-0.540587	2.610471
O	0.443865	4.225555	-3.073956	O	2.371047	2.075527	-1.110611
C	0.782194	4.873404	-2.061756	C	3.570121	2.937708	-1.129583
O	1.964094	5.688986	-2.304200	C	4.921242	2.306219	-0.968941
C	2.345445	6.526180	-1.211582	C	2.614408	3.013847	-0.002510
O	0.299875	4.924936	-0.895005	C	5.056279	-0.936659	-3.580462
H	3.167660	7.157957	-1.579859	H	-1.273995	0.070071	-0.859205
H	1.510645	7.158007	-0.870929	H	0.481605	2.110811	-2.311431
H	2.699947	5.944874	-0.343143	H	-1.753564	0.241590	-3.267085
82				H	-0.763652	1.320315	-4.289557
1a'-cis-B1-RPO C2 dE=6.16 pre-reactive				H	-1.509451	3.298211	-3.062660

H	-1.487837	2.541574	-4.876425	C	1.791387	-3.023155	-1.752548
H	-2.525484	1.534204	-2.840876	C	1.747465	-2.687051	-3.143863
H	-2.334713	3.283606	-2.632264	C	1.923142	-3.685850	-4.123323
H	-0.274774	2.956632	-1.291286	C	2.168296	-5.008678	-3.779258
H	-1.643606	2.029733	-0.585133	C	2.207983	-5.330369	-2.403014
H	-0.299561	1.575570	0.903860	C	2.021681	-4.388634	-1.398497
H	3.527748	0.217337	5.098516	C	1.401352	-1.341739	-3.518204
H	0.074958	1.849134	3.125644	N	1.554781	-0.326495	-2.728985
H	5.129488	-1.087708	3.927989	C	0.775477	0.907149	-2.845074
H	5.378201	-0.520255	2.248517	C	-0.127436	0.834672	-1.588458
H	4.478935	-1.999935	2.527590	C	-0.959387	2.108464	-1.444582
H	0.929183	-1.182706	-4.493910	C	-1.776836	2.339946	-2.728125
H	2.411961	-6.365594	-2.109972	C	-0.878462	2.391232	-3.971588
H	1.889052	-3.394226	-5.176263	C	-0.056327	1.099454	-4.107541
H	1.135465	-4.565505	0.563437	N	0.777176	0.494456	-0.469010
H	2.822906	-4.074026	0.564111	Co	2.351664	-0.429908	-1.018435
H	2.395297	-5.782350	0.205147	O	3.983395	-1.335385	-1.565117
H	1.138965	0.934351	6.354279	C	4.520916	-1.438788	-2.756238
H	2.032845	2.417474	5.981052	O	4.335830	-0.710275	-3.746611
H	1.683733	-6.899644	-4.732441	C	2.403600	-6.071064	-4.825061
H	2.308255	-5.654368	-5.836933	C	2.100688	-4.733747	0.061896
H	0.340091	2.251612	5.468834	O	1.590977	-2.156770	-0.781955
H	3.411614	-6.507519	-4.738291	C	0.579591	0.944729	0.730145
H	4.305366	1.179640	-2.852285	C	1.413649	0.710770	1.871000
H	3.867656	2.957743	-2.332063	C	2.632217	-0.041759	1.799364
H	5.024562	0.674404	-0.506606	C	3.386430	-0.208211	3.012465
H	5.741269	2.986589	0.414067	C	2.929876	0.356914	4.191487
H	4.109081	3.599744	0.028518	C	1.732662	1.110174	4.272757
H	4.334947	2.365396	1.317464	C	1.003434	1.270237	3.108051
H	4.821632	-3.540259	-3.005628	O	3.124088	-0.580374	0.719530
H	6.137884	-2.539629	-3.692845	C	1.288265	1.708813	5.584658
H	6.000906	-2.796165	-1.908204	C	4.663714	-0.996128	2.937328
O	1.440489	3.869414	-2.365057	O	3.107606	1.403236	-1.075242
C	2.207349	4.836456	-2.611328	C	4.517943	1.624417	-0.689210
O	1.509155	5.937786	-3.229733	C	4.678659	2.712255	0.332128
C	2.346153	7.056134	-3.535475	C	4.093447	1.914595	-2.072641
O	3.439921	4.978834	-2.415421	C	5.450474	-2.650640	-2.846221
H	1.705841	7.788836	-4.048491	H	-0.792610	-0.039929	-1.728023
H	2.769133	7.509099	-2.623954	H	1.437787	1.778331	-2.715126
H	3.185476	6.769194	-4.187484	H	-0.732994	0.237458	-4.253103
82				H	0.608202	1.152962	-4.983380
1a'-cis-B2-RPO C1, C2 dE=3.58 pre-reactive				H	-0.188358	3.242896	-3.867723

H	-2.288411	2.098000	-4.322950	C	2.359493	-2.406750	-1.331424
H	-3.011524	0.947360	-2.256530	C	2.307711	-2.043182	-2.716358
H	-3.198352	2.692552	-2.045627	C	2.786484	-2.920150	-3.711940
H	-1.082531	2.801744	-0.705916	C	3.329314	-4.154146	-3.382933
H	-2.191772	1.587032	-0.031353	C	3.354398	-4.518232	-2.017262
H	-0.935481	0.876557	1.459724	C	2.883705	-3.693883	-1.001406
H	3.047075	0.072732	5.660235	C	1.639065	-0.828831	-3.095660
H	-0.744996	0.663965	3.724869	N	1.468218	0.154446	-2.264872
H	4.835129	-0.922478	2.805529	C	0.363950	1.107373	-2.360659
H	5.054768	-0.173965	4.418145	C	-0.462488	0.794619	-1.094683
H	5.081901	0.813917	2.926191	C	-1.567151	1.834816	-0.902975
H	1.237524	-0.746746	-4.110565	C	-2.450057	1.893616	-2.162271
H	3.783029	-5.486735	-1.737860	C	-1.628650	2.112097	-3.442299
H	2.765555	-2.564356	-4.744865	C	-0.525106	1.054703	-3.596634
H	3.411415	-3.289197	1.042166	N	0.501284	0.642149	0.018383
H	3.501520	-5.023384	0.580759	Co	2.235550	0.244866	-0.536557
H	1.931472	-4.220825	0.866893	O	4.070079	-0.305333	-1.156030
H	0.543418	-0.549660	6.758429	C	4.821922	0.345439	-2.271070
H	0.772043	1.206110	6.843419	C	5.498923	-0.608646	-3.203189
H	3.748676	-4.649957	-5.441244	C	3.904418	-5.067998	-4.438182
H	4.988828	-5.209859	-4.301190	C	2.941452	-4.087129	0.448503
H	-0.700761	0.538761	6.106372	O	1.926281	-1.641048	-0.345122
H	3.440865	-6.067535	-4.409590	C	0.123199	0.674776	1.257281
H	4.978162	1.461369	-0.362700	C	0.956801	0.490536	2.406668
H	6.068381	-0.051914	-0.468566	C	2.375424	0.302728	2.306685
H	4.259428	1.160014	-2.728448	C	3.117065	0.157104	3.528718
H	5.919087	-1.461654	-2.652332	C	2.455791	0.191331	4.745879
H	4.795286	-0.954450	-3.971007	C	1.054993	0.370113	4.857274
H	6.297013	-0.068986	-3.732776	C	0.338916	0.519340	3.681996
H	3.215319	4.628235	-1.875104	O	3.043410	0.261411	1.189100
H	2.871187	5.281012	-0.249895	C	0.383729	0.392768	6.208884
H	4.247048	4.144486	-0.516637	C	4.603548	-0.043033	3.425386
O	3.016611	-0.329397	-5.594720	O	2.830307	2.074694	-0.794634
C	3.289975	0.875223	-5.360238	C	2.261155	3.228369	-0.552514
O	2.075495	1.689041	-5.253153	O	1.085459	3.443526	-0.213406
C	2.311160	3.029074	-4.817896	C	5.236689	0.532000	-0.868907
O	4.372684	1.477573	-5.191000	C	3.218284	4.398721	-0.799261
H	1.326412	3.519434	-4.772568	H	-0.908914	-0.205576	-1.256060
H	2.775474	3.053721	-3.817775	H	0.778600	2.117640	-2.244109
H	2.968380	3.576247	-5.510631	H	-0.979092	0.052186	-3.687306
82				H	0.086843	1.230652	-4.491839
1a'-trans-SPO C1, C2 dE=2.26 pre-reactive				H	-1.163457	3.111609	-3.410343

H	-2.547066	-0.044690	-0.707172	C	-2.776776	0.36364.2	-3.266033
H	-0.654793	0.690021	1.538984	C	-1.547521	0.397743	-2.565503
H	-1.936790	-2.020502	0.984801	C	-0.348076	0.776833	-3.246412
H	-2.789389	-0.464021	1.232145	C	-0.440359	1.088108	-4.644321
H	-2.725121	-1.780147	3.362991	C	-1.670744	1.026497	-5.281390
H	-1.902989	-0.211355	3.481138	C	-2.866170	0.666741	-4.614903
H	-0.538564	-2.941143	3.108248	C	-1.564019	0.084332	-1.167046
H	-0.529950	-1.963190	4.585197	N	-0.520281	-0.039822	-0.410281
H	1.595817	-1.724898	3.281839	Co	1.263421	0.193641	-0.968753
H	0.746528	-0.164400	3.427140	O	1.341838	2.138520	-0.413120
H	0.545316	-2.054769	1.000270	C	1.210171	2.768499	0.920937
H	5.082294	0.503745	2.605176	C	2.340300	3.690272	1.268629
H	7.197245	2.110589	-0.775773	O	0.825188	0.898400	-2.682253
H	6.202813	2.204111	-2.939685	C	0.820844	1.482223	-5.361311
H	4.409374	2.305733	-2.940389	C	-4.180293	0.626112	-5.356012
H	5.184722	0.768838	-3.271574	C	-0.645476	-0.295374	1.036151
H	2.998227	-0.454813	2.393455	C	0.618935	-1.053820	1.456688
H	-5.001631	0.341612	-4.684264	C	0.694785	-1.170211	2.976811
H	-4.430407	1.606653	-5.792305	C	-0.558074	-1.904306	3.485826
H	7.702554	2.747475	1.891205	C	-1.846131	-1.211474	3.022975
H	7.280157	1.387208	2.953172	C	-1.896036	-1.044736	1.494994
H	0.876384	2.081819	1.700859	N	1.736931	-0.385213	0.770247
H	-0.781308	2.577631	-0.013185	C	2.880960	-0.162690	1.342760
H	-4.158401	-0.100189	-6.184943	C	4.017852	0.452718	0.725330
H	8.378128	1.139748	1.578418	C	4.048247	0.754400	-0.678551
H	2.071754	-3.444413	-3.168732	C	5.245788	1.359711	-1.200422
H	0.923167	-4.616455	-2.409270	C	6.304887	1.636719	-0.352526
H	0.345999	-3.426802	-3.604475	C	6.284179	1.342228	1.034579
H	0.278024	3.962587	-0.706306	C	5.140111	0.750074	1.540095
H	2.053194	4.307186	2.133030	O	3.083142	0.517504	-1.515737
H	3.237636	3.113445	1.534106	C	7.470137	1.670127	1.908431
H	2.583850	4.348239	0.423813	C	5.274579	1.684085	-2.666927
O	-2.597290	2.143021	0.864428	O	1.440453	-1.506009	-1.798987
C	-2.446981	2.277730	2.104004	C	0.724853	-2.595381	-1.667231
O	-3.689405	2.513729	2.786765	C	1.057250	-3.594073	-2.782384
C	-3.564831	2.648125	4.204587	O	-0.134828	-2.876941	-0.817387
O	-1.405472	2.222054	2.817989	C	0.208109	3.043320	-0.120144
H	-4.576532	2.857469	4.582153	H	-3.676403	0.090256	-2.708069
H	-3.180647	1.725535	4.670099	H	-1.713782	1.268698	-6.348912
H	-2.885178	3.470459	4.478464	H	1.235929	2.412910	-4.943757
82				H	1.599935	0.718487	-5.221990
1a'-cis-B1-SPO C1, C2 dE=10.86 pre-reactive				H	0.635634	1.625973	-6.434538

H	-2.773289	1.582787	-4.714842	C	0.407290	1.351243	3.113970
H	-3.349014	0.368948	-2.625859	C	0.855321	0.792754	1.888522
H	-3.692420	2.094988	-2.428999	C	2.155741	0.187493	1.809986
H	-1.584523	2.441647	-1.172744	C	2.946613	0.154807	3.012464
H	-2.551455	1.130531	-0.424858	C	2.453342	0.715026	4.178224
H	-1.023348	1.281498	0.961319	C	1.178224	1.330550	4.261910
H	3.082646	0.685043	5.074190	C	-0.038836	0.838583	0.772413
H	-0.583942	1.814474	3.134084	N	0.219902	0.412137	-0.427064
H	4.825498	-0.423244	3.899562	Co	1.927601	-0.184463	-1.013580
H	4.914260	-0.007838	2.155807	O	2.682544	1.674116	-0.897671
H	4.218914	-1.543918	2.640395	C	2.018447	2.998967	-0.736676
H	0.738816	-1.051148	-4.555635	C	2.504607	3.783333	0.443733
H	3.448076	-5.806708	-2.364789	O	2.680860	-0.334662	0.741098
H	2.334593	-2.883695	-5.320885	C	4.303135	-0.486668	2.935205
H	3.068180	-3.636385	0.437474	C	0.696749	1.932278	5.559011
H	3.196312	-5.368516	-0.027699	C	-0.791002	0.459808	-1.503527
H	1.610452	-4.610643	0.292489	C	-0.008436	0.785992	-2.797347
H	1.361497	2.740503	5.904641	C	-0.920074	0.697401	-4.017868
H	-0.310300	2.355978	5.444928	C	-2.103221	1.661236	-3.844591
H	3.377853	-4.909140	-6.051336	C	-2.877216	1.366493	-2.553549
H	4.596500	-5.518767	-4.912610	C	-1.967458	1.415110	-1.314266
H	0.655428	1.181797	6.365076	N	1.106441	-0.165900	-2.730853
H	3.034494	-6.343083	-5.057992	C	1.235987	-1.135153	-3.583132
H	0.935802	2.993714	-0.888875	C	1.908280	-2.367218	-3.270368
H	2.347306	2.521106	-2.870825	C	1.959911	-2.768982	-1.897136
H	6.161758	-0.639224	-3.710577	C	2.513364	-4.047369	-1.589403
H	6.096640	-1.305577	-2.032783	C	2.994050	-4.844118	-2.622673
H	5.249892	-2.138713	-3.351155	C	2.948453	-4.457248	-3.981349
H	3.871396	3.070140	-1.980326	C	2.386853	-3.221738	-4.282228
H	3.601246	3.777994	0.505592	O	1.484886	-2.033077	-0.911201
H	2.147619	4.818898	0.346657	C	3.516567	-5.352382	-5.055800
H	2.092883	3.367591	1.374373	C	2.607955	-4.448202	-0.144197
O	0.236397	3.850287	-3.354763	O	3.677142	-0.733591	-1.604138
C	-0.338241	4.592278	-2.520734	C	4.259873	-0.347683	-2.712133
O	-0.636946	5.892660	-3.052602	C	5.540243	-1.149663	-2.965844
C	-1.297144	6.765909	-2.131853	O	3.876638	0.511319	-3.521909
O	-0.685588	4.371750	-1.325343	C	2.839383	2.718291	-1.922640
H	-1.437838	7.719838	-2.661925	H	-1.160511	-0.578097	-1.616366
H	-2.275729	6.365379	-1.820126	H	0.361684	1.824803	-2.734207
H	-0.696659	6.929318	-1.222586	H	-1.290887	-0.336931	-4.136308
82				H	-0.350664	0.958825	-4.922011
1a'-cis-B2-SPO C1, C2 dE=14.45 pre-reactive				H	-1.704174	2.685551	-3.819109

H	-3.638052	0.361463	-4.056710	C	0.654910	-0.234200	3.388583
H	-3.693256	-0.824930	-1.881567	C	0.990318	-0.028544	2.024543
H	-4.295962	0.824351	-1.675982	C	2.331793	0.333460	1.667186
H	-2.085299	1.551995	-0.716609	C	3.289627	0.512470	2.722973
H	-2.728190	0.152331	0.168090	C	2.899879	0.283427	4.033324
H	-1.060983	-0.329015	1.451230	C	1.585394	-0.100572	4.401323
H	3.650262	0.409227	4.820476	C	-0.051766	-0.157060	1.055831
H	-0.376343	-0.510255	3.629580	N	0.088909	-0.071221	-0.230948
H	5.178963	0.248633	1.667003	Co	1.754843	0.051687	-1.092904
H	5.304273	1.037245	3.262136	O	1.658764	1.929068	-1.542620
H	4.673032	1.911779	1.842717	C	0.901642	2.870910	-1.039625
H	0.359165	-1.794111	-4.162902	C	1.544619	4.250586	-1.188459
H	4.365670	-5.446573	-1.960376	O	2.746591	0.534490	0.445012
H	2.057497	-3.395958	-4.952753	C	4.681963	0.942155	2.362624
H	2.972323	-3.836555	0.852490	C	1.232698	-0.347753	5.847598
H	4.404964	-2.916809	0.418663	C	-1.050030	-0.262266	-1.151203
H	4.440080	-4.699200	0.293460	C	-0.541976	0.149699	-2.553371
H	1.446019	0.532766	6.474741	C	-1.575133	-0.180075	-3.623062
H	0.165908	-0.587300	5.957674	C	-2.870364	0.584203	-3.300026
H	4.827083	-5.485076	-4.770808	C	-3.391449	0.237584	-1.896630
H	3.513647	-6.574411	-4.295154	C	-2.337668	0.485983	-0.804720
H	1.808978	-1.188556	6.266619	N	0.769777	-0.491792	-2.615450
H	3.252969	-5.377734	-5.584999	C	1.015678	-1.559913	-3.314359
H	4.609003	-0.661146	-0.592865	C	2.029302	-2.517784	-2.978998
H	4.220734	1.729381	-1.002660	C	2.492499	-2.605735	-1.623332
H	2.129866	4.318071	-2.113475	C	3.332828	-3.712790	-1.269990
H	0.777057	5.032279	-1.148126	C	3.700953	-4.625169	-2.246303
H	2.240071	4.391423	-0.347751	C	3.273625	-4.533753	-3.593901
H	4.893141	1.580622	-2.726984	C	2.428379	-3.488921	-3.927859
H	5.233665	-2.178442	-2.585759	O	2.170406	-1.766646	-0.670314
H	5.617589	-0.707052	-3.534955	C	3.738190	-5.544202	-4.613548
H	6.594087	-1.117151	-2.088874	C	3.817216	-3.806505	0.149036
O	6.941413	1.933692	-1.244238	O	3.398475	0.112044	-2.202407
C	7.299010	1.250618	-0.256368	C	4.727934	-0.319036	-1.618556
O	8.112488	2.018958	0.672442	C	5.586093	-1.140093	-2.526647
C	8.573279	1.273215	1.799448	C	4.484679	1.096804	-1.843905
O	7.076578	0.049710	0.059747	O	-0.209750	2.746276	-0.494826
H	9.210853	1.955943	2.383525	H	-1.251747	-1.351123	-1.200305
H	7.741014	0.920075	2.431202	H	-0.367035	1.233906	-2.527958
H	9.157446	0.388592	1.495869	H	-1.780646	-1.264559	-3.639649
83				H	-1.195140	0.098871	-4.617737
1b'-trans-RPO C1,C2 dE=0.00 pre-reactive				H	-2.669667	1.666690	-3.355945

H	3.589172	2.375797	-4.035750	C	3.965867	0.874544	0.699437
H	-1.857841	0.143899	-2.254994	C	3.258339	0.700618	1.937342
H	-1.189202	0.608628	0.527090	C	3.810674	1.190416	3.146945
H	-1.982800	-2.141000	-0.536861	C	5.020418	1.863450	3.186373
H	-2.909508	-0.620585	-0.724927	C	5.708146	2.036534	1.959153
H	-3.787657	-1.949314	1.209693	C	5.226648	1.564758	0.748458
H	-3.168917	-0.354915	1.681960	C	2.001782	0.011934	1.992700
H	-1.681739	-3.027072	1.989895	N	1.299209	-0.345046	0.962251
H	-2.397317	-2.076408	3.302615	C	0.030750	-1.079922	1.059254
H	0.078780	-1.720347	3.136291	C	-0.923829	-0.373884	0.091354
H	-0.813366	-0.202518	2.847047	C	-2.217647	-1.170493	-0.073907
H	0.226384	-2.080046	0.638112	C	-2.871379	-1.347021	1.306402
H	3.246270	1.034900	4.071920	C	-1.916068	-1.999119	2.314984
H	6.661934	2.575192	1.962638	C	-0.603310	-1.206266	2.440962
H	5.300163	2.251190	-1.285930	N	-0.158007	-0.090161	-1.138975
H	6.247343	0.804572	-0.993149	Co	1.690111	0.119952	-0.827908
H	6.858791	2.380286	-0.402892	O	2.203969	-1.649818	-1.325161
H	1.608909	-0.215641	2.991074	C	1.455344	-2.675607	-1.618048
H	-2.462803	1.769858	-6.585194	O	0.286533	-2.939808	-1.330806
H	-1.323116	3.034715	-7.090300	C	5.591278	2.408131	4.473228
H	6.600423	2.012284	4.670255	C	5.957879	1.768705	-0.548112
H	5.675533	3.507009	4.448216	O	3.558259	0.443242	-0.459622
H	0.178979	2.243621	1.247386	C	-0.766711	0.206945	-2.243607
H	1.469886	3.574965	1.041915	C	-0.145212	0.698104	-3.439002
H	-0.580800	2.453714	-1.035060	C	1.265098	0.915315	-3.539609
H	1.658280	4.604977	-1.371944	C	1.772278	1.474302	-4.760564
H	0.835060	3.777924	-2.730700	C	0.895689	1.790197	-5.787940
H	-0.090044	4.867293	-1.672870	C	-0.501481	1.584438	-5.698648
H	-1.177488	1.397932	-7.755519	C	-0.990437	1.040765	-4.522293
H	4.955314	2.143619	5.329395	O	2.135201	0.671382	-2.594415
H	3.460846	-2.326640	-3.354028	C	-1.412384	1.965119	-6.840143
H	4.156356	-3.147704	-1.933043	C	3.252022	1.722580	-4.854903
H	3.815686	-4.094721	-3.426885	O	1.507970	2.086850	-0.481794
O	-2.631821	2.099421	-0.905396	C	0.355945	2.979022	-0.807062
C	-2.961093	2.251761	0.297824	C	0.723469	4.127113	-1.694599
O	-4.359570	2.527513	0.456193	C	0.812410	2.832926	0.583578
C	-4.779258	2.677956	1.815720	O	2.151068	-3.636946	-2.356877
O	-2.268769	2.186010	1.353647	C	3.478049	-3.267939	-2.789168
H	-5.853808	2.908570	1.779416	H	-2.065446	0.887413	-4.397378
H	-4.618996	1.755078	2.396707	H	1.307720	2.229064	-6.703225
H	-4.237313	3.491720	2.322233	H	3.817027	0.785305	-4.739217
83				H	3.514191	2.183594	-5.816814

H	0.958568	1.572509	-5.007312	1b'-cis-B1-RPO C1 dE=9.00 pre-reactive			
H	-0.434497	3.419548	-4.183629	C	2.820175	-3.004745	-4.040121
H	-1.347551	2.492657	-5.384011	C	2.219480	-2.128130	-3.115813
H	-2.591878	1.299132	-3.604635	C	1.821340	-2.597808	-1.823380
H	-2.759828	3.046940	-3.374664	C	2.055364	-3.967769	-1.502562
H	-1.020310	3.046900	-1.610214	C	2.668951	-4.787232	-2.442704
H	-2.309787	1.858943	-1.222188	C	3.068671	-4.333070	-3.720252
H	-1.217328	1.700553	0.507730	C	1.852517	-0.788615	-3.482662
H	1.419436	0.162732	5.490031	N	1.626400	0.145186	-2.611038
H	-1.358249	2.000740	2.770831	C	0.704742	1.255643	-2.886013
H	3.275841	-1.108413	4.709696	C	-0.426621	0.989043	-1.868884
H	3.906634	-0.592627	3.110134	C	-1.482942	2.091338	-1.911702
H	2.902235	-2.024264	3.216286	C	-2.036656	2.218118	-3.341053
H	1.666311	-0.577048	-4.541282	C	-0.922476	2.453145	-4.368822
H	2.871192	-5.827659	-2.167563	C	0.143855	1.349538	-4.303039
H	3.113834	-2.612598	-5.017773	N	0.244371	0.744866	-0.575068
H	2.035200	-5.472275	0.042153	Co	1.935529	-0.093553	-0.741223
H	0.592797	-4.416356	0.026128	O	3.690577	-0.911152	-0.857935
H	2.117755	-3.775783	0.627558	C	4.589118	-0.635817	-1.743893
H	-1.714678	2.278495	5.120940	O	4.611786	0.216765	-2.641006
H	-1.162483	0.925853	6.132979	O	1.206762	-1.839518	-0.934487
H	3.229974	-6.206663	-4.808119	C	1.682381	-4.446214	-0.127591
H	3.883994	-4.794105	-5.669339	C	3.775845	-5.259009	-4.679583
H	-0.202164	2.412838	6.042366	C	-0.283870	1.128256	0.549423
H	4.786596	-5.512561	-4.320362	C	0.239849	0.872183	1.854008
H	1.437845	3.228426	-0.630266	C	-0.468516	1.394815	2.967418
H	2.686580	3.471971	0.725641	C	-0.070912	1.161583	4.270735
H	3.204505	2.543793	-2.213188	C	1.085760	0.363050	4.466226
H	5.565428	2.153278	-1.395037	C	1.818680	-0.174402	3.422785
H	5.204823	3.900177	-1.352327	C	1.416120	0.075933	2.063264
H	5.162237	2.950047	0.164049	O	2.148002	-0.445003	1.124358
H	7.144368	-0.304762	-2.466585	C	3.042244	-1.018451	3.640227
H	7.484079	-2.065016	-2.291161	C	-0.825892	1.723084	5.450472
H	6.344808	-1.470484	-3.553508	O	2.906648	1.609721	-0.289239
O	1.749091	4.166176	-3.268482	C	3.501934	2.645615	-1.170903
C	0.923604	4.912940	-2.689595	C	4.950497	2.923665	-0.913434
O	0.704496	6.146044	-3.394469	C	2.432488	3.011471	-0.231981
C	-0.246655	7.016301	-2.774259	O	5.674721	-1.509545	-1.564800
O	0.263789	4.743225	-1.624449	C	6.717754	-1.316934	-2.530491
H	-0.298063	7.914379	-3.407209	H	-0.882412	0.021321	-2.156206
H	-1.242978	6.549948	-2.708722	H	1.187086	2.222437	-2.655571
H	0.060623	7.295307	-1.754007	H	-0.304421	0.381701	-4.592417

H	1.461595	0.402018	-4.820252	83			
H	2.852534	1.487107	-4.573840		1b'-cis-B1-RPO C2 dE=6.70 pre-reactive		
H	1.296284	3.414413	-4.217394	C	3.788023	-3.276264	-3.016702
H	1.010427	2.661371	-5.814571	C	2.951024	-2.339971	-2.374133
H	-0.933887	1.404036	-4.875932	C	2.148197	-2.733180	-1.254825
H	-1.145177	3.145171	-4.626239	C	2.236301	-4.088359	-0.810106
H	-0.380490	2.975010	-2.282311	C	3.095204	-4.963237	-1.461967
H	-1.739323	1.832126	-2.579472	C	3.888731	-4.585725	-2.570458
H	-1.399059	1.765753	-0.507296	C	2.804814	-1.010130	-2.895925
H	-0.769646	0.780904	5.215879	N	2.350326	-0.020378	-2.191637
H	-2.362645	2.247193	1.502121	C	1.684656	1.141617	-2.792345
H	1.182888	-0.573056	5.286647	C	0.213944	0.913455	-2.359386
H	2.373935	-0.148979	4.018531	C	-0.687147	2.059829	-2.813511
H	1.418663	-1.607571	3.841527	C	-0.535125	2.278986	-4.329467
H	3.029454	-0.843187	-3.955554	C	0.929251	2.510005	-4.726973
H	3.175291	-5.987384	-1.083016	C	1.799592	1.317590	-4.301493
H	4.387307	-2.940742	-3.867722	N	0.280035	0.657243	-0.904888
H	1.670013	-5.513420	0.705466	Co	1.907355	-0.153761	-0.351738
H	0.350997	-4.420652	0.190620	O	3.591293	-0.909759	0.313635
H	1.631851	-3.792573	1.220910	C	4.703137	-1.115365	-0.314196
H	-3.502229	2.809103	3.527803	O	5.259072	-0.456873	-1.206167
H	-3.395119	1.588498	4.815766	O	1.302360	-1.930352	-0.639916
H	4.313858	-6.499775	-3.505662	C	1.430845	-4.487875	0.392959
H	5.292453	-5.146274	-4.115916	C	4.831354	-5.572473	-3.214090
H	-2.402513	3.055198	4.900074	C	-0.586737	1.165819	-0.083684
H	5.645460	-5.857999	-2.527949	C	-0.583772	1.033884	1.340713
H	4.490380	1.420047	-0.631501	C	-1.621339	1.673334	2.065654
H	3.839396	3.177093	-0.704341	C	-1.711939	1.601953	3.443855
H	3.620340	1.132616	1.675698	C	-0.720055	0.852171	4.124142
H	1.997770	2.864685	2.621185	C	0.319628	0.209674	3.472738
H	3.635245	3.565850	2.617253	C	0.422833	0.294327	2.042088
H	2.472558	4.018783	1.328501	O	1.438449	-0.305140	1.486289
H	7.270437	-1.788107	-0.385224	C	1.374751	-0.570330	4.205155
H	6.915578	-3.497970	0.066435	C	-2.809261	2.298498	4.210061
H	6.370092	-2.838369	-1.516726	O	2.450307	1.721085	0.001220
O	1.296372	4.239951	-2.071518	C	3.324096	2.046212	1.155267
C	2.078644	4.922105	-1.364832	C	2.821603	3.197166	1.972986
O	3.418158	4.978992	-1.971753	C	3.839153	2.196760	-0.221317
C	4.343099	5.801079	-1.256485	O	5.306887	-2.270438	0.195001
O	1.936142	5.517776	-0.276194	C	6.541768	-2.608288	-0.455345
H	5.282419	5.781589	-1.828770	H	-0.106680	-0.036164	-2.829447
H	3.981241	6.837466	-1.166441	H	2.022909	2.066337	-2.300364

H	-0.755285	0.568777	-2.889799	H	4.526603	5.427163	-0.234908
H	-2.000142	-2.223358	-3.254997	83			
H	-1.585416	-1.108461	-4.575992	1b'-cis-B2-RPO C1, C2 dE=10.33 pre-reactive			
H	-3.102390	0.620183	-3.668180	C	2.571628	-3.919350	-3.544177
H	-4.010159	-0.878971	-3.902490	C	2.074807	-2.856654	-2.750597
H	-3.864962	-1.409325	-1.492148	C	2.661429	-2.577237	-1.470206
H	-4.543572	0.209378	-1.697595	C	3.744673	-3.405040	-1.023471
H	-2.325385	1.242020	-1.131447	C	4.198463	-4.417804	-1.855149
H	-2.824895	0.116440	0.141773	C	3.637977	-4.696485	-3.126815
H	-1.056263	-0.207892	1.421768	C	0.893684	-2.152233	-3.151008
H	3.701001	1.737880	4.180952	N	0.541607	-1.001244	-2.659539
H	-0.229897	0.126700	3.525929	C	-0.826617	-0.500790	-2.639918
H	4.386771	2.582716	0.810549	C	-1.221423	-0.600975	-1.148245
H	5.093516	0.994843	1.132251	C	-2.515975	0.179788	-0.911836
H	5.152111	2.262248	2.393642	C	-3.624063	-0.382872	-1.819451
H	0.220598	-2.645443	-3.865312	C	-3.214200	-0.413590	-3.301685
H	5.045684	-5.020137	-1.512008	C	-1.883652	-1.157791	-3.517936
H	2.103511	-4.109600	-4.514639	N	-0.049586	-0.160107	-0.371550
H	5.014062	-2.201662	0.243707	Co	1.533697	-0.016455	-1.371994
H	5.018728	-3.943245	0.622618	O	3.053721	0.072468	-2.625632
H	3.620490	-2.914439	1.069829	C	4.027637	1.196529	-2.531421
H	1.615500	1.941703	5.955269	C	4.334810	1.868628	-3.833453
H	0.437167	0.622112	5.770958	O	2.240291	-1.635966	-0.656943
H	3.640143	-5.904319	-4.920547	C	4.382750	-3.106880	0.302840
H	5.257314	-5.598321	-4.250129	C	4.206974	-5.799160	-3.985172
H	2.152774	0.256405	6.053977	C	-0.100975	-0.006298	0.917494
H	4.185958	-6.770033	-3.464628	C	0.971461	0.426720	1.750743
H	4.612039	-0.409726	-1.137758	C	0.740290	0.469547	3.152543
H	5.033412	-0.736340	-2.918909	C	1.696981	0.921641	4.038991
H	3.795298	1.844572	-1.684957	C	2.929684	1.369960	3.496511
H	4.483921	1.126851	-4.629307	C	3.216923	1.362306	2.141889
H	3.522349	2.552594	-4.114789	C	2.233480	0.863719	1.218752
H	5.266340	2.442266	-3.716965	O	2.548992	0.866207	-0.046073
H	1.032283	4.589042	0.229664	C	4.534325	1.826939	1.596509
H	-0.718337	4.479273	-0.100236	C	1.462426	0.937133	5.529694
H	-0.028257	3.692164	1.372787	O	0.997762	1.661212	-2.238840
O	7.063475	0.303735	-1.815693	C	0.667730	2.795321	-1.693522
C	7.174401	0.085245	-0.588293	O	0.589556	3.877396	-2.284109
O	8.403884	0.611598	-0.037576	C	4.490977	-0.144406	-2.186774
C	8.550172	0.403866	1.368482	O	0.357756	2.688366	-0.340661
O	6.403571	-0.497834	0.228695	C	0.146230	3.945223	0.320195
H	9.527945	0.828449	1.642748	H	-1.391459	-1.673476	-0.927709

H	-2.544508	-0.491224	-3.964444
H	0.279282	0.348793	-7.097070
H	2.541374	0.924091	-6.609084
H	2.635270	1.992358	-5.177112
H	3.177838	0.329369	-5.038727
H	-2.011986	-0.225033	-1.742168
H	-0.830414	1.023741	0.783889
H	-1.822251	-1.827270	0.343945
H	-2.761724	-0.317356	0.117106
H	-3.225571	-1.315720	2.368375
H	-2.515302	0.308952	2.454790
H	-1.009068	-2.341906	2.856546
H	-1.430559	-1.181658	4.127746
H	0.956108	-0.955781	3.404312
H	0.040200	0.541167	3.085816
H	0.580049	-1.669799	1.000770
H	4.317281	1.624747	3.304714
H	7.124691	3.001938	0.353164
H	6.782427	2.608570	-1.970683
H	5.065112	2.401853	-2.456604
H	6.087021	0.987763	-2.278302
H	2.471444	0.350539	2.731432
H	-3.290483	-0.623909	-6.233343
H	-2.462394	0.448502	-7.382107
H	7.686303	2.646694	3.062830
H	6.731005	4.129580	2.893660
H	0.508684	2.564813	1.067819
H	-0.558636	2.645311	-1.111644
H	-2.046456	-1.273742	-7.321908
H	6.220613	2.873721	4.041672
H	2.033720	-2.136850	-4.011154
H	3.496593	-2.729352	-3.175302
H	2.554664	-3.847268	-4.229418
H	0.625063	3.978361	-1.702504
H	2.787777	3.750184	1.416675
H	2.452354	4.733478	-0.034292
H	1.434122	4.913780	1.426405
O	-2.512411	2.234463	-0.650167
C	-2.710224	2.576767	0.541946
O	-4.089374	2.866005	0.810314
C	-4.362027	3.228449	2.166819
O	-1.905370	2.685544	1.511566

H	7.756584	0.908050	1.943337
H	8.521346	-0.666014	1.629924
83			
1b'-trans-SPO C1, C2 dE=0.00 pre-reactive			
C	-1.542880	-0.209421	-4.300620
C	-0.561880	0.050547	-3.314383
C	0.755158	0.448832	-3.706748
C	1.036635	0.546447	-5.110019
C	0.038179	0.266944	-6.031801
C	-1.271297	-0.114881	-5.655896
C	-0.949565	-0.059511	-1.938311
N	-0.153265	0.038120	-0.921421
Co	1.705740	0.328856	-1.026588
O	1.597876	2.314869	-0.791413
C	1.048506	3.139712	0.313529
C	1.991161	4.196586	0.805253
O	1.720043	0.763175	-2.881773
C	2.420999	0.967484	-5.518129
C	-2.320897	-0.405683	-6.700858
C	-0.651797	-0.019898	0.463061
C	0.482582	-0.614765	1.309250
C	0.150349	-0.517529	2.794860
C	-1.165589	-1.269345	3.062408
C	-2.306123	-0.738568	2.184813
C	-1.952396	-0.789019	0.689657
N	1.712307	0.043545	0.845662
C	2.634707	0.468355	1.653425
C	3.850959	1.115466	1.257863
C	4.255327	1.186610	-0.117164
C	5.477756	1.882759	-0.413902
C	6.210246	2.457618	0.612071
C	5.824278	2.383822	1.973770
C	4.654243	1.703508	2.266322
O	3.601205	0.663723	-1.114178
C	6.657166	3.040455	3.047217
C	5.886298	1.983920	-1.855886
O	2.080976	-1.467993	-1.555614
C	1.367060	-2.552228	-1.444060
O	1.670862	-3.484791	-2.437669
C	2.493747	-3.008117	-3.524997
O	0.522716	-2.892900	-0.611600
C	0.404140	3.164297	-1.008629

C	1.536686	2.785073	-2.596030
H	-0.234715	-1.981116	-1.836444
H	-0.123680	0.745561	-3.168848
H	-0.396976	-2.038579	-4.424744
H	-0.171739	-0.512178	-5.311807
H	-2.284125	0.386980	-4.304462
H	-2.600184	-1.125298	-5.200731
H	-2.558992	-2.412476	-3.063141
H	-3.769049	-1.122516	-2.980727
H	-2.259042	0.327800	-1.657438
H	-2.398184	-1.271210	-0.882673
H	-1.340253	0.200589	0.362178
H	2.180522	2.683585	4.313706
H	-1.397661	1.467249	2.260114
H	4.395276	2.095449	1.655242
H	4.429238	0.623010	2.611350
H	4.337346	2.204750	3.446571
H	1.755349	-1.755468	-4.680505
H	5.966126	-4.633151	-1.765937
H	4.052982	-2.753779	-5.131123
H	5.322326	-4.123495	0.480691
H	3.543972	-4.008941	0.614546
H	4.505061	-2.540041	0.715920
H	-0.305703	3.898910	4.565344
H	-1.619003	2.740736	4.271193
H	5.841994	-4.307564	-5.537791
H	7.132479	-4.063379	-4.344215
H	-0.370483	2.386766	5.486704
H	6.155716	-5.541690	-4.295644
H	-0.208367	2.306987	-1.351930
H	1.158497	2.235913	-3.453994
H	6.122335	-1.157842	-2.197450
H	7.501305	-0.044450	-2.509715
H	6.332896	0.294538	-1.180296
H	2.281584	3.549778	-2.820193
H	1.852869	4.442616	-0.431591
H	0.080353	4.693725	-0.556184
H	0.726572	3.571346	0.656021
O	-2.358139	2.343732	-1.125555
C	-2.366536	2.796929	-2.299960
O	-3.210636	3.947349	-2.444553
C	-3.226711	4.499512	-3.765069

H	-5.435174	3.464395	2.210833
H	-4.137748	2.403087	2.862268
H	-3.771984	4.102877	2.481077

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1b'-cis-B1-SPO C1, C2 dE=7.03 pre-reactive

C	1.893264	0.919088	1.390159
C	0.459814	0.873703	1.339299
C	-0.309081	1.491563	2.357353
C	0.276625	2.145429	3.426810
C	1.692787	2.165263	3.480907
C	2.495764	1.576679	2.517269
C	-0.250135	0.231660	0.275621
N	0.295326	-0.267039	-0.792084
Co	2.115557	-0.031602	-1.273881
O	1.938925	1.959549	-1.451617
C	0.741154	2.847499	-1.362020
C	0.871411	3.954958	-0.362600
C	-0.546615	2.826481	4.491822
C	3.996299	1.634656	2.571568
O	2.695123	0.417201	0.491502
C	-0.503729	-0.907734	-1.854126
C	0.080476	-0.336860	-3.172007
C	-0.592793	-0.951432	-4.393948
C	-2.105777	-0.699832	-4.313166
C	-2.686711	-1.314346	-3.033015
C	-2.018691	-0.742988	-1.772152
N	1.514385	-0.599607	-2.988197
C	2.148655	-1.487269	-3.693534
C	3.266763	-2.238428	-3.189238
C	4.144456	-2.922074	-4.054803
C	5.128314	-3.773307	-3.567626
C	5.196550	-3.966489	-2.168714
C	4.346363	-3.329731	-1.272540
C	3.362670	-2.422971	-1.771202
O	2.560398	-1.841726	-0.904217
C	4.445257	-3.517599	0.215593
C	6.112767	-4.457513	-4.483834
O	3.963496	0.228790	-1.810488
C	4.330954	0.761618	-2.938703
O	5.711983	0.667583	-3.158566
C	6.451205	-0.109075	-2.194797
O	3.670743	1.320965	-3.816690

C	4.243060	1.600979	-1.963888	O	-1.747089	2.406621	-3.328578
O	0.959548	4.527202	-1.019290	H	-3.851138	5.403312	-3.711476
H	-1.505520	-0.876046	-1.282647	H	-2.214316	4.762746	-4.106521
H	-0.582615	1.770836	-2.477934	H	-3.655613	3.795629	-4.496683
H	-2.105902	-0.629177	-3.661345	83			
H	-1.549006	0.784242	-4.583392	1b'-cis-B2-SPO C1, C2 dE=9.64 pre-reactive			
H	-2.917079	2.300356	-3.181784	C	2.301344	0.450432	1.519784
H	-3.955430	1.040510	-3.860840	C	0.969759	0.073018	1.906694
H	-3.921113	-0.213686	-1.730735	C	0.689298	-0.238162	3.265720
H	-4.442406	1.446781	-1.426067	C	1.663417	-0.188257	4.241380
H	-2.151929	2.041623	-0.586115	C	2.969987	0.200257	3.844209
H	-2.787249	0.638188	0.287441	C	3.310605	0.518989	2.541190
H	-1.105257	-0.171057	1.410257	C	-0.114642	0.038935	0.984675
H	3.758581	0.241753	4.602082	N	-0.038830	0.251658	-0.295838
H	-0.333373	-0.527810	3.528742	Co	1.583658	0.457032	-1.210390
H	5.157000	0.085836	1.519913	O	1.321448	2.367172	-1.550939
H	5.345825	1.020303	3.026044	C	1.019023	3.327868	-0.726469
H	4.719750	1.804779	1.545003	O	0.732897	2.882978	0.559584
H	0.051974	-1.070901	-4.401066	C	0.464317	3.928523	1.505545
H	4.260019	-4.815883	-2.822913	C	1.375120	-0.540703	5.679003
H	1.780076	-2.496125	-5.461837	C	4.708979	0.881841	2.143074
H	4.186538	-4.499094	-0.455143	O	2.662350	0.756112	0.304337
H	2.957218	-3.401436	0.253983	C	-1.226364	0.189810	-1.166039
H	4.528919	-2.760344	-0.254124	C	-0.780329	0.691357	-2.559088
H	1.975625	-1.402682	6.009609	C	-1.877609	0.448261	-3.588349
H	1.611115	0.294607	6.357565	C	-3.134964	1.220158	-3.149675
H	4.642617	-4.399759	-5.651421	C	-3.578697	0.835849	-1.728510
H	3.459038	-5.655677	-5.252295	C	-2.445796	0.986348	-0.698107
H	0.315761	-0.798102	5.818266	N	0.520658	0.057126	-2.736500
H	3.020408	-4.342686	-6.371620	C	0.745699	-0.921906	-3.562373
H	4.523841	-0.342204	-0.999169	C	1.793632	-1.880745	-3.387379
H	4.034459	2.093550	-1.015069	C	2.189405	-2.705212	-4.469078
H	-0.432378	4.500833	1.222834	C	3.086928	-3.743210	-4.294946
H	0.309527	3.416987	2.463629	C	3.557120	-3.992099	-2.980834
H	1.313832	4.622080	1.577669	C	3.194718	-3.231978	-1.878491
H	4.579645	2.231649	-2.789453	C	2.317024	-2.112826	-2.070248
H	6.356599	-0.634856	-2.632669	O	2.007436	-1.394346	-1.015325
H	4.928903	-1.492151	-3.266465	C	3.743148	-3.495258	-0.507611
H	5.363282	0.103320	-3.961533	C	3.573813	-4.579078	-5.452248
O	6.017885	-1.402962	0.216191	O	3.180465	0.670786	-2.385457
C	7.171917	-0.930315	0.038442	C	4.543273	0.163504	-1.967002
O	7.812168	-0.609671	1.298021	C	5.338754	-0.498531	-3.042239

H	-1.485100	0.547400	0.670200
H	-2.374600	-2.241900	-0.243100
H	-3.378400	-0.769900	-0.320400
H	-3.884500	-2.099700	1.743500
H	-3.271900	-0.480700	2.120300
H	-1.643500	-3.092000	2.193300
H	-2.176800	-2.152100	3.595200
H	0.231600	-1.764900	3.012600
H	-0.711400	-0.244600	2.896800
H	-0.001000	-2.120500	0.579000
H	4.200300	-1.095800	2.823100
H	7.039400	1.216200	0.579800
H	4.823900	3.432900	-0.694100
H	4.778300	2.267600	-2.015800
H	6.336200	2.645700	-1.209100
H	2.011000	-1.086400	2.381400
C	-2.932200	1.936300	-7.106000
H	-2.081300	0.126500	-7.943300
H	-3.301200	-0.165900	-6.691800
C	-3.269000	2.676900	-5.789300
H	-2.166300	2.519700	-7.647000
H	-3.828700	1.935300	-7.748300
C	-2.005300	3.185300	-5.102000
H	-3.935000	3.517600	-6.041300
H	-3.827500	2.006700	-5.115000
H	-1.479900	2.369300	-4.605500
H	-1.321200	3.610700	-5.847600
C	6.921400	-2.272500	2.327700
H	7.858700	-0.325300	2.134200
H	6.859600	-0.506300	3.582400
C	6.787700	-2.731800	0.852500
H	7.858300	-2.662300	2.757800
H	6.105600	-2.725300	2.916500
C	5.357000	-3.204700	0.630800
H	7.051300	-1.900000	0.183700
H	7.495400	-3.551900	0.654500
H	5.156200	-4.085500	1.251900
H	4.645500	-2.438400	0.952200
N	-2.152600	4.254900	-4.033400
C	-2.633800	5.550400	-4.659600
C	-3.152300	3.849500	-2.959200
C	-0.779700	4.430700	-3.385200

C	9.081179	0.031025	1.161125
O	7.823930	-0.693419	-1.007231
H	9.465045	0.176939	2.182093
H	9.790138	-0.579267	0.578247
H	8.990204	1.009173	0.659227

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2-trans-a-RPO

N	-0.739500	-0.115300	-1.124000
C	-1.376600	-0.269500	-2.232000
C	-0.881400	0.117100	-3.520000
C	-1.717700	-0.104000	-4.635100
C	-1.384000	0.341000	-5.901000
C	-0.089900	0.880700	-6.083800
C	0.760500	1.139000	-5.023400
C	0.322200	0.875800	-3.683100
O	1.020400	1.380100	-2.708700
N	1.060500	-0.362600	0.708200
C	2.100900	-0.499300	1.462700
C	3.403700	0.022500	1.175000
C	4.453800	-0.411100	2.011800
C	5.771900	-0.067700	1.766400
C	6.013100	0.874600	0.746900
C	5.008000	1.396500	-0.054700
C	3.678100	0.893200	0.075500
O	2.791800	1.291600	-0.799100
Co	1.046000	0.501900	-0.979700
C	-1.291700	-0.433900	0.194300
C	-0.173300	-1.113000	0.991900
C	-0.564800	-1.248400	2.457900
C	-1.859200	-2.066700	2.543800
C	-2.986400	-1.462400	1.699900
C	-2.566100	-1.265100	0.235600
C	2.126700	1.729800	-5.197400
C	5.260600	2.485400	-1.053700
C	6.904600	-0.738600	2.503700
C	-2.442400	0.472300	-6.959200
H	-2.692900	-0.568900	-4.466700
H	0.231200	1.154000	-7.093900
H	2.203900	2.712800	-4.711100
H	2.871200	1.086800	-4.703100
H	2.383300	1.833200	-6.260600
H	-2.379200	-0.711500	-2.205500

H	3.958700	-1.682100	-0.910800	C	-2.733500	6.731800	-3.687100
C	5.537000	-4.868200	-2.861200	H	-1.949400	5.749600	-5.495000
H	6.868400	-3.806800	-1.526800	H	-3.621000	5.323500	-5.086400
H	6.135300	-5.253200	-0.807800	C	-2.694400	2.689500	-2.093800
C	3.609900	-5.650500	-0.028700	H	-3.318600	4.725800	-2.311300
H	2.940400	-3.626800	-0.039700	H	-4.083300	3.620200	-3.497100
H	3.161500	-4.309900	-1.686100	C	0.293500	5.046300	-4.266600
C	5.122800	-0.424800	-3.105200	H	-0.956600	5.012700	-2.466400
H	6.257900	-0.894000	-1.328400	H	-0.461700	3.422100	-3.089200
H	6.472100	-2.054800	-2.663000	C	-4.180200	7.140800	-3.390600
C	6.184500	0.465500	-3.744000	H	-2.230500	6.505400	-2.731300
H	4.564600	-0.971400	-3.885000	H	-2.192600	7.589600	-4.122100
H	4.368000	0.177000	-2.575100	C	-4.250800	8.280300	-2.377900
H	6.767200	0.998700	-2.977700	H	-4.682100	7.426200	-4.334000
H	6.890500	-0.127600	-4.348600	H	-4.721700	6.272500	-2.980100
H	5.729400	1.220000	-4.403200	H	-3.828200	7.940600	-1.421100
C	6.673300	-5.650200	-3.524200	H	-3.687200	9.160500	-2.726700
H	4.641900	-5.507200	-2.801600	H	-5.291600	8.590300	-2.202100
H	5.268000	-4.007200	-3.494100	C	-3.818700	2.212300	-1.167900
C	6.296800	-6.138200	-4.922500	H	-2.360400	1.851100	-2.717000
H	7.572100	-5.010800	-3.583400	H	-1.841200	3.000100	-1.476400
H	6.944700	-6.512400	-2.889400	C	-4.906700	1.421400	-1.894300
H	5.416500	-6.798300	-4.884300	H	-3.365600	1.581400	-0.386500
H	6.050500	-5.291000	-5.581100	H	-4.250700	3.086400	-0.651800
H	7.121300	-6.699900	-5.385400	H	-5.437100	2.038300	-2.636500
C	2.175200	-6.192600	0.027800	H	-4.476000	0.559100	-2.430200
H	4.250100	-6.357900	-0.584800	H	-5.663400	1.038800	-1.192300
H	3.966700	-5.573100	1.011200	C	1.601600	5.151400	-3.462500
C	2.094300	-7.506900	0.801200	H	0.471100	4.427500	-5.161600
H	1.553800	-5.429800	0.525700	H	0.006500	6.056400	-4.604700
H	1.787800	-6.332000	-0.997500	C	1.571200	6.254200	-2.401600
H	2.728100	-8.283700	0.343400	H	1.805900	4.172900	-2.995600
H	2.432500	-7.356200	1.837600	H	2.430600	5.337800	-4.166200
H	1.062500	-7.888600	0.832300	H	0.741100	6.132000	-1.691800
O	0.232800	2.144900	-0.111900	H	2.509700	6.269300	-1.827400
C	0.893800	3.467600	-0.201500	H	1.455100	7.242200	-2.875900
C	0.917600	2.732800	1.068000	N	4.918400	-3.544400	-0.784800
C	0.005000	3.047000	2.206700	C	4.595400	-2.280100	-1.574500
H	1.791500	3.435700	-0.819400	C	5.946000	-4.399100	-1.474300
H	0.162300	4.276000	-0.336400	C	3.573800	-4.276100	-0.669500
H	1.842700	2.202600	1.301000	C	5.731100	-1.438600	-2.125000
H	-0.886200	3.589000	1.860400	H	3.955800	-2.603300	-2.404300

C	-3.509500	-0.883700	1.439200	H	-0.279500	2.122300	2.730500
C	-2.270500	-0.434600	1.872800	H	0.535400	3.691000	2.926000
C	-1.202400	-1.368800	2.040300	O	-3.609900	5.583700	-0.526800
O	-0.004600	-0.874300	2.223100	C	-2.443000	5.499200	-0.082500
Co	1.520800	-1.924200	1.745700	O	-2.278300	5.201200	1.293400
C	2.784300	-4.412900	1.279000	O	-1.338600	5.627700	-0.679800
C	1.733100	-4.608900	2.382300	C	-3.506100	5.036900	2.014100
C	1.242600	-6.049400	2.416400	H	-3.220300	4.869600	3.061000
C	2.435500	-6.983800	2.649600	H	-4.137600	5.932800	1.932300
C	3.537200	-6.775000	1.606100	H	-4.078800	4.175200	1.639700
C	3.989900	-5.309800	1.538600	O	1.878300	-0.960400	-1.917500
C	3.009500	2.395500	0.976800	C	1.433700	-2.114600	-2.302300
C	-1.957200	1.021100	2.045600	O	0.337200	-2.579200	-1.618400
C	-4.980100	-2.701300	0.429400	C	-0.166100	-3.835300	-2.105600
C	7.654900	0.865600	-0.311600	O	1.972100	-2.791600	-3.184900
H	6.582000	-1.589000	0.312200	H	-0.417300	-3.761200	-3.172400
H	5.622200	2.594200	0.233600	H	0.570100	-4.634400	-1.958200
H	3.448500	3.383000	0.780900	H	-1.062200	-4.042100	-1.508300
H	2.110100	2.272600	0.354800	O	1.965300	-3.363200	1.745800
H	2.660100	2.352500	2.021300	C	2.716400	-3.516200	2.741000
H	5.021700	-3.184900	0.716400	O	2.378700	-2.582100	3.794300
H	2.295100	-4.692600	0.326200	O	3.677500	-4.281900	2.954500
H	4.454600	-5.003400	2.493600	C	3.199300	-2.678100	4.962200
H	4.749600	-5.198900	0.751400	H	3.130000	-3.677800	5.415600
H	4.404300	-7.419700	1.826100	H	4.258500	-2.485100	4.731100
H	3.155300	-7.078200	0.616200	H	2.827300	-1.917000	5.661300
H	2.852200	-6.799300	3.656700		187		
H	2.093000	-8.031000	2.631800		2-trans-n2-RPO		
H	0.502000	-6.177200	3.220300	N	3.039500	-2.962700	1.206700
H	0.724200	-6.286100	1.471200	C	4.201600	-2.483000	0.902900
H	2.217900	-4.346500	3.342400	C	4.529800	-1.096200	0.757100
H	-3.009100	-4.226200	1.447600	C	5.862300	-0.770400	0.409100
H	-4.282400	-0.141800	1.214900	C	6.273500	0.533500	0.195400
H	-1.534500	1.213300	3.043500	C	5.312000	1.554200	0.371900
H	-2.854900	1.639400	1.909100	C	4.001200	1.301100	0.730100
H	-1.186500	1.343000	1.326400	C	3.561800	-0.050200	0.927800
H	-0.917400	-4.817600	2.241600	O	2.313400	-0.226600	1.219100
C	7.812300	0.537700	-1.813300	N	0.727700	-3.580600	2.151100
H	7.851500	1.938800	-0.148900	C	-0.543100	-3.793100	2.139600
H	8.422800	0.316900	0.258500	C	-1.516900	-2.759300	1.952300
C	6.714600	1.203700	-2.664800	C	-2.809900	-3.162700	1.570800
H	8.808300	0.859700	-2.163000	C	-3.788600	-2.248600	1.226300

C	1.454600	2.804400	-2.856000	H	7.794000	-0.554700	-1.930600
H	1.341400	0.643300	-2.927900	C	6.246300	0.476300	-3.920600
H	2.241800	1.278300	-1.544700	H	5.840400	1.411600	-2.032200
H	1.263700	2.978800	-3.926900	H	7.070400	2.193900	-2.997300
H	0.498200	2.911100	-2.323000	H	5.788000	1.190500	-4.618200
H	2.128700	3.599000	-2.498200	H	7.080700	-0.014500	-4.442000
C	4.919800	-2.348400	-7.194700	C	-4.650400	-2.692000	-1.083100
H	6.475900	-1.114300	-6.311700	H	-5.261700	-3.726900	0.722300
H	6.132800	-2.620700	-5.433300	H	-5.851700	-2.050100	0.610500
C	3.971300	-3.497200	-6.841600	C	-3.479600	-3.616400	-1.445400
H	4.351200	-1.535600	-7.680000	H	-5.551800	-3.001600	-1.644200
H	5.668900	-2.690200	-7.928800	H	-4.420600	-1.654800	-1.391100
H	4.528500	-4.336600	-6.393300	C	-3.261900	-3.603000	-2.947000
H	3.190700	-3.183100	-6.132100	H	-2.567500	-3.283300	-0.930700
H	3.468600	-3.875900	-7.744100	H	-3.683400	-4.633300	-1.071200
N	-2.257700	-4.621200	-3.469400	H	-4.199800	-3.810000	-3.485600
C	-0.868100	-4.295200	-2.911600	H	-2.891600	-2.623900	-3.281000
C	-2.619200	-6.033600	-3.012800	N	5.184900	-0.600200	-3.723500
C	-2.270600	-4.571500	-4.987400	C	5.772500	-1.770000	-2.958100
C	0.275200	-5.010600	-3.627300	C	3.987600	-0.094200	-2.922600
H	-0.729200	-3.213000	-3.030100	C	4.672300	-1.044100	-5.088700
H	-0.920400	-4.564600	-1.845900	C	4.886000	-2.994600	-2.804000
C	-4.070800	-6.437300	-3.202500	H	6.710300	-2.032800	-3.467700
H	-1.955100	-6.704100	-3.577300	H	6.014900	-1.375400	-1.965500
H	-2.341800	-6.089600	-1.948100	C	3.372900	1.214800	-3.383200
C	-2.032900	-3.194900	-5.594700	H	3.249200	-0.899800	-3.018800
H	-1.501300	-5.283100	-5.312200	H	4.314200	-0.023600	-1.875400
H	-3.246500	-4.972200	-5.294500	C	5.664900	-1.780200	-5.972400
C	1.494800	-5.188600	-2.710900	H	3.776900	-1.651600	-4.881600
H	-0.030200	-6.012400	-3.973500	H	4.318900	-0.133500	-5.588200
H	0.573400	-4.419700	-4.503700	C	5.714400	-4.108800	-2.155700
C	1.389100	-6.426800	-1.822600	H	4.015800	-2.768500	-2.169200
H	2.388500	-5.242900	-3.350600	H	4.483400	-3.337500	-3.767900
H	1.622600	-4.282100	-2.097300	C	4.908100	-5.386500	-1.949100
H	1.303000	-7.338000	-2.438500	H	6.599100	-4.322600	-2.783000
H	2.286100	-6.545000	-1.198100	H	6.107000	-3.751900	-1.186700
H	0.513800	-6.378100	-1.156100	H	4.574400	-5.802800	-2.911200
C	-4.270300	-7.868400	-2.688700	H	5.497600	-6.157100	-1.430800
H	-4.725700	-5.777600	-2.612000	H	4.008700	-5.183700	-1.353800
H	-4.388700	-6.373400	-4.258200	C	2.057400	1.423200	-2.621200
C	-5.733900	-8.299800	-2.761000	H	4.049100	2.063500	-3.185000
H	-3.641200	-8.564500	-3.271900	H	3.153600	1.187400	-4.461800

O	-3.457900	-6.421000	0.122900	H	-3.925000	-7.894900	-1.641900
C	-3.102600	-7.033300	2.629100	H	-5.864400	-9.327100	-2.389200
H	-2.713700	-7.281800	3.625200	H	-6.360500	-7.638600	-2.141300
H	-3.845000	-6.225400	2.710400	H	-6.117500	-8.261900	-3.793900
H	-3.592600	-7.910000	2.182400	C	-1.557700	-3.302100	-7.052900
187				H	-2.965700	-2.610000	-5.561700
2-trans-n1-RPO				H	-1.280900	-2.627700	-5.022800
N	1.997000	-0.526500	-1.547700	C	-0.101100	-3.751500	-7.194900
C	3.266100	-0.304700	-1.434800	H	-2.221500	-3.982500	-7.617600
C	4.006400	0.586100	-2.282300	H	-1.671800	-2.310000	-7.520100
C	5.312500	0.926300	-1.881700	H	0.191500	-3.797100	-8.255300
C	6.055500	1.880400	-2.554100	H	0.577100	-3.051600	-6.686300
C	5.502100	2.435500	-3.724400	H	0.070000	-4.750500	-6.766600
C	4.253200	2.073400	-4.210800	O	0.630700	-2.111300	-0.110900
C	3.458000	1.144600	-3.477300	C	1.373000	-1.588300	-1.261400
O	2.280600	0.828300	-3.962600	C	0.250300	-0.812000	-0.728900
Co	0.837600	0.357700	-2.785300	C	-1.099100	-0.773100	-1.363000
N	-0.572900	-0.229000	-1.645800	H	2.382000	-1.271200	-1.002400
C	-1.802400	-0.388300	-2.006200	H	1.258700	-2.174700	-2.174800
C	-2.346600	0.052000	-3.258700	H	0.515000	0.008200	-0.058200
C	-3.732200	-0.128600	-3.445600	H	-1.174800	0.130500	-1.987900
C	-4.419100	0.506200	-4.467300	H	-1.245800	-1.631300	-2.021400
C	-3.668300	1.247900	-5.401600	H	-1.880500	-0.743700	-0.593000
C	-2.298200	1.420300	-5.291500	O	2.023400	-2.327600	-4.264400
C	-1.600500	0.851700	-4.179700	C	1.170300	-1.470800	-4.623200
O	-0.331800	1.141400	-4.086300	O	1.649200	-0.633800	-5.674600
C	1.246800	-1.385200	-0.617200	O	0.017800	-1.256900	-4.194800
C	1.969700	-1.780900	0.662000	C	0.700900	0.348300	-6.112300
C	1.022700	-2.546400	1.593500	H	-0.206600	-0.125200	-6.515300
C	-0.262100	-1.761900	1.869600	H	0.401300	1.010800	-5.287300
C	-0.989900	-1.408400	0.568600	H	1.202200	0.926300	-6.900400
C	-0.055200	-0.616500	-0.331200	O	2.369800	-1.717400	3.443400
C	3.707800	2.605400	-5.503400	C	1.745800	-1.707000	4.594700
C	-1.505300	2.249200	-6.256200	O	0.501600	-2.280000	4.562100
C	7.375300	2.374700	-2.012500	C	-0.230900	-2.170400	5.792700
C	-5.915200	0.665700	-4.398700	O	2.249300	-1.267000	5.624900
H	5.719100	0.484800	-0.970700	H	-1.215300	-2.600500	5.577400
H	6.080100	3.179100	-4.282500	H	0.270300	-2.722900	6.599400
H	3.901200	1.896100	-6.326600	H	-0.330100	-1.117900	6.089100
H	2.617800	2.716600	-5.432900	O	-1.259900	-5.866500	-0.119800
H	4.170500	3.566200	-5.769500	C	-2.271300	-6.287900	0.498700
H	3.822600	-0.799700	-0.627900	O	-1.969100	-6.623500	1.853500

C	3.986600	5.755700	0.148600	H	0.958800	-2.291400	-1.187500
H	3.629600	5.304800	2.234300	H	2.365900	-0.886100	1.172100
H	5.338600	5.536800	1.834200	H	2.852700	-2.397600	0.434400
C	2.195200	3.017500	2.289800	H	1.552900	-2.765200	2.534100
H	2.837700	3.230600	0.240200	H	0.759000	-3.519700	1.139100
H	3.534200	1.828700	1.124100	H	-0.014800	-0.830300	2.408200
C	4.950600	3.791600	3.966500	H	-0.938000	-2.338200	2.521800
H	5.017500	2.014500	2.681700	H	-1.887700	-0.817500	0.787300
H	6.350400	3.158900	2.457900	H	-1.309900	-2.332400	0.053100
N	-3.525600	3.732100	-1.605600	H	0.225800	0.324600	0.169000
C	-3.526700	4.986800	-2.441600	H	-4.282700	-0.648700	-2.658400
C	-4.318300	3.885400	-0.310100	H	-4.194100	1.748000	-6.221400
C	-2.110100	3.233000	-1.279600	H	-0.977600	3.055300	-5.723900
C	-2.761800	4.866600	-3.752900	H	-2.149600	2.681800	-7.033700
H	-4.583200	5.230900	-2.630900	H	-0.719800	1.648300	-6.741900
H	-3.103500	5.789300	-1.830000	H	-2.524000	-0.807000	-1.295800
C	-4.245200	5.228600	0.406100	C	7.293100	3.788300	-1.391600
H	-5.365200	3.672800	-0.563400	H	7.754000	1.663500	-1.258900
H	-3.951700	3.057000	0.319400	H	8.116200	2.400000	-2.830700
C	-1.300600	4.019100	-0.265900	C	6.770200	3.846200	0.055100
H	-2.281000	2.236200	-0.848300	H	8.298900	4.242400	-1.397800
H	-1.584200	3.120200	-2.235300	H	6.656100	4.423000	-2.034500
C	3.559800	7.211600	0.347000	C	5.395600	3.205600	0.188800
H	4.824800	5.721800	-0.566700	H	7.484500	3.319300	0.708500
H	3.159700	5.201800	-0.314900	H	6.760300	4.903600	0.366800
C	3.089800	7.833100	-0.968200	H	4.761300	3.408500	-0.683500
H	2.742600	7.252000	1.088400	H	5.518000	2.122600	0.311200
H	4.394400	7.801500	0.767900	C	-6.328700	1.531100	-3.183700
H	2.268900	7.239200	-1.397800	H	-6.272300	1.142600	-5.327300
H	2.736700	8.865300	-0.825300	H	-6.424500	-0.310000	-4.323500
H	3.906700	7.853300	-1.707200	C	-5.527200	2.841800	-3.003900
C	1.016600	2.115200	1.898400	H	-7.399100	1.779900	-3.281200
H	2.580700	2.682000	3.263500	H	-6.219400	0.939400	-2.259200
H	1.839400	4.056600	2.398900	C	-4.155100	2.578300	-2.385100
C	-0.232600	2.334500	2.745800	H	-5.433300	3.365600	-3.972200
H	0.787400	2.279800	0.834100	H	-6.124000	3.497000	-2.347300
H	1.356300	1.069800	1.975700	H	-4.205000	1.751100	-1.652600
H	-0.057900	2.050700	3.796500	H	-3.414800	2.334700	-3.149000
H	-0.527800	3.395900	2.732800	N	4.572300	3.618800	1.404300
H	-1.088300	1.760200	2.359900	C	4.391300	5.117000	1.466400
C	5.455500	2.935700	5.133100	C	3.243500	2.887400	1.201000
H	5.428100	4.785700	4.012800	C	5.273400	3.087700	2.654800

H	-0.253000	-2.082200	-7.026300
H	-0.694800	-2.945100	-5.521700
O	6.381000	0.401600	1.167800
C	5.324800	-0.228100	1.413600
O	5.226500	-1.563000	0.900900
O	4.279400	0.130100	2.012300
C	6.416000	-2.042200	0.258400
H	6.218100	-3.092600	0.002000
H	6.644700	-1.475800	-0.658000
H	7.283300	-1.972700	0.930800
O	1.045900	1.961400	-1.734600
C	1.351400	3.141800	-2.166500
O	1.864100	4.014500	-1.452500
O	1.015000	3.414500	-3.464900
C	1.463500	4.707900	-3.909000
H	0.942700	5.513900	-3.371900
H	2.544900	4.817200	-3.753500
H	1.225600	4.746600	-4.977600
O	-3.042100	1.434500	1.081500
C	-3.853400	0.518000	0.764700
O	-4.203600	-0.410200	1.766000
O	-4.392900	0.283700	-0.343700
C	-3.630200	-0.142500	3.053600
H	-3.947800	0.838800	3.437000
H	-3.994000	-0.940600	3.714100
H	-2.531300	-0.158100	3.020400

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N	2.233900	0.620500	-2.430000
C	3.275200	-0.028700	-2.839000
C	3.519000	-1.411100	-2.556800
C	4.560200	-2.039800	-3.266000
C	4.760800	-3.409200	-3.198300
C	3.938100	-4.147200	-2.325000
C	2.941400	-3.565700	-1.553500
C	2.708100	-2.162600	-1.651200
O	1.780100	-1.647100	-0.885100
N	-0.198700	1.396000	-2.094900
C	-1.339900	1.787800	-1.642500
C	-2.093100	1.144000	-0.609700
C	-3.311900	1.750000	-0.232500
C	-4.149100	1.202100	0.722900

H	3.869900	3.952200	4.090400
C	5.226700	3.608100	6.485500
H	4.945300	1.958200	5.101900
H	6.530400	2.724400	4.995300
H	5.760000	4.570000	6.545700
H	4.155900	3.807500	6.650200
H	5.581300	2.974300	7.311600
C	-2.803800	6.187800	-4.523000
H	-1.710800	4.600000	-3.563300
H	-3.182000	4.062400	-4.377400
C	-2.033300	6.102400	-5.839900
H	-3.853800	6.467600	-4.722200
H	-2.379300	6.991400	-3.894900
H	-2.064100	7.056200	-6.387000
H	-0.977900	5.849200	-5.657500
H	-2.453700	5.320900	-6.490600
C	-4.748100	5.065100	1.851400
H	-3.218500	5.617000	0.442900
H	-4.857900	5.981000	-0.118700
C	-3.749800	4.333400	2.754000
H	-4.959000	6.066700	2.262600
H	-5.711700	4.524400	1.843600
H	-2.805400	4.897800	2.819900
H	-4.148000	4.233000	3.775300
H	-3.517900	3.323200	2.383700
C	-0.814700	5.432400	-0.591300
H	-1.808400	3.993700	0.709300
H	-0.404400	3.394000	-0.131500
C	0.140600	5.930800	0.492700
H	-0.293500	5.430100	-1.561000
H	-1.650500	6.144900	-0.677600
H	-0.342000	5.905300	1.483100
H	1.027600	5.285900	0.524200
H	0.467100	6.962700	0.300400
O	0.582900	-1.387400	-3.785600
C	1.700900	-1.986500	-4.527900
C	0.643000	-1.282400	-5.262200
C	-0.492400	-1.957700	-5.959100
H	2.649000	-1.469800	-4.372500
H	1.694400	-3.076900	-4.461500
H	0.888300	-0.260800	-5.563100
H	-1.400900	-1.342800	-5.877100

H	6.121600	-4.340700	-6.252700	C	-3.747900	-0.016500	1.312600
C	2.925500	-3.177700	-5.569300	C	-2.578900	-0.669900	0.965500
H	4.018100	-4.038800	-7.214800	C	-1.707300	-0.104400	-0.022900
H	3.759500	-5.184600	-5.888900	O	-0.655800	-0.799500	-0.341900
H	2.713200	-3.334900	-4.506500	Co	0.760100	-0.121100	-1.469400
H	3.281400	-2.151100	-5.703300	C	1.991200	2.028600	-2.774300
C	-5.074900	2.738800	2.478100	C	0.513400	2.058100	-3.193900
H	-5.769000	2.584800	0.419800	C	0.044600	3.457100	-3.568400
H	-6.179900	1.190700	1.431100	C	0.970800	4.046700	-4.639800
C	-4.103700	3.888600	2.179800	C	2.426900	4.053200	-4.169200
H	-6.008800	3.136100	2.912200	C	2.903300	2.638100	-3.827900
H	-4.649600	2.053400	3.224600	C	2.071300	-4.355400	-0.624600
C	-3.287000	4.414800	3.357400	C	-2.197100	-1.993100	1.555100
H	-3.411500	3.567400	1.389200	C	-5.381300	1.917700	1.209200
H	-4.670500	4.732900	1.752100	C	5.701500	-4.099800	-4.152800
H	-3.091000	5.489500	3.255500	H	5.143900	-1.430300	-3.956900
H	-3.808800	4.267200	4.313600	H	4.073900	-5.231300	-2.268100
N	1.535400	-3.209400	-6.226700	H	2.250200	-4.061500	0.422500
C	0.647800	-4.234400	-5.543900	H	1.010300	-4.149500	-0.831600
C	0.948600	-1.825000	-5.952800	H	2.262800	-5.432800	-0.719600
C	1.610500	-3.463600	-7.712700	H	4.005600	0.479200	-3.479800
C	1.227700	-5.626900	-5.367600	H	2.066100	2.598600	-1.829300
H	0.384100	-3.793300	-4.572900	H	2.903600	1.997000	-4.727800
H	-0.276200	-4.284600	-6.137600	H	3.941000	2.668400	-3.458400
C	-0.468200	-1.602300	-6.455100	H	3.076700	4.473700	-4.953100
H	0.990200	-1.708600	-4.860500	H	2.523000	4.712000	-3.285400
H	1.663000	-1.103500	-6.371200	H	0.895600	3.441200	-5.558700
C	2.352800	-2.370600	-8.470400	H	0.637400	5.066500	-4.893100
H	2.097100	-4.439800	-7.840800	H	-0.992500	3.421400	-3.942400
H	0.572700	-3.569000	-8.060300	H	0.055900	4.100200	-2.671900
C	0.217400	-6.531900	-4.644700	H	0.423900	1.390100	-4.069500
H	1.497300	-6.071800	-6.339800	H	-3.597700	2.680300	-0.733000
H	2.139800	-5.580500	-4.754000	H	-4.396900	-0.475500	2.064800
C	-0.007100	-6.127300	-3.185400	H	-2.951100	-2.340100	2.274900
H	-0.741800	-6.528500	-5.192400	H	-1.220000	-1.938100	2.060100
H	0.595100	-7.567600	-4.688300	H	-2.079900	-2.748100	0.761600
H	0.951400	-6.103600	-2.645400	H	-1.798900	2.678900	-2.086000
H	-0.464700	-5.131600	-3.096600	C	5.404000	-3.781000	-5.628000
H	-0.664100	-6.847800	-2.675500	H	6.746600	-3.811200	-3.939400
C	-0.918000	-0.165200	-6.135800	H	5.640600	-5.189700	-3.988700
H	-0.530600	-1.753800	-7.547600	C	3.985900	-4.132700	-6.119700
H	-1.168300	-2.300400	-5.971600	H	5.576800	-2.714200	-5.843100

H	-0.789900	6.304300	6.591500	C	-0.119100	0.912600	-6.871200
H	2.002600	5.518000	5.521300	H	-1.987900	-0.077800	-6.391300
H	1.632900	5.957600	7.207800	H	-0.852400	-0.007400	-5.047900
H	0.981700	4.459900	6.499500	H	-0.180800	0.770700	-7.963300
C	-2.701600	0.330000	5.178500	H	-0.522900	1.912400	-6.648200
H	-2.283300	2.304300	5.963800	H	0.945800	0.903200	-6.594700
H	-3.807800	2.199900	5.052600	C	2.870600	-2.872200	-9.819600
C	-1.360700	-0.177200	5.715300	H	1.685000	-1.508000	-8.630500
H	-3.520300	-0.014300	5.832100	H	3.206400	-1.979900	-7.887300
H	-2.898400	-0.102600	4.181600	C	3.611800	-1.766700	-10.571800
H	-1.242500	0.093100	6.776000	H	3.555700	-3.722800	-9.648600
H	-1.291900	-1.272000	5.633500	H	2.037500	-3.260300	-10.434300
H	-0.508200	0.268500	5.185000	H	2.934100	-0.930300	-10.803500
O	1.240500	0.916100	0.193600	H	4.429800	-1.369000	-9.952100
C	2.571700	0.895800	0.822800	H	4.033000	-2.135500	-11.518800
C	1.507400	0.050100	1.375600	N	-1.924400	3.773400	3.517500
C	0.709500	0.420800	2.572100	C	-1.073600	3.849100	2.243000
H	3.338700	0.430000	0.201300	C	-1.205900	4.409000	4.710100
H	2.797800	1.849700	1.308500	C	-2.019600	2.278600	3.810100
H	1.542700	-0.999500	1.076500	C	-1.145600	5.130700	1.423900
H	0.703600	1.507900	2.697400	H	-0.039600	3.646500	2.587900
H	-0.316700	0.044000	2.469800	H	-1.399700	3.002000	1.620700
H	1.158100	-0.014100	3.477900	C	-0.592200	5.780400	4.491500
O	4.832900	-0.864900	-6.911800	H	-1.957600	4.453500	5.512700
C	4.312100	-0.002100	-6.171500	H	-0.420600	3.677900	4.978900
O	5.194000	0.769900	-5.340400	C	-2.757900	1.867100	5.071200
O	3.108500	0.299800	-5.980900	H	-2.474900	1.817700	2.922000
C	6.584900	0.492700	-5.537400	H	-0.970400	1.964400	3.889300
H	6.877400	0.655300	-6.584600	C	-0.478900	4.905200	0.056700
H	7.129200	1.183100	-4.879500	H	-2.184900	5.451000	1.250100
H	6.836400	-0.546300	-5.272600	H	-0.632200	5.955700	1.936500
O	0.241500	-1.220800	-2.965400	C	0.953600	4.376200	0.148500
C	-0.962800	-1.711400	-3.054200	H	-1.093600	4.196000	-0.522500
O	-1.946800	-0.793600	-2.810600	H	-0.501200	5.861900	-0.492300
C	-3.263300	-1.348200	-2.644000	H	1.462400	4.462000	-0.822300
O	-1.222200	-2.864700	-3.405700	H	1.544200	4.930300	0.894100
H	-3.242200	-2.160800	-1.905700	H	0.966600	3.317400	0.439300
H	-3.880500	-0.521500	-2.273500	C	-0.004200	6.304600	5.813300
H	-3.650300	-1.733400	-3.597600	H	0.228200	5.699800	3.763000
O	1.784000	3.393300	3.265100	H	-1.331100	6.506300	4.110500
C	1.848800	2.799600	4.379000	C	1.215600	5.513700	6.291300
O	3.118800	2.613600	4.948500	H	0.277800	7.360500	5.662200

H	1.600600	1.552200	1.960400	O	0.917800	2.324500	5.079300
H	1.066100	4.043700	0.261300	C	4.207900	3.109500	4.159900
H	2.619000	3.673300	1.051600	H	5.109200	2.972100	4.771300
H	1.258000	5.236200	2.453000	H	4.310200	2.545600	3.219900
H	1.574100	3.705000	3.283400	H	4.073300	4.171600	3.911200
H	-1.039700	4.480800	1.859800	187			
H	-0.807200	4.346100	3.609900	2-trans-a-SPO			
H	-1.949000	2.332100	2.639700	N	1.553000	1.314900	-0.101800
H	-0.390700	1.888300	3.390800	C	2.714400	1.514200	-0.633800
H	-0.858600	2.439200	0.410500	C	3.287200	0.744300	-1.692700
H	-3.904200	-1.057900	2.313900	C	4.511400	1.213500	-2.212700
H	-4.070800	-4.535000	-0.213100	C	5.145800	0.588300	-3.268300
H	-0.830800	-4.959900	-0.657800	C	4.524000	-0.547400	-3.829600
H	-0.981400	-3.834600	-2.011300	C	3.323900	-1.051300	-3.353700
H	-2.258300	-5.060000	-1.715300	C	2.668400	-0.415800	-2.250500
H	-2.250200	0.389200	2.266500	O	1.550800	-0.946900	-1.839900
C	7.585200	-0.007800	-3.249500	Co	0.437400	-0.191500	-0.451200
H	6.593000	1.163200	-4.775200	N	-0.649100	0.472700	0.961000
H	6.734800	2.006600	-3.221600	C	-1.677700	-0.116700	1.475700
C	7.425700	-0.489300	-1.799200	C	-2.211000	-1.376200	1.036200
H	7.500100	-0.898200	-3.895300	C	-3.473700	-1.724000	1.560100
H	8.599400	0.399600	-3.409000	C	-4.195100	-2.795600	1.060600
C	7.791000	0.594600	-0.796300	C	-3.546200	-3.642100	0.141900
H	6.379300	-0.805800	-1.662600	C	-2.267500	-3.395000	-0.339900
H	8.061100	-1.376300	-1.661300	C	-1.611100	-2.177800	0.017000
H	8.870500	0.805300	-0.836800	O	-0.498600	-1.880600	-0.606400
H	7.249000	1.539900	-0.980800	C	1.139500	2.066400	1.096100
C	-6.510600	-1.769600	0.888600	C	-0.365700	1.890600	1.234500
H	-6.028800	-3.889400	0.928300	C	-0.859500	2.450500	2.561400
H	-5.806000	-3.061800	2.478800	C	-0.480700	3.934700	2.640900
C	-6.244000	-1.384400	-0.589000	C	1.020900	4.159900	2.440400
H	-7.575500	-2.019100	1.024200	C	1.528400	3.541600	1.130700
H	-6.317900	-0.889800	1.520800	C	2.647600	-2.238900	-3.969700
C	-5.354400	-0.144500	-0.635700	C	-1.554800	-4.362200	-1.239200
H	-5.775500	-2.239500	-1.102600	C	-5.657900	-2.957900	1.389900
H	-7.199200	-1.185800	-1.100500	C	6.524900	1.028100	-3.681700
H	-5.913900	0.737700	-0.302000	H	4.978000	2.090800	-1.757100
H	-4.499700	-0.241900	0.040500	H	5.001100	-1.055400	-4.674400
N	7.478700	0.227900	0.661300	H	3.218800	-2.623400	-4.825900
C	8.304800	1.113300	1.586400	H	2.515400	-3.048500	-3.234200
C	5.982100	0.447000	0.881500	H	1.635400	-1.966700	-4.304100
C	7.810400	-1.218000	0.961200	H	3.347800	2.324900	-0.244800

H	-4.144100	-1.835300	-2.043100	C	7.960800	2.585900	1.527000
C	-5.516400	1.077500	-4.291000	H	8.166000	0.710100	2.600700
H	-6.028500	-0.796600	-3.300500	H	9.352400	0.946300	1.298900
H	-6.711800	0.656000	-2.547600	C	5.495500	0.195300	2.299100
C	-4.868300	2.730500	-1.488900	H	5.755100	1.490100	0.593300
H	-3.282500	1.359400	-1.027700	H	5.474000	-0.214600	0.167400
H	-3.432600	1.676800	-2.762900	C	9.268000	-1.615900	0.765100
C	-1.933400	-1.892600	-3.725600	H	7.516300	-1.389800	2.004700
H	-3.841500	-1.162000	-4.427800	H	7.144100	-1.814100	0.325600
H	-2.675600	0.104600	-3.920600	C	8.836600	3.405200	2.476400
C	-1.197700	-1.829100	-5.062700	H	8.075000	2.964500	0.499900
H	-1.230100	-1.677600	-2.906000	H	6.903600	2.748500	1.787100
H	-2.324400	-2.910200	-3.556600	C	8.511300	4.895400	2.355200
H	-1.877800	-2.024100	-5.908600	H	8.675900	3.069800	3.517300
H	-0.756800	-0.830900	-5.208100	H	9.905700	3.235500	2.251600
H	-0.386600	-2.571000	-5.106400	H	7.440400	5.078500	2.530900
C	-6.538300	0.776000	-5.396600	H	9.092200	5.494100	3.072300
H	-5.556100	2.146900	-4.039400	H	8.738200	5.258000	1.341600
H	-4.506400	0.882400	-4.671000	C	4.033800	0.641500	2.415000
C	-6.349100	-0.594600	-6.051000	H	5.573900	-0.870000	2.579700
H	-7.562700	0.863400	-4.991100	H	6.094300	0.767800	3.027400
H	-6.448000	1.558500	-6.168000	C	3.446500	0.340400	3.791200
H	-7.084100	-0.753700	-6.854000	H	3.985100	1.720000	2.197300
H	-5.343900	-0.678700	-6.492500	H	3.437700	0.134400	1.642400
H	-6.468900	-1.419800	-5.332600	H	3.515400	-0.734000	4.030100
C	-4.066500	4.021200	-1.734700	H	3.976900	0.891700	4.584300
H	-5.793800	2.764100	-2.086400	H	2.384700	0.623500	3.841100
H	-5.132300	2.677400	-0.421700	C	9.424400	-3.144400	0.806800
C	-2.736600	4.060400	-0.972100	H	9.652100	-1.241200	-0.197500
H	-3.874000	4.136300	-2.816800	H	9.889400	-1.170700	1.557200
H	-4.694700	4.874400	-1.428800	C	8.815600	-3.865000	-0.397600
H	-2.026100	3.330900	-1.388200	H	10.500600	-3.376700	0.862000
H	-2.271000	5.055000	-1.049100	H	8.979500	-3.531400	1.741100
H	-2.897900	3.813100	0.087200	H	8.983700	-4.949900	-0.327900
O	1.712900	-1.128200	0.870900	H	7.729200	-3.709900	-0.474900
C	1.347300	-2.265900	1.717600	H	9.272600	-3.516200	-1.336800
C	2.132400	-2.487000	0.495500	N	-4.734000	0.200500	-1.985000
C	3.617700	-2.670100	0.465700	C	-3.682700	-0.868800	-2.279700
H	1.842100	-2.225400	2.690900	C	-5.817300	0.250200	-3.042800
H	1.566900	-2.839600	-0.370500	C	-4.002200	1.530200	-1.837300
H	0.283100	-2.505600	1.710700	C	-3.086500	-0.884800	-3.673800
H	4.020600	-2.173700	-0.430900	H	-2.888400	-0.679300	-1.548400

C	-4.526300	-2.823600	-1.056600	H	4.089300	-2.241900	1.361300
C	-4.268800	-3.689300	-2.146700	H	3.866300	-3.741300	0.409200
C	-3.061400	-3.701600	-2.816700	O	4.949300	3.304100	0.610600
C	-2.003000	-2.822600	-2.401400	C	5.691100	3.942100	-0.188000
O	-0.836600	-3.003000	-2.938000	O	5.621900	5.330200	-0.008600
C	1.825500	0.524700	-1.616200	O	6.468100	3.493400	-1.071900
C	0.337200	0.820600	-1.805200	C	6.444700	6.086700	-0.908600
C	-0.143100	1.874700	-0.816000	H	6.273900	7.140400	-0.655100
C	0.701900	3.147100	-0.973100	H	7.507900	5.835600	-0.783000
C	2.197400	2.855600	-0.824700	H	6.166800	5.896600	-1.955400
C	2.674200	1.775700	-1.803000	O	-0.791800	0.648700	-1.670700
C	2.556600	-5.315100	-5.020100	C	-0.470000	1.329700	-2.735200
C	-2.801000	-4.577000	-4.003700	O	0.854400	1.596000	-2.851000
C	-5.705600	-3.050500	-0.150300	C	1.262900	2.212900	-4.083600
C	7.189600	-3.266500	-4.776900	O	-1.295600	1.719800	-3.569200
H	5.746700	-1.169100	-3.741400	H	2.358200	2.226100	-4.040400
H	5.259800	-5.123100	-5.348300	H	0.919000	1.620400	-4.940900
H	1.794000	-4.910500	-5.705900	H	0.860600	3.231800	-4.160800
H	3.102500	-6.122700	-5.525900	O	-3.778600	1.877500	1.201500
H	2.002100	-5.732400	-4.170800	C	-4.407100	1.476600	2.210200
H	4.077900	-0.032100	-2.803400	O	-5.829200	1.570500	2.039900
H	1.966000	0.168300	-0.576700	O	-3.985700	0.988600	3.284300
H	2.572500	2.125800	-2.846300	C	-6.581100	1.212000	3.205500
H	3.733000	1.545900	-1.617000	H	-6.360200	1.889100	4.044700
H	2.782600	3.776900	-0.977500	H	-7.639600	1.296700	2.924300
H	2.405900	2.517200	0.206800	H	-6.358300	0.185500	3.533900
H	0.511500	3.578300	-1.972300	187			
H	0.378700	3.899000	-0.234400	2-trans-n2-SPO			
H	-1.205900	2.109300	-0.988300	N	2.133100	-0.620000	-2.484900
H	-0.044400	1.480900	0.212700	C	3.317300	-0.798000	-2.972500
H	0.200800	1.197900	-2.837300	C	3.761500	-1.978200	-3.649000
H	-3.779600	-1.111200	-0.004300	C	5.131000	-2.036900	-3.986600
H	-5.045100	-4.397100	-2.454200	C	5.702400	-3.169400	-4.540700
H	-2.669700	-3.949400	-4.900600	C	4.841800	-4.241000	-4.853400
H	-3.629700	-5.277200	-4.175700	C	3.481400	-4.218600	-4.588500
H	-1.862500	-5.134600	-3.889900	C	2.912600	-3.097500	-3.907900
H	-1.942900	0.148600	-0.653000	O	1.662800	-3.199700	-3.544900
C	8.047100	-3.185900	-3.499800	Co	0.651200	-1.796000	-2.703800
H	7.404800	-4.220700	-5.288000	N	-0.348200	-0.474100	-1.786200
H	7.514200	-2.466200	-5.465600	C	-1.507100	-0.661000	-1.248100
C	7.668900	-4.224600	-2.417200	C	-2.334600	-1.808300	-1.448300
H	9.102600	-3.323900	-3.785800	C	-3.579100	-1.855900	-0.779900

C	7.167400	-0.953800	3.255400	H	7.977600	-2.175300	-3.062100
H	5.576800	-1.028500	1.789500	C	6.711000	-3.568000	-1.432600
H	5.361100	-2.152600	3.155900	H	7.232500	-5.112800	-2.898800
H	7.732800	-1.623000	3.924500	H	8.582200	-4.549200	-1.894500
H	7.879100	-0.476900	2.564500	H	7.211900	-2.722500	-0.941500
H	6.713200	-0.164600	3.873100	H	5.845800	-3.144700	-1.956200
C	3.638400	-6.914000	-2.007600	C	-5.620400	-4.377700	0.638300
H	5.427700	-5.953500	-2.739200	H	-5.774300	-2.213400	0.565400
H	5.688400	-7.047200	-1.354000	H	-6.650000	-3.054700	-0.722900
C	3.694600	-8.100600	-2.963000	C	-4.319400	-4.598300	1.440600
H	3.210300	-7.209700	-1.035400	H	-6.472700	-4.419100	1.337500
H	2.970200	-6.143100	-2.418600	H	-5.753300	-5.224000	-0.058700
H	4.096900	-7.798700	-3.942100	C	-3.172300	-4.977100	0.513000
H	4.339700	-8.900200	-2.564600	H	-4.078300	-3.685600	2.009100
H	2.694400	-8.526600	-3.127700	H	-4.502400	-5.401600	2.172800
N	-1.870400	-5.418400	1.152300	H	-3.482000	-5.801200	-0.142000
C	-2.052300	-6.779600	1.811400	H	-2.895200	-4.137500	-0.126600
C	-0.819400	-5.470700	0.052900	N	6.104300	-4.427100	-0.322800
C	-1.413000	-4.422100	2.209900	C	7.102900	-5.416300	0.215800
C	-0.784000	-7.451400	2.343200	C	5.630700	-3.460800	0.768100
H	-2.761500	-6.597300	2.629500	C	4.843100	-5.114300	-0.823900
H	-2.555600	-7.414000	1.067200	C	6.580800	-6.257500	1.371500
C	-1.160700	-6.358600	-1.131500	H	7.396900	-6.047900	-0.629400
H	-0.703800	-4.436800	-0.294200	H	7.984900	-4.833100	0.517300
H	0.116100	-5.787100	0.540500	C	6.725700	-2.828300	1.607200
C	-1.330100	-2.978400	1.737200	H	5.110200	-2.654900	0.223300
H	-2.127300	-4.530300	3.038200	H	4.922900	-4.028900	1.386100
H	-0.415900	-4.759400	2.541700	C	5.014600	-6.283700	-1.774900
C	-0.086400	-8.419500	1.380500	H	4.269000	-5.433800	0.057900
H	-0.056900	-6.700900	2.698900	H	4.282200	-4.312200	-1.317300
H	-1.091800	-8.020500	3.238700	C	7.516600	-7.435200	1.670900
C	1.062600	-9.155700	2.067300	H	6.476600	-5.631500	2.268900
H	-0.823300	-9.145700	0.988300	H	5.572200	-6.642200	1.158900
H	0.330300	-7.871400	0.524700	C	7.504000	-8.516200	0.586500
H	0.712600	-9.710100	2.952400	H	8.546900	-7.067300	1.825300
H	1.534500	-9.874100	1.380600	H	7.202600	-7.882500	2.628200
H	1.831900	-8.435000	2.380000	H	6.481600	-8.893800	0.428500
C	0.027500	-6.392500	-2.099900	H	7.878800	-8.142400	-0.378800
H	-1.384700	-7.387000	-0.804500	H	8.138300	-9.369300	0.870800
H	-2.041900	-5.976300	-1.668500	C	6.106700	-1.718400	2.466800
C	-0.184600	-7.414000	-3.215600	H	7.225400	-3.567600	2.256700
H	0.174800	-5.384500	-2.524500	H	7.477300	-2.350400	0.960100

O	2.260300	-6.179800	1.106700	H	0.939700	-6.642700	-1.535600
C	3.888600	-4.758000	3.871900	H	0.649200	-7.405400	-3.931200
H	4.972600	-4.677300	4.029600	H	-0.269900	-8.433200	-2.805100
H	3.438100	-3.755300	3.858800	H	-1.106000	-7.202100	-3.780700
H	3.432200	-5.334000	4.690300	C	-0.924100	-2.061500	2.899500
187				H	-0.590100	-2.875500	0.930600
2-trans-n1-SPO				H	-2.290100	-2.629500	1.327500
N	0.105400	-0.009200	-0.210900	C	-2.003900	-1.912400	3.973300
C	0.072300	0.006700	1.086000	H	0.007300	-2.438000	3.354100
C	1.242600	-0.067300	1.917900	H	-0.690500	-1.069200	2.479700
C	1.094900	0.240600	3.289100	H	-2.948500	-1.551700	3.534700
C	2.182600	0.243800	4.144300	H	-2.209800	-2.864400	4.485400
C	3.433400	-0.164500	3.634600	H	-1.696000	-1.191200	4.745600
C	3.623200	-0.509600	2.308100	O	0.975400	-2.629700	-0.815700
C	2.525400	-0.420500	1.402500	C	1.914700	-3.760000	-0.719100
O	2.760700	-0.694700	0.146200	C	2.311700	-2.471400	-0.156200
Co	1.713100	0.131400	-1.229200	C	2.251000	-2.179900	1.308800
N	0.613800	0.771300	-2.644100	H	1.607900	-4.558800	-0.046200
C	0.960600	0.825000	-3.888900	H	3.000700	-1.852600	-0.731700
C	2.291000	0.577900	-4.370300	H	2.277400	-4.059400	-1.698500
C	2.508600	0.761200	-5.752900	H	1.712700	-2.955700	1.869000
C	3.784300	0.833300	-6.285900	H	3.277800	-2.112300	1.693500
C	4.874500	0.600800	-5.424300	H	1.781000	-1.199800	1.482400
C	4.716100	0.354800	-4.070700	O	7.162500	-0.643600	-0.657100
C	3.406700	0.371900	-3.497900	C	5.999400	-0.305600	-0.957000
O	3.346800	0.223300	-2.202200	O	5.858100	0.711300	-1.964500
C	-1.081700	0.119000	-1.068800	O	4.881000	-0.708600	-0.543100
C	-2.377800	0.498700	-0.366500	C	7.093500	1.190700	-2.505400
C	-3.496100	0.722100	-1.391000	H	7.655300	0.384400	-3.002200
C	-3.095700	1.758500	-2.444800	H	6.825000	1.963600	-3.238000
C	-1.803400	1.362600	-3.167700	H	7.733000	1.616000	-1.718800
C	-0.701700	1.163500	-2.137800	O	0.435400	-1.040300	-4.432500
C	4.949300	-0.943200	1.760400	C	-0.751100	-0.708900	-4.876300
C	5.872500	0.111900	-3.148900	O	-0.640300	-0.513900	-6.243300
C	2.088900	0.854800	5.516400	C	-1.872000	-0.078800	-6.847700
C	4.005800	1.421400	-7.653500	O	-1.806400	-0.547600	-4.275800
H	0.104000	0.537300	3.640300	H	-1.648400	0.026100	-7.915200
H	4.298000	-0.185200	4.305300	H	-2.667000	-0.819700	-6.688800
H	5.765000	-0.713600	2.460400	H	-2.199700	0.882300	-6.426600
H	4.957900	-2.029700	1.568900	O	1.481600	-5.123100	2.971700
H	5.131200	-0.455900	0.791600	C	2.363800	-5.587700	2.209500
H	-0.880900	0.121900	1.620800	O	3.718300	-5.423200	2.613200

C	0.917600	6.495100	1.961800	H	-1.203800	-0.849800	-1.592400
H	2.043900	5.827700	3.674900	H	-2.213600	1.425300	0.203400
H	2.186300	4.766100	2.241800	H	-2.666100	-0.269600	0.368000
C	-0.457400	3.663700	1.100000	H	-4.410500	1.039800	-0.864700
H	1.005800	2.724300	2.304900	H	-3.732600	-0.234000	-1.893400
H	-0.613700	2.676900	3.040900	H	-2.945500	2.736200	-1.950500
C	-0.547900	6.193300	4.980600	H	-3.903200	1.896900	-3.181200
H	-1.272300	5.486500	3.074300	H	-1.529600	2.138500	-3.901700
H	-1.360200	4.263600	4.376000	H	-1.956400	0.421200	-3.727900
N	3.296300	4.784200	-4.290800	H	-0.538300	2.110000	-1.595000
C	4.700000	5.036900	-3.787000	H	1.645700	1.016700	-6.369400
C	2.792900	6.032200	-5.006600	H	5.889100	0.648100	-5.832400
C	2.407600	4.422200	-3.101100	H	6.830900	0.279000	-3.660100
C	5.363600	3.882700	-3.048900	H	5.859100	-0.922900	-2.767200
H	5.295000	5.318300	-4.668600	H	5.803700	0.760900	-2.264000
H	4.631200	5.915900	-3.129600	H	0.240200	1.170700	-4.644700
C	2.471800	7.218500	-4.112100	C	2.887100	2.178800	5.559600
H	3.583400	6.308600	-5.716500	H	1.030100	1.030000	5.765300
H	1.908700	5.717100	-5.591100	H	2.492200	0.176100	6.287700
C	0.923800	4.364900	-3.426700	C	2.531500	3.141800	4.414100
H	2.749600	3.441300	-2.748300	H	2.737800	2.674200	6.535700
H	2.635600	5.153900	-2.314200	H	3.963300	1.949100	5.487400
C	2.008300	7.493000	1.542300	C	1.138000	3.708200	4.636500
H	0.457100	6.074500	1.060900	H	3.280300	3.949100	4.368600
H	0.134600	7.049100	2.501800	H	2.590300	2.587800	3.465800
C	3.135600	6.887800	0.703000	H	0.403300	2.932300	4.905400
H	1.518100	8.298300	0.969800	H	1.176000	4.451600	5.443600
H	2.431100	7.972400	2.444400	C	3.568200	2.901700	-7.697500
H	3.732700	6.161600	1.272400	H	5.075600	1.343600	-7.913300
H	2.733000	6.340800	-0.160500	H	3.447000	0.866100	-8.425900
H	3.812900	7.675700	0.339400	C	4.098700	3.778200	-6.538700
C	-1.839200	4.311900	0.945000	H	3.907400	3.339000	-8.651800
H	0.306500	4.211900	0.537300	H	2.466500	2.964500	-7.686600
H	-0.487800	2.679400	0.604100	C	3.260800	3.610000	-5.270000
C	-2.971500	3.663400	1.744100	H	5.163200	3.555900	-6.343100
H	-1.792700	5.392900	1.170400	H	4.039000	4.818800	-6.888800
H	-2.085900	4.259900	-0.130000	H	2.201800	3.474800	-5.542500
H	-2.886000	3.857400	2.821600	H	3.583100	2.750500	-4.677400
H	-3.947800	4.047900	1.411600	N	0.497800	4.413600	3.439300
H	-2.966700	2.570000	1.641300	C	1.494400	5.384600	2.830000
C	-1.828100	7.025300	5.110600	C	0.088000	3.300000	2.467700
H	-0.302700	5.767500	5.966400	C	-0.760500	5.087700	3.955100

H	0.626600	-4.873900	-1.044900
H	-0.603300	-3.588800	-1.023900
O	-1.539800	2.200500	4.907900
C	-2.266800	1.395200	4.262800
O	-3.467300	1.087000	4.925200
O	-2.060600	0.866500	3.138500
C	-4.312200	0.168900	4.217800
H	-4.636100	0.587100	3.252900
H	-3.793800	-0.782000	4.026400
H	-5.182000	0.001800	4.866300
O	1.835900	1.971700	-0.647300
C	2.789300	2.598000	-0.041300
O	2.700500	3.787700	0.302200
O	3.924400	1.871500	0.189200
C	4.872100	2.534200	1.044500
H	5.127400	3.530000	0.656700
H	4.465000	2.632800	2.061200
H	5.754100	1.884900	1.062500
O	0.318400	2.818700	-6.253400
C	-0.226600	3.944900	-6.144500
O	-1.492600	3.864200	-5.482700
O	0.185500	5.084500	-6.465100
C	-2.139000	5.123400	-5.282500
H	-3.117900	4.897200	-4.837900
H	-1.565800	5.768600	-4.597000
H	-2.267000	5.665100	-6.231100

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N	2.024700	0.953400	-1.680100
C	3.197300	0.923000	-2.225700
C	3.679500	-0.156500	-3.035200
C	4.896600	0.044800	-3.716000
C	5.360500	-0.857100	-4.659500
C	4.613000	-2.033400	-4.863900
C	3.445900	-2.314900	-4.169300
C	2.951600	-1.374800	-3.216500
O	1.880200	-1.709000	-2.546700
Co	0.672300	-0.378500	-1.876100
N	-0.510600	0.944200	-1.189800
C	-1.707800	0.724300	-0.761500
C	-2.402000	-0.524700	-0.845700
C	-3.732500	-0.566800	-0.367900

H	0.285000	6.858800	4.697200
C	-1.710500	8.114300	6.175200
H	-2.062300	7.482800	4.132800
H	-2.670700	6.354100	5.351200
H	-2.633100	8.709100	6.240200
H	-1.521600	7.676300	7.167300
H	-0.880900	8.802000	5.946800
C	6.735800	4.333300	-2.535000
H	4.753200	3.555400	-2.193500
H	5.479900	3.012400	-3.713900
C	7.484400	3.218400	-1.807300
H	7.345700	4.697600	-3.381400
H	6.600200	5.194100	-1.855400
H	8.442500	3.579900	-1.404500
H	6.887100	2.829900	-0.970300
H	7.693300	2.377600	-2.483800
C	1.703500	8.272300	-4.918600
H	1.839700	6.913100	-3.269400
H	3.386000	7.668700	-3.686700
C	1.291700	9.463200	-4.055000
H	2.321200	8.617000	-5.766600
H	0.812400	7.792800	-5.359300
H	0.728400	10.204400	-4.640700
H	0.652800	9.137100	-3.219400
H	2.171800	9.969200	-3.626600
C	0.051500	4.561300	-2.186700
H	0.650500	5.121200	-4.174100
H	0.698000	3.396400	-3.886800
C	-0.035900	6.012800	-1.716900
H	-0.961300	4.209200	-2.439400
H	0.432400	3.921300	-1.379100
H	-0.735500	6.117000	-0.874700
H	0.937500	6.398700	-1.378500
H	-0.396700	6.665700	-2.528300
O	1.395600	-1.703800	-2.029000
C	1.421500	-2.897000	-1.154400
C	2.547200	-2.615600	-2.052600
C	0.354300	-3.895100	-1.468900
H	1.575700	-2.616700	-0.109400
H	2.633800	-3.135600	-3.008900
H	3.447500	-2.165500	-1.632600
H	0.226700	-4.003300	-2.554800

H	7.064000	0.936300	-7.084700	C	-4.548600	-1.667700	-0.552500
C	3.682700	0.991500	-6.303800	C	-4.018900	-2.755600	-1.281700
H	5.003200	1.653600	-7.878000	C	-2.716200	-2.789100	-1.735400
H	4.846000	-0.107300	-7.806200	C	-1.849400	-1.671200	-1.501800
H	3.382300	0.077400	-5.781100	O	-0.637900	-1.778500	-1.957400
H	3.901600	1.760300	-5.555800	C	1.565500	2.071000	-0.843400
C	-5.813000	-2.767000	1.297200	C	0.101600	2.277700	-1.255500
H	-6.270500	-0.819400	0.428500	C	-0.572100	3.392500	-0.468200
H	-6.634800	-2.195600	-0.628100	C	0.254700	4.678900	-0.588800
C	-4.977600	-2.189000	2.449900	C	1.693900	4.458700	-0.117900
H	-6.823300	-3.026200	1.658300	C	2.382700	3.351800	-0.922000
H	-5.355800	-3.706700	0.945300	C	2.659200	-3.572300	-4.379000
C	-4.312900	-3.249400	3.332100	C	-2.153300	-3.956900	-2.485000
H	-4.206000	-1.528800	2.032600	C	-5.899700	-1.804100	0.096100
H	-5.613400	-1.543700	3.078300	C	6.501900	-0.497300	-5.573900
H	-4.457800	-3.038500	4.398500	H	5.415400	0.990300	-3.557100
H	-4.733600	-4.246400	3.134900	H	4.955600	-2.747700	-5.618800
N	2.385700	1.461900	-6.983900	H	3.043600	-4.145200	-5.233700
C	1.588300	0.279500	-7.502100	H	2.702000	-4.212800	-3.483100
C	1.573100	2.112000	-5.863000	H	1.597700	-3.333000	-4.540300
C	2.650500	2.461300	-8.084100	H	3.869600	1.781000	-2.104600
C	2.340100	-0.739600	-8.340000	H	1.551700	1.699200	0.199700
H	1.149500	-0.191200	-6.611600	H	2.513400	3.646200	-1.978500
H	0.757000	0.703100	-8.083700	H	3.396600	3.178400	-0.528200
C	0.202600	2.626000	-6.272600	H	2.273500	5.390200	-0.217100
H	1.471200	1.332600	-5.094200	H	1.687400	4.197000	0.957300
H	2.212300	2.898400	-5.438800	H	0.268600	5.003600	-1.642600
C	3.318200	3.734700	-7.582100	H	-0.227000	5.481700	-0.007100
H	3.270300	1.950000	-8.832500	H	-1.593100	3.561200	-0.848500
H	1.677900	2.666900	-8.553600	H	-0.649400	3.101200	0.592500
C	1.381200	-1.848600	-8.801500	H	0.112900	2.546000	-2.327700
H	2.809400	-0.265800	-9.218500	H	-4.122700	0.313900	0.151500
H	3.138000	-1.204700	-7.741400	H	-4.664600	-3.616600	-1.482400
C	0.862500	-2.710600	-7.647700	H	-1.709700	-3.629200	-3.438200
H	0.534000	-1.398500	-9.349500	H	-2.925300	-4.712800	-2.683500
H	1.916800	-2.483600	-9.527100	H	-1.331600	-4.423200	-1.917800
H	0.249900	-3.543100	-8.025700	H	-2.276400	1.563800	-0.345200
H	1.704600	-3.139900	-7.084000	C	6.229300	0.787300	-6.377700
H	0.248200	-2.132800	-6.942000	H	7.434200	-0.358300	-4.997900
C	-0.490800	3.287600	-5.069600	H	6.683900	-1.337600	-6.266000
H	0.283600	3.373900	-7.081500	C	4.917700	0.801200	-7.189200
H	-0.431800	1.800000	-6.627700	H	6.223500	1.668300	-5.715300

H	-1.254800	-6.174800	1.986900	C	0.198500	4.565300	-4.587400
H	-2.925900	-7.789600	0.945100	H	-1.533900	3.508100	-5.354500
H	-2.561800	-7.105900	-0.657100	H	-0.548000	2.553700	-4.249400
H	-1.303600	-7.985100	0.242900	H	-0.377400	5.034100	-3.774600
C	-0.776300	-0.037000	3.398000	H	1.218600	4.376200	-4.222200
H	-1.069100	-1.485100	1.844500	H	0.269200	5.302400	-5.405100
H	-2.513300	-0.524900	2.192500	C	4.047500	4.477500	-8.702600
C	-0.333200	1.099500	2.482000	H	2.563100	4.398800	-7.130500
H	-1.315900	0.370800	4.271900	H	4.042200	3.525400	-6.774800
H	0.098200	-0.573800	3.802600	C	4.713400	5.748500	-8.173900
H	0.374300	1.774000	2.987200	H	4.817500	3.812200	-9.134300
H	0.148100	0.695500	1.581100	H	3.350100	4.723200	-9.524400
H	-1.199000	1.697600	2.158500	H	5.289000	6.259700	-8.959600
O	1.038600	-0.972600	0.023500	H	3.959200	6.453300	-7.790400
C	1.441300	-2.385200	0.249200	H	5.389600	5.502900	-7.341200
C	2.440600	-1.321600	0.375000	N	-2.814200	-3.372400	3.152800
C	2.890400	-0.771700	1.688600	C	-2.306600	-4.542200	3.996900
H	1.004600	-2.830900	1.152500	C	-2.423600	-3.632600	1.703600
H	3.110400	-1.190500	-0.477200	C	-2.093800	-2.104300	3.664900
H	1.433700	-2.961100	-0.677200	C	-2.512500	-4.406100	5.497100
H	3.778000	-1.326400	2.026200	H	-2.814700	-5.440400	3.620800
H	3.155000	0.292000	1.593800	H	-1.232800	-4.589900	3.752500
H	2.113100	-0.899100	2.450900	C	-2.860600	-4.982400	1.131300
O	5.397000	3.598800	-5.023600	H	-2.829500	-2.801600	1.117600
C	4.641000	3.551700	-4.029100	H	-1.327400	-3.569000	1.716900
O	5.257300	3.368500	-2.742500	C	-1.663000	-1.047900	2.658200
O	3.389500	3.593000	-3.943700	H	-2.767300	-1.662600	4.413000
C	6.688200	3.324400	-2.774400	H	-1.188700	-2.475800	4.178300
H	7.057800	2.484000	-3.381900	C	-1.664000	-5.461100	6.216700
H	7.105300	4.252300	-3.192300	H	-2.176600	-3.417900	5.845800
H	7.013000	3.197500	-1.733200	H	-3.573700	-4.529100	5.776200
O	0.403700	0.111500	-3.724700	C	-1.852300	-5.413900	7.731800
C	-0.709600	-0.107200	-4.361600	H	-1.917000	-6.467800	5.837900
O	-1.827300	0.190900	-3.632200	H	-0.608700	-5.266100	5.962600
C	-3.066800	-0.246300	-4.216800	H	-1.568000	-4.426100	8.126500
O	-0.779700	-0.472100	-5.538500	H	-2.900800	-5.603100	8.012700
H	-3.821500	-0.102200	-3.434800	H	-1.227800	-6.167500	8.233600
H	-3.306800	0.344500	-5.111400	C	-1.706600	-5.980900	1.001300
H	-3.006700	-1.307900	-4.488200	H	-3.687500	-5.432100	1.707800
O	0.520500	-3.121600	4.899300	H	-3.274000	-4.792700	0.128900
C	1.024100	-3.437500	3.793500	C	-2.147400	-7.287300	0.347600
O	2.413300	-3.272600	3.621300	H	-0.906800	-5.509900	0.405200

H	-0.865100	-0.705400	1.988300
H	0.808000	-3.231200	2.476100
H	-0.971800	-3.169300	2.461600
H	-0.095700	-3.092700	4.802400
H	-1.020800	-1.639900	4.383800
H	2.045900	-1.872800	4.431000
H	1.046600	-0.986700	5.594200
H	2.086900	0.532400	3.888300
H	0.305800	0.587100	3.788200
H	2.150300	-1.136900	2.046300
H	3.442900	3.696000	1.933300
H	3.721800	5.256100	-2.061300
H	0.817100	3.823300	-3.160700
H	1.977100	2.624100	-3.729300
H	2.380400	4.366400	-3.824200
H	2.234700	1.913200	2.454000
C	-3.247300	-4.627800	-4.914400
H	-1.772400	-6.145800	-4.489700
H	-2.816000	-5.762300	-3.111100
C	-3.937100	-3.340700	-4.404400
H	-2.724300	-4.389400	-5.857700
H	-4.029000	-5.361500	-5.174700
C	-2.962600	-2.171800	-4.433100
H	-4.800400	-3.139600	-5.059800
H	-4.326700	-3.502700	-3.386200
H	-2.200300	-2.287300	-3.662200
H	-2.450900	-2.145400	-5.402800
C	6.160900	4.616200	0.869500
H	5.227000	6.069600	-0.450400
H	4.627200	6.111300	1.216100
C	6.541600	3.462600	-0.095700
H	7.015600	5.300100	0.999600
H	5.953700	4.191400	1.863800
C	6.141500	2.134100	0.533900
H	6.026000	3.607700	-1.055000
H	7.624400	3.482100	-0.298500
H	6.773600	1.916400	1.405100
H	5.110600	2.164600	0.901100
N	-3.505400	-0.776100	-4.214700
C	-4.428100	-0.364500	-5.345700
C	-4.279800	-0.680300	-2.905500
C	-2.298600	0.161600	-4.147000

O	0.455400	-3.886200	2.756800
C	3.087000	-2.732300	4.767000
H	2.955900	-3.377900	5.647500
H	4.148900	-2.676800	4.494300
H	2.709400	-1.729500	5.018000

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N	0.098400	-1.581300	0.368200
C	-0.568000	-2.529000	-0.204800
C	-0.575300	-2.814300	-1.607100
C	-1.290100	-3.941200	-2.066600
C	-1.224600	-4.364500	-3.384000
C	-0.268800	-3.738400	-4.220700
C	0.417900	-2.602300	-3.833300
C	0.146800	-2.016900	-2.550000
O	0.587000	-0.818200	-2.326300
N	1.359300	0.546100	1.173800
C	1.964000	1.661900	1.418100
C	2.374900	2.608700	0.421500
C	3.210500	3.657000	0.865500
C	3.792500	4.543500	-0.023200
C	3.354000	4.498800	-1.361300
C	2.468700	3.541700	-1.833900
C	2.073500	2.475600	-0.969200
O	1.442800	1.465300	-1.509600
Co	0.907300	-0.109400	-0.542700
C	0.024600	-1.343000	1.819500
C	1.250200	-0.508800	2.188100
C	1.192600	-0.057000	3.641000
C	1.109600	-1.296100	4.538700
C	-0.082200	-2.186400	4.175300
C	-0.064500	-2.589500	2.694200
C	1.455900	-1.935600	-4.686400
C	1.893800	3.590600	-3.216900
C	4.934000	5.432700	0.401500
C	-2.250600	-5.312300	-3.944800
H	-1.941800	-4.466600	-1.361700
H	-0.102700	-4.137100	-5.226700
H	1.205800	-0.883500	-4.878600
H	2.422800	-1.914600	-4.156200
H	1.584400	-2.461300	-5.643200
H	-1.142900	-3.217300	0.425200

H	4.225800	1.367700	-0.949200	C	-4.776200	1.120100	-5.358700
C	7.757200	-0.571300	-1.698000	H	-3.930300	-0.671800	-6.275200
H	7.749600	1.601000	-1.580100	H	-5.338000	-0.972200	-5.232800
H	8.270100	0.797500	-0.090300	C	-3.576900	-1.244000	-1.681800
C	6.673800	-0.655400	1.653800	H	-4.475700	0.394700	-2.748500
H	4.775900	-0.053300	0.846300	H	-5.233000	-1.202800	-3.079600
H	5.693600	-1.134200	-0.228000	C	-1.443500	0.205200	-5.404600
C	4.384400	1.126900	-3.784300	H	-2.684400	1.153000	-3.869800
H	5.212800	2.783400	-2.659300	H	-1.683600	-0.210900	-3.320900
H	6.398300	1.545600	-3.130700	C	-5.946000	1.404900	-6.307500
C	4.409700	1.879400	-5.110400	H	-5.026900	1.474300	-4.345900
H	4.622600	0.061000	-3.944800	H	-3.901600	1.707100	-5.681600
H	3.372400	1.138500	-3.346900	C	-5.654100	1.063300	-7.770200
H	4.155100	2.940300	-4.966700	H	-6.840100	0.855100	-5.963200
H	5.408000	1.833800	-5.576000	H	-6.192400	2.475700	-6.223000
H	3.686300	1.454400	-5.822700	H	-5.497600	-0.016200	-7.920800
C	9.058900	-0.565400	-2.510100	H	-6.488300	1.364300	-8.421100
H	7.773900	-1.412800	-0.988700	H	-4.750100	1.587200	-8.119800
H	6.904300	-0.750200	-2.372900	C	-4.344800	-0.820300	-0.424500
C	9.030700	0.379900	-3.712900	H	-3.499400	-2.341700	-1.724100
H	9.906300	-0.308400	-1.849200	H	-2.548500	-0.865700	-1.600000
H	9.246600	-1.592700	-2.863200	C	-3.621100	-1.242900	0.851400
H	8.198900	0.124700	-4.387900	H	-4.471700	0.275700	-0.444800
H	8.909900	1.431900	-3.413300	H	-5.363300	-1.248800	-0.448200
H	9.965300	0.312800	-4.289600	H	-3.502200	-2.337500	0.900000
C	6.314800	-2.073000	2.141000	H	-2.621600	-0.787200	0.875200
H	7.742000	-0.645200	1.377500	H	-4.170200	-0.923000	1.749400
H	6.502800	0.060900	2.471400	C	-0.353300	1.282900	-5.269900
C	4.829100	-2.258500	2.474800	H	-0.961600	-0.770700	-5.563500
H	6.614300	-2.807700	1.371100	H	-2.049900	0.428500	-6.299500
H	6.923200	-2.287900	3.035600	C	-0.890100	2.708000	-5.407000
H	4.658900	-3.236400	2.951100	H	0.162900	1.152700	-4.303200
H	4.484400	-1.455900	3.142400	H	0.403600	1.094100	-6.050300
H	4.208100	-2.221800	1.567000	H	-0.064800	3.434600	-5.390100
O	-0.913900	0.660200	-0.345500	H	-1.418100	2.830700	-6.367900
C	-1.523100	1.607100	-1.487600	H	-1.577300	2.972800	-4.589000
C	-1.143700	2.108400	-0.178300	N	6.190000	0.910800	-0.363000
C	-2.167000	2.453900	0.857300	C	5.113300	0.967700	-1.451000
H	-0.798400	1.657700	-2.289600	C	7.569100	0.733500	-0.935500
H	-2.520300	1.220300	-1.638900	C	5.779900	-0.301600	0.481000
H	-0.217100	2.685200	-0.134000	C	5.374100	1.699300	-2.757300
H	-2.508700	3.485400	0.678900	H	4.886400	-0.080700	-1.677800

C	4.867100	4.148400	-0.709700	H	-3.035900	1.786000	0.783200
C	3.731400	3.657600	-1.336900	H	-1.737700	2.387200	1.867900
C	2.943800	2.661500	-0.680500	O	-4.552300	2.292500	-2.151700
O	2.030500	2.061100	-1.393500	C	-3.672700	3.192900	-2.109700
Co	0.940300	0.621900	-0.742900	O	-3.955200	4.360500	-1.387900
C	-0.380000	-0.677100	1.339700	O	-2.502700	3.174200	-2.586100
C	1.069800	-0.487400	1.821300	C	-5.244400	4.373200	-0.757000
C	1.154800	-0.327600	3.333200	H	-5.336600	3.552700	-0.029900
C	0.504400	-1.542200	4.003200	H	-5.315800	5.340600	-0.244400
C	-0.933600	-1.759300	3.526700	H	-6.052600	4.272700	-1.495800
C	-1.007300	-1.898800	1.999500	O	2.736900	-0.768300	-0.664000
C	1.445500	-0.180700	-5.022000	C	3.116900	-1.902200	-1.157000
C	3.310000	4.102700	-2.705900	O	2.235900	-2.929300	-0.942700
C	6.584300	4.166100	1.178200	C	2.552500	-4.156500	-1.622700
C	-1.954300	-3.936100	-5.080300	O	4.192800	-2.090300	-1.743500
H	-1.943100	-3.438400	-2.391800	H	2.799800	-3.964300	-2.674200
H	0.150000	-2.398400	-5.991400	H	3.400300	-4.661000	-1.137700
H	1.796500	-0.636700	-5.957900	H	1.643500	-4.765800	-1.557200
H	1.072600	0.830400	-5.234600	O	4.291100	0.823200	2.848800
H	2.295900	-0.055300	-4.335100	C	4.363300	1.880700	3.521600
H	-1.556300	-2.291400	-0.396600	O	5.715000	2.312200	3.714600
H	-0.940200	0.237100	1.615000	O	3.451900	2.605200	3.984100
H	-0.450400	-2.798000	1.678900	C	5.842300	3.478900	4.536900
H	-2.055500	-2.019800	1.685100	H	5.464700	3.292400	5.553600
H	-1.367200	-2.657300	3.997400	H	6.915200	3.712000	4.571900
H	-1.558300	-0.902300	3.838400	H	5.283700	4.330600	4.120800
H	1.107600	-2.437900	3.772100	187			
H	0.539600	-1.417800	5.096700	2-trans-a-RPO TS; i=2			
H	2.203200	-0.255400	3.666000	N	-0.298800	-0.686600	-0.126400
H	0.636100	0.603000	3.629000	C	-0.909600	-1.545300	-0.869900
H	1.613500	-1.398100	1.519200	C	-0.730800	-1.655900	-2.289200
H	4.604000	2.647600	2.320100	C	-1.290500	-2.764900	-2.955300
H	5.504300	4.845600	-1.263300	C	-1.076200	-2.989800	-4.306200
H	2.365300	4.670000	-2.649600	C	-0.132600	-2.165000	-4.959900
H	3.111900	3.244900	-3.363400	C	0.408600	-1.039000	-4.360400
H	4.070000	4.748400	-3.167100	C	-0.005900	-0.676500	-3.037300
H	2.933400	1.226500	2.478600	O	0.289000	0.510700	-2.587400
C	-2.942900	-3.204800	-6.023200	N	1.626500	0.605200	1.016100
H	-1.353800	-4.631000	-5.694000	C	2.550600	1.388500	1.461300
H	-2.528700	-4.555700	-4.370700	C	3.245400	2.373800	0.686500
C	-3.809500	-2.095500	-5.383100	C	4.376300	2.959100	1.299000
H	-2.377700	-2.763800	-6.863400	C	5.242600	3.778600	0.598900

C	-4.177900	-0.849000	0.186300	H	-3.615100	-3.958500	-6.466900
H	-5.162700	0.690600	-0.963300	C	-2.974900	-0.849000	-5.124400
H	-5.782400	-0.933400	-1.273000	H	-4.637800	-1.870600	-6.075200
H	-3.891500	-1.909100	0.103500	H	-4.254500	-2.468600	-4.445800
H	-3.266900	-0.264900	0.386100	H	-2.261300	-1.028100	-4.320200
H	-4.842100	-0.746500	1.057300	H	-2.401600	-0.592100	-6.023500
C	-0.641400	2.864200	-4.920900	C	7.402500	2.945100	1.658100
H	-1.178700	1.027800	-5.913200	H	7.160000	4.702600	0.404200
H	-2.275500	2.385500	-6.262400	H	6.462900	4.867300	2.022600
C	-1.213800	4.198000	-4.438900	C	7.470500	1.813700	0.596600
H	-0.095900	2.364300	-4.103700	H	8.417000	3.280600	1.927000
H	0.095000	3.045600	-5.722400	H	6.957400	2.546900	2.585100
H	-0.403700	4.855300	-4.088600	C	6.731700	0.584000	1.109900
H	-1.736700	4.722600	-5.256300	H	7.000000	2.178200	-0.323900
H	-1.924900	4.068300	-3.610600	H	8.517700	1.571800	0.351600
N	6.280500	-0.422300	0.062700	H	7.351100	0.027600	1.828300
C	5.334700	0.197300	-0.975000	H	5.822900	0.856300	1.665400
C	7.473800	-1.070600	-0.588000	N	-3.687700	0.422700	-4.711600
C	5.402100	-1.457500	0.772400	C	-4.541000	0.963500	-5.843300
C	5.893700	0.913400	-2.198000	C	-4.597900	0.181400	-3.514300
H	4.728400	-0.640000	-1.332500	C	-2.603300	1.431100	-4.328000
H	4.675800	0.855100	-0.399700	C	-5.069000	2.376400	-5.611700
C	7.121200	-2.216500	-1.527700	H	-3.921400	0.904200	-6.748500
H	8.005700	-0.267500	-1.111500	H	-5.375300	0.255300	-5.957300
H	8.125500	-1.417100	0.226800	C	-3.934100	-0.459000	-2.308400
C	6.072200	-2.285700	1.854200	H	-5.002900	1.165600	-3.231100
H	4.577500	-0.868900	1.198300	H	-5.423100	-0.445800	-3.884700
H	5.001700	-2.099500	-0.023500	C	-1.700200	1.887700	-5.463600
C	4.820600	0.861500	-3.295700	H	-3.110700	2.261900	-3.818100
H	6.135600	1.963900	-1.981100	H	-1.981400	0.928100	-3.578300
H	6.808500	0.435900	-2.580100	C	-6.241600	2.688200	-6.548900
C	5.224500	1.657400	-4.531900	H	-5.392700	2.519100	-4.568100
H	4.635800	-0.194600	-3.558100	H	-4.262300	3.106800	-5.783600
H	3.867500	1.230500	-2.885000	C	-5.889800	2.609700	-8.035800
H	5.395200	2.715600	-4.280500	H	-7.077600	2.001800	-6.323500
H	6.154600	1.264100	-4.974900	H	-6.604100	3.700800	-6.308500
H	4.440800	1.618300	-5.304200	H	-5.613300	1.588400	-8.342300
C	8.314700	-2.614700	-2.406400	H	-6.741700	2.916400	-8.660600
H	6.798700	-3.087900	-0.937200	H	-5.043000	3.273400	-8.273700
H	6.265900	-1.948500	-2.168200	C	-4.857100	-0.358200	-1.089300
C	8.669500	-1.577100	-3.473400	H	-3.668700	-1.510500	-2.500200
H	9.194900	-2.815100	-1.768800	H	-2.994600	0.055700	-2.072500

O	4.191400	-0.839800	4.970900
C	6.735500	-1.014700	5.513200
H	7.828900	-0.925800	5.571300
H	6.279900	-0.708900	6.466300
H	6.451900	-2.061700	5.322900

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N	-1.318500	-2.636100	-0.180500
C	-1.617100	-2.139000	-1.338200
C	-1.268800	-2.699300	-2.604600
C	-1.569200	-1.940500	-3.755000
C	-1.266600	-2.385300	-5.030500
C	-0.694600	-3.669100	-5.147500
C	-0.375500	-4.454400	-4.051800
C	-0.605600	-3.959400	-2.732400
O	-0.169200	-4.687700	-1.743700
Co	-0.344400	-4.239800	0.117000
N	-0.471900	-3.816100	1.961600
C	0.163600	-4.418600	2.912400
C	0.977100	-5.585200	2.761600
C	1.645100	-6.083500	3.905100
C	2.324600	-7.286100	3.891400
C	2.216600	-8.085500	2.727500
C	1.607900	-7.637900	1.573700
C	1.053200	-6.309600	1.526300
O	0.650300	-5.879700	0.376500
C	-1.519100	-1.855700	1.052600
C	-1.559700	-2.859200	2.202200
C	-1.578800	-2.146300	3.549200
C	-2.785100	-1.198500	3.605600
C	-2.785800	-0.212900	2.434400
C	-2.728700	-0.928700	1.079200
C	0.255600	-5.805400	-4.184000
C	1.480800	-8.480300	0.342300
C	3.298600	-7.651100	4.976200
C	-1.349800	-1.461900	-6.221000
H	-2.014000	-0.952600	-3.614300
H	-0.465500	-4.053100	-6.146400
H	0.402100	-6.079100	-5.237800
H	1.224700	-5.826100	-3.665900
H	-0.360200	-6.573400	-3.688700
H	-2.121900	-1.171100	-1.365100

H	8.069800	-3.569500	-2.900100
H	8.986800	-0.619000	-3.034300
H	9.496500	-1.931300	-4.107100
H	7.804500	-1.379400	-4.125600
C	5.181900	-3.493900	2.198600
H	7.048600	-2.668400	1.512100
H	6.249100	-1.673800	2.751100
C	3.754700	-3.125400	2.612300
H	5.153500	-4.171500	1.325100
H	5.668900	-4.054600	3.013800
H	3.202800	-2.672800	1.775800
H	3.200500	-4.027000	2.916700
H	3.755600	-2.416500	3.456100
O	-0.277100	2.014900	-0.107100
C	-1.812300	2.299700	-0.811200
C	-0.600600	3.060000	-1.068000
C	-0.403000	4.449400	-0.540300
H	-1.977500	1.407500	-1.397100
H	-2.442400	2.526700	0.042300
H	-0.127400	2.878000	-2.036400
H	0.672700	4.664400	-0.460500
H	-0.869200	5.173700	-1.224200
H	-0.861600	4.558500	0.452600
O	-5.543600	2.918100	-2.296200
C	-4.515700	3.105600	-1.614300
O	-4.634700	3.246900	-0.222700
O	-3.307300	3.162400	-2.007500
C	-5.985300	3.219700	0.267500
H	-5.913500	3.403300	1.346500
H	-6.592100	3.997800	-0.215200
H	-6.459200	2.245100	0.080600
O	2.378800	-0.563400	-1.352600
C	2.603700	-1.827900	-1.299200
O	1.746400	-2.543800	-0.484600
C	1.901000	-3.969800	-0.579100
O	3.543000	-2.392200	-1.879400
H	2.930200	-4.273100	-0.348200
H	1.207400	-4.390100	0.158900
H	1.637200	-4.311600	-1.590400
O	4.594900	0.645500	3.292000
C	4.902000	-0.121300	4.247800
O	6.323200	-0.157100	4.442400

C	5.828600	-0.936400	-5.202900	H	-0.612200	-1.231800	1.176600
H	4.123800	-1.453600	-6.458500	H	-3.644600	-1.522900	0.908800
H	4.392600	0.291000	-6.276000	H	-2.637300	-0.179300	0.280500
C	4.012000	1.751900	-3.862400	H	-3.679900	0.429600	2.477700
H	2.994600	0.185900	-2.791300	H	-1.909200	0.455500	2.514800
H	4.726200	-0.153800	-3.112200	H	-3.711500	-1.799800	3.578400
C	3.075500	-3.219100	-4.930700	H	-2.784900	-0.655100	4.564300
H	3.914200	-2.115300	-3.275200	H	-1.642900	-2.873500	4.374400
H	2.173700	-1.830200	-3.495300	H	-0.642500	-1.574500	3.675900
C	6.801200	-1.325700	-6.316000	H	-2.483300	-3.460700	2.088300
H	6.209400	-0.038000	-4.693000	H	1.646900	-5.472800	4.812100
H	5.809300	-1.724000	-4.432500	H	2.668100	-9.082600	2.728600
C	8.200700	-1.595300	-5.763600	H	1.918300	-7.977100	-0.529700
H	6.428600	-2.226700	-6.835500	H	0.416200	-8.627900	0.098400
H	6.842100	-0.524600	-7.076800	H	1.959300	-9.460000	0.478100
H	8.603600	-0.701100	-5.263300	H	0.029600	-4.058400	3.938300
H	8.170900	-2.404200	-5.017600	C	-0.251800	-0.374600	-6.139900
H	8.900100	-1.884600	-6.561800	H	-1.238000	-2.046000	-7.150700
C	4.163300	2.530100	-2.548500	H	-2.335300	-0.968700	-6.270600
H	4.904400	1.907700	-4.494900	C	1.148700	-0.992300	-5.981500
H	3.144200	2.163200	-4.400800	H	-0.300800	0.287100	-7.021500
C	4.426700	4.017600	-2.768900	H	-0.455200	0.245200	-5.251700
H	3.239900	2.393000	-1.960000	C	2.058000	-0.042500	-5.221200
H	4.980700	2.090500	-1.955700	H	1.019100	-1.901500	-5.384100
H	5.364200	4.176900	-3.325100	H	1.561100	-1.289000	-6.961100
H	3.610000	4.481800	-3.343800	H	2.331300	0.830200	-5.829600
H	4.508500	4.552000	-1.810600	H	1.521600	0.298200	-4.325300
C	4.381900	-4.007700	-5.059300	C	4.763500	-7.587300	4.485900
H	2.314100	-3.882100	-4.484700	H	3.172600	-6.958900	5.826000
H	2.686700	-2.990700	-5.933700	H	3.107700	-8.668000	5.362300
C	4.167800	-5.306500	-5.834600	C	5.180900	-6.265800	3.805600
H	5.147100	-3.408500	-5.574000	H	5.428600	-7.759400	5.349200
H	4.785700	-4.210000	-4.054200	H	4.947900	-8.419400	3.783700
H	5.095600	-5.894000	-5.901700	C	4.622100	-6.153700	2.389800
H	3.405500	-5.933100	-5.350300	H	4.845400	-5.414900	4.420800
H	3.824000	-5.101500	-6.861900	H	6.282200	-6.236400	3.784400
N	5.198000	-5.055100	1.511500	H	4.785900	-7.092300	1.846400
C	6.638400	-5.408100	1.178800	H	3.548200	-5.965800	2.400900
C	4.342400	-4.971000	0.245300	N	3.370500	-0.618000	-4.678100
C	5.126700	-3.706700	2.212500	C	4.431100	-0.673200	-5.747600
C	7.355000	-4.538800	0.147200	C	3.809100	0.285700	-3.523300
H	7.179900	-5.393400	2.134900	C	3.121200	-1.984800	-4.026600

H	2.451700	0.162400	-0.018300
H	1.943300	-0.710900	1.437600
O	-0.565500	0.553900	-0.946000
C	0.198200	0.485500	-1.927500
O	-0.113500	1.258800	-3.080800
O	1.249500	-0.197000	-2.087900
C	-1.328800	2.010500	-2.974300
H	-1.288600	2.714900	-2.131300
H	-1.432200	2.555500	-3.921700
H	-2.195900	1.348900	-2.827500
O	-1.926000	-5.311800	0.417600
C	-2.844800	-5.613500	-0.458300
O	-2.957500	-4.704600	-1.477400
C	-3.786600	-5.118600	-2.574200
O	-3.574200	-6.595800	-0.365600
H	-4.846400	-5.132000	-2.283200
H	-3.607200	-4.379200	-3.364000
H	-3.498000	-6.121300	-2.917600
O	5.569300	-1.602600	0.014700
C	5.734500	-1.802500	-1.209000
O	6.457500	-0.816700	-1.939200
O	5.361800	-2.760400	-1.936500
C	6.922400	0.279700	-1.140600
H	6.100100	0.735300	-0.571600
H	7.693200	-0.049200	-0.427100
H	7.354200	1.005700	-1.842500

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N	1.574800	-0.447800	-2.372000
C	2.725000	-0.355700	-2.950100
C	3.374000	-1.428700	-3.648100
C	4.600700	-1.136700	-4.277900
C	5.331300	-2.106900	-4.947000
C	4.749900	-3.383600	-5.070200
C	3.537300	-3.718300	-4.487300
C	2.857900	-2.762600	-3.671800
O	1.829300	-3.179900	-2.985200
Co	0.458200	-1.980100	-2.370000
N	-0.891900	-0.834900	-1.678900
C	-1.977400	-1.237800	-1.108800
C	-2.487900	-2.575900	-1.162200
C	-3.691900	-2.869300	-0.484500

H	6.595300	-6.451000	0.837700
C	4.403400	-6.192400	-0.651900
H	3.313200	-4.804000	0.587300
H	4.680500	-4.078100	-0.300400
C	3.745200	-3.370100	2.751200
H	5.872300	-3.742300	3.021800
H	5.428000	-2.959900	1.459700
C	8.164600	-3.366600	0.711500
H	8.054100	-5.215100	-0.378000
H	6.659800	-4.173400	-0.625600
C	9.008000	-2.708000	-0.380500
H	7.488100	-2.613900	1.140800
H	8.821600	-3.732200	1.522600
H	9.583000	-1.858900	0.017700
H	9.724400	-3.425800	-0.813400
H	8.370900	-2.336400	-1.197000
C	3.424100	-6.039500	-1.823300
H	5.419800	-6.328400	-1.058600
H	4.135700	-7.108000	-0.099200
C	3.525000	-7.238300	-2.765500
H	2.397900	-5.931500	-1.433300
H	3.660400	-5.110200	-2.366300
H	3.360200	-8.182900	-2.222200
H	2.776600	-7.190300	-3.567900
H	4.520500	-7.290500	-3.234800
C	3.754900	-2.024200	3.477700
H	3.009400	-3.321900	1.932400
H	3.390000	-4.142200	3.450300
C	2.373900	-1.716700	4.057700
H	4.507200	-2.035900	4.287700
H	4.060100	-1.230300	2.776700
H	2.334500	-0.716900	4.515400
H	1.610200	-1.766800	3.268200
H	2.097500	-2.455400	4.827400
O	1.494500	-3.248900	0.144600
C	2.031200	-2.828600	-1.145200
C	1.514900	-1.683900	-0.420300
C	2.387700	-0.833900	0.439900
H	3.118800	-2.938200	-1.213400
H	0.477500	-1.424000	-0.517100
H	1.481100	-3.224400	-1.996000
H	3.403500	-1.243600	0.518800

H	7.606600	-0.720400	-3.793700	C	-4.360300	-4.070800	-0.651500
C	6.835300	-2.359300	-2.109000	C	-3.885100	-4.939900	-1.663400
H	7.351300	-3.743500	-3.724500	C	-2.685900	-4.725800	-2.314100
H	8.743200	-3.016700	-2.893900	C	-1.874800	-3.589700	-1.966100
H	7.270000	-1.468600	-1.636200	O	-0.662300	-3.561300	-2.416100
H	5.851600	-2.048200	-2.477800	C	1.002000	0.636400	-1.572400
C	-5.035600	-5.720100	1.171800	C	-0.513400	0.574600	-1.806700
H	-5.700800	-3.663600	0.961000	C	-1.245500	1.570200	-0.915400
H	-6.366000	-4.779000	-0.242100	C	-0.692100	2.982700	-1.150900
C	-3.700500	-5.587000	1.939800	C	0.822800	3.039800	-0.935000
H	-5.839300	-5.905600	1.904300	C	1.562700	2.030100	-1.819600
H	-4.984900	-6.622500	0.537300	C	2.863700	-5.035500	-4.730900
C	-2.521100	-5.750800	0.992300	C	-2.185800	-5.610800	-3.414600
H	-3.661900	-4.608500	2.446200	C	-5.441800	-4.507800	0.299300
H	-3.678100	-6.365200	2.721300	C	6.729100	-1.841000	-5.443500
H	-2.642100	-6.664800	0.396400	H	4.993000	-0.122400	-4.178400
H	-2.461600	-4.912700	0.296700	H	5.268100	-4.140500	-5.667900
N	6.522900	-3.350200	-0.996100	H	3.555100	-5.770600	-5.166400
C	7.756900	-4.092400	-0.556100	H	2.431500	-5.437700	-3.807800
C	5.943800	-2.529500	0.165600	H	2.017100	-4.891000	-5.423600
C	5.414100	-4.309300	-1.417600	H	3.277000	0.585800	-2.896100
C	7.516100	-5.027900	0.619500	H	1.171600	0.361100	-0.514700
H	8.123200	-4.639100	-1.430900	H	1.428600	2.288400	-2.886100
H	8.506600	-3.327200	-0.308500	H	2.641700	2.047400	-1.602900
C	6.946800	-1.670700	0.920900	H	1.199400	4.055500	-1.136200
H	5.207500	-1.849000	-0.294600	H	1.049700	2.822100	0.125200
H	5.439200	-3.253000	0.814800	H	-0.923900	3.288200	-2.187600
C	5.776400	-5.465600	-2.340300	H	-1.204800	3.697100	-0.486200
H	4.985100	-4.686800	-0.485200	H	-2.327100	1.552600	-1.125800
H	4.649100	-3.677400	-1.891100	H	-1.100900	1.282000	0.142400
C	8.778100	-5.823300	0.974600	H	-0.694800	0.824900	-2.870800
H	7.182000	-4.456100	1.497100	H	-4.091800	-2.124200	0.210000
H	6.702700	-5.732500	0.389200	H	-4.464600	-5.835300	-1.909700
C	9.205100	-6.817000	-0.108300	H	-1.155800	-5.941400	-3.229000
H	9.607500	-5.127100	1.194100	H	-2.149300	-5.036600	-4.355000
H	8.580500	-6.371700	1.910800	H	-2.836100	-6.485800	-3.554300
H	10.063000	-7.420200	0.224400	H	-2.616500	-0.500100	-0.610800
H	8.381500	-7.507700	-0.348400	C	7.765000	-1.683300	-4.309400
H	9.504900	-6.312800	-1.039300	H	7.039100	-2.676300	-6.095000
C	6.224800	-0.906400	2.041900	H	6.751000	-0.931100	-6.067500
H	7.756800	-2.273700	1.366400	C	7.722100	-2.818600	-3.257100
H	7.378800	-0.923500	0.236400	H	8.770300	-1.634100	-4.760000

H	1.891800	-6.664500	-1.005600	C	5.764600	-1.796400	3.198300
H	0.098000	-7.933200	-3.174900	H	6.912900	-0.135300	2.426700
H	1.851500	-7.684900	-3.292700	H	5.377800	-0.364500	1.590800
H	1.197200	-8.833900	-2.101000	H	6.625300	-2.285900	3.685100
C	-0.736900	-2.155200	2.837100	H	5.234000	-1.209500	3.963900
H	-0.583900	-3.142100	0.943300	H	5.086700	-2.595200	2.865900
H	-2.210700	-3.175500	1.631200	C	4.679800	-6.540700	-2.247900
C	-1.613000	-2.051000	4.086200	H	5.859200	-5.115800	-3.378100
H	0.317600	-2.291600	3.129500	H	6.737300	-5.927400	-2.063900
H	-0.782300	-1.211400	2.270300	C	4.711700	-7.349600	-0.950200
H	-1.526400	-2.941700	4.727400	H	3.700500	-6.051100	-2.351500
H	-1.324900	-1.184000	4.699100	H	4.778100	-7.218100	-3.112200
H	-2.673900	-1.931600	3.813500	H	5.683400	-7.853900	-0.821900
O	0.934100	-2.215700	-0.473000	H	4.527600	-6.714800	-0.070400
C	2.014900	-3.643400	0.114400	H	3.933900	-8.129900	-0.962000
C	2.327600	-2.229900	-0.098800	N	-1.136800	-5.837500	1.601900
C	2.630700	-1.369300	1.102800	C	-0.978100	-7.109700	2.412800
H	1.444700	-3.866400	1.003900	C	-0.138300	-5.807400	0.452700
H	3.002500	-2.024700	-0.936700	C	-0.861300	-4.637400	2.506700
H	1.966200	-4.274000	-0.766500	C	0.456400	-7.425200	2.815100
H	2.851300	-0.340500	0.790400	H	-1.610300	-6.983100	3.303200
H	1.784400	-1.392300	1.802000	H	-1.407000	-7.921100	1.806600
H	3.517100	-1.753400	1.622900	C	-0.201700	-6.941800	-0.552400
O	6.765500	0.602100	-1.430500	H	-0.307800	-4.857300	-0.067800
C	5.520100	0.705500	-1.440100	H	0.848100	-5.775400	0.928400
O	4.961100	1.743100	-2.267800	C	-1.144500	-3.281700	1.879700
O	4.621400	0.045000	-0.861400	H	-1.479700	-4.800600	3.401000
C	5.928000	2.516200	-2.984400	H	0.199600	-4.706500	2.789000
H	5.360700	3.274800	-3.540300	C	0.509600	-8.540800	3.862000
H	6.639300	2.998500	-2.298700	H	1.035800	-7.738700	1.931900
H	6.502900	1.892900	-3.687000	H	0.963700	-6.532800	3.212400
O	0.095100	-1.618400	-4.231300	C	1.951700	-8.852700	4.262200
C	-1.115000	-1.639500	-4.706500	H	-0.064400	-8.234300	4.754200
O	-1.031200	-1.589300	-6.096500	H	0.022500	-9.452000	3.470800
C	-2.318900	-1.557100	-6.732900	H	1.996700	-9.648500	5.020100
O	-2.199700	-1.677400	-4.131300	H	2.541200	-9.177600	3.391200
H	-2.908600	-2.448300	-6.476000	H	2.437000	-7.956500	4.676800
H	-2.888400	-0.666700	-6.430000	C	0.940600	-6.735300	-1.559900
H	-2.111600	-1.530000	-7.809200	H	-0.085700	-7.925600	-0.065100
O	2.399700	-4.754100	2.887500	H	-1.160800	-6.941400	-1.092800
C	3.403600	-4.859200	2.161700	C	1.026500	-7.859800	-2.587600
O	4.647200	-5.155200	2.710900	H	0.794300	-5.765100	-2.066400

H	4.012900	-6.161600	4.439200	O	3.504300	-4.731200	0.888000
H	5.686100	-5.499400	4.418900	C	4.642300	-5.311800	4.141000
				H	4.273300	-4.401900	4.632400