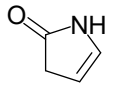
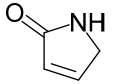
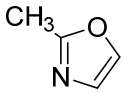
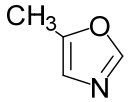
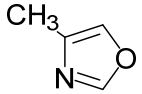
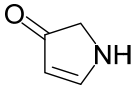
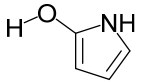
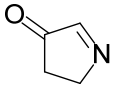
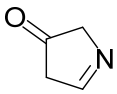
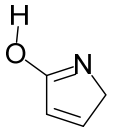
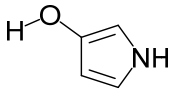
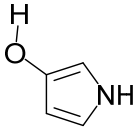
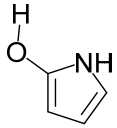
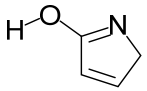
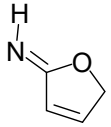
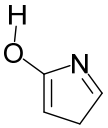
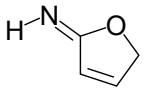
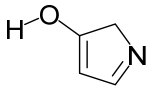
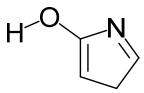
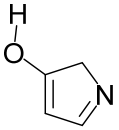
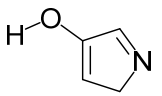
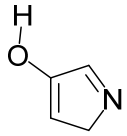
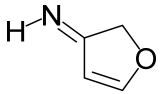
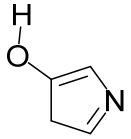
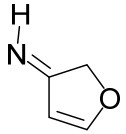
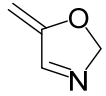
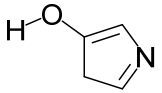
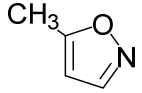
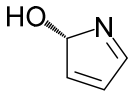
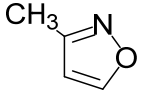
Table S1. Molecules C_4H_5NO containing 5-membered heterocycles and their thermodynamic parameters

Structure	E(zpve), a.u.	ΔE(zpve), kcal/mol	H, a.u.	ΔH(kcal/mol)	G(298), a.u.	ΔG(kcal/mol)
 **000**	-285.229335	0	-285.223367	0	-285.257581	0
 **001**	-285.229061	0.17	-285.223032	0.21	-285.257548	0.02
 **002**	-285.220611	5.47	-285.214513	5.56	-285.249214	5.25
 **003**	-285.218815	6.60	-285.212765	6.65	-285.247266	6.47
 **004**	-285.217305	7.55	-285.211248	7.60	-285.245791	7.40
 **005**	-285.213312	10.05	-285.208309	9.45	-285.241513	10.08
 **006**	-285.212644	10.47	-285.206465	10.61	-285.240877	10.48
 **007**	-285.209030	12.74	-285.203052	12.75	-285.237651	12.51
 **008**	-285.208787	12.89	-285.202817	12.90	-285.237320	12.71
 **009**	-285.209240	12.61	-285.203516	12.46	-285.237152	12.82

 **010**	-285.208165	13.28	-285.201927	13.45	-285.236503	13.23
 **011**	-285.207693	13.58	-285.201520	13.71	-285.235890	13.61
 **012**	-285.206885	14.09	-285.201149	13.94	-285.234783	14.31
 **013**	-285.200612	18.02	-285.194710	17.98	-285.228657	18.15
 **014**	-285.200473	18.11	-285.194736	17.97	-285.228525	18.23
 **015**	-285.198230	19.52	-285.192314	19.49	-285.226266	19.65
 **016**	-285.195834	21.02	-285.190090	20.88	-285.223902	21.13
 **017**	-285.195373	21.31	-285.189527	21.23	-285.223389	21.46
 **018**	-285.193806	22.29	-285.187914	22.25	-285.221826	22.44
 **019**	-285.193250	22.64	-285.187290	22.64	-285.221368	22.72

 **020**	-285.192141	23.34	-285.186252	23.29	-285.220187	23.47
 **021**	-285.190268	24.51	-285.184214	24.57	-285.218487	24.53
 **022**	-285.188657	25.53	-285.182835	25.43	-285.216878	25.54
 **023**	-285.188653	25.53	-285.182706	25.52	-285.216720	25.64
 **024**	-285.186932	26.61	-285.181113	26.51	-285.215140	26.63
 **025**	-285.181691	29.90	-285.180747	26.74	-285.214770	26.86
 **026**	-285.185720	27.37	-285.179546	27.50	-285.214053	27.31
 **027**	-285.183883	28.52	-285.178466	28.18	-285.211669	28.81
 **028**	-285.182308	29.51	-285.176323	29.52	-285.210557	29.51
 **029**	-285.180719	30.51	-285.175338	30.14	-285.208469	30.82

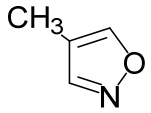
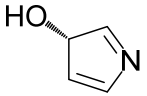
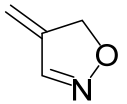
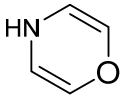
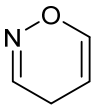
 **030**	-285.178201	32.09	-285.172060	32.20	-285.206918	31.79
 **031**	-285.173373	35.12	-285.167368	35.14	-285.201652	35.10
 **032**	-285.142275	54.63	-285.136263	54.66	-285.170717	54.51

Table S2. Molecules C_4H_5NO containing 6-membered heterocycles and their thermodynamic parameters

Structure	E(zpve). a.u.	ΔE(zpve), kcal/mol	H, a.u.	ΔH(kcal/mol)	G(298). a.u.	ΔG(kcal/mol)
 **100**	-285.186593	26.82	-285.180805	26.71	-285.215020	26.71
 **101**	-285.185214	27.69	-285.179395	27.59	-285.213585	27.61
 **102**	-285.181749	29.86	-285.176103	29.66	-285.209692	30.05
 **103**	-285.173018	35.34	-285.167415	35.11	-285.200858	35.59
 **104**	-285.161914	42.31	-285.156031	42.25	-285.190256	42.25
 **105**	-285.137756	57.47	-285.131843	57.43	-285.166604	57.09

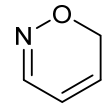
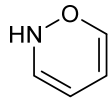
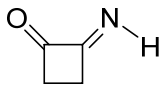
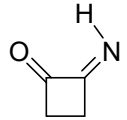
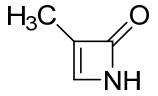
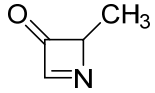
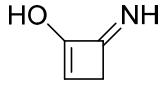
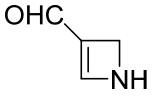
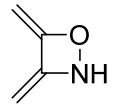
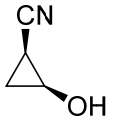
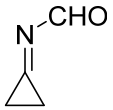
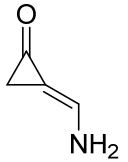
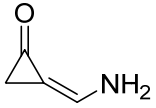
 **106**	-285.128733	63.13	-285.123531	62.65	-285.156322	63.54
 **107**	-285.115525	71.42	-285.109668	71.35	-285.143535	71.57

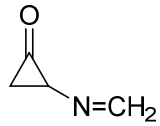
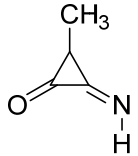
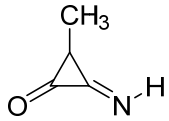
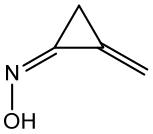
Table S3. Molecules C_4H_5NO containing 4-membered heterocycles and their thermodynamic parameters

Structure	E(zpve). a.u.	ΔE(zpve), kcal/mol	H, a.u.	ΔH(kcal/mol)	G(298). a.u.	ΔG(kcal/mol)
 **200**	-285.182089	29.65	-285.175665	29.93	-285.211225	29.09
 **201**	-285.181981	29.72	-285.175566	30.00	-285.211083	29.18
 **202** [a]	-285.177060	32.80	-285.170390	33.24	-285.206128	32.29
 **203**[a]	-285.172826	35.46	-285.166249	35.84	-285.201867	34.96
 **204**[a.b]	-285.164083	40.95	-285.157723	41.19	-285.192740	40.69
 **205** [a]	-285.158320	44.56	-285.151832	44.89	-285.187334	44.08
 **206** [a]	-285.090918	86.86	-285.089974	83.71	-285.124975	83.21

[a]Positional isomer neglected;[b]rotamer neglected.

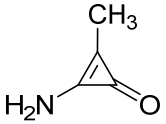
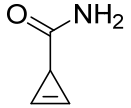
Table S4. Molecules C_4H_5NO containing saturated 3-membered cycles and their thermodynamic parameters.

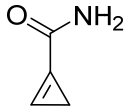
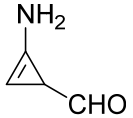
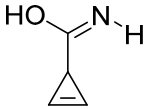
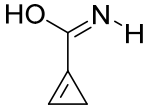
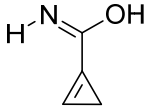
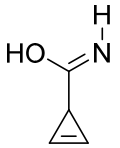
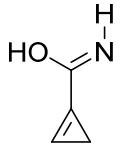
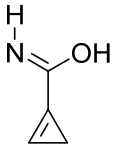
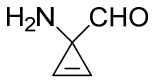
Structure	E(zpve). a.u.	ΔE(zpve), kcal/mol	H, a.u.	ΔH(kcal/mol)	G(298). a.u.	ΔG(kcal/mol)
 **300**	-285.199137	18.95	-285.192356	19.46	-285.229628	17.54
 **301**[a]	-285.173826	34.83	-285.167011	35.36	-285.203084	34.20
 **302**	-285.170962	36.63	-285.164610	36.87	-285.199725	36.31
 **303**[b]	-285.157401	45.14	-285.150456	45.75	-285.187228	44.15
 **304**	-285.149779	49.92	-285.143849	49.90	-285.178174	49.83
 **305**	-285.146515	51.97	-285.139109	52.87	-285.176552	50.85
 **306**	-285.145812	52.41	-285.138411	53.31	-285.175883	51.27

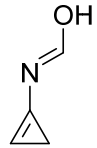
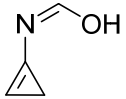
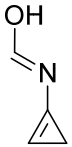
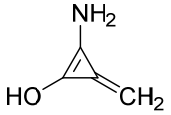
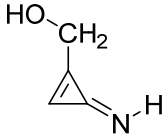
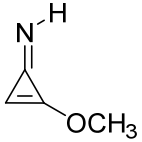
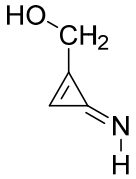
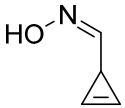
 **307** [b]	-285.135249	59.04	-285.128359	59.62	-285.164931	58.14
 **308**	-285.132579	60.72	-285.125136	61.64	-285.162826	59.46
 **309**	-285.131205	61.58	-285.123797	62.48	-285.161392	60.36
 **310**	-285.079089	94.28	-285.072104	94.92	-285.108475	93.57

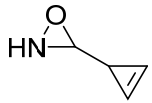
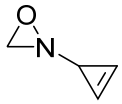
[a]Positional isomer neglected;[b]rotamer neglected.

Table S5. Molecules C_4H_5NO containing unsaturated 3-membered cycles and their thermodynamic parameters

Structure	E(zpve). a.u.	ΔE(zpve), kcal/mol	H, a.u.	ΔH(kcal/mol)	G(298). a.u.	ΔG(kcal/mol)
 **400**	-285.167990	38.49	-285.159793	39.89	-285.202046	34.85
 **401**	-285.157527	45.06	-285.150189	45.92	-285.187639	43.89

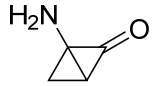
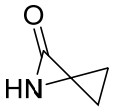
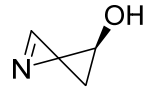
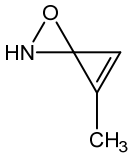
 **402** [b]	-285.154099	47.21	-285.146418	48.29	-285.185658	45.13
 **403** [a]	-285.136616	58.18	-285.129322	59.01	-285.166376	57.23
 **404**	-285.135031	59.18	-285.128290	59.66	-285.164466	58.43
 **405**	-285.134187	59.71	-285.127284	60.29	-285.163876	58.80
 **406**	-285.132766	60.60	-285.125837	61.20	-285.162779	59.49
 **407**	-285.129321	62.76	-285.122511	63.29	-285.158725	62.03
 **408**	-285.127080	64.17	-285.120095	64.80	-285.156831	63.22
 **409**	-285.126148	64.75	-285.119158	65.39	-285.156083	63.69
 **410** [a]	-285.122136	67.27	-285.114737	68.17	-285.152455	65.97

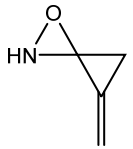
 **411**	-285.118767	69.38	-285.111768	70.03	-285.148270	68.59
 **412**	-285.116870	70.57	-285.109797	71.27	-285.147091	69.33
 **413**	-285.115440	71.47	-285.108310	72.20	-285.145278	70.47
 **414**	-285.112647	73.22	-285.105165	74.17	-285.142344	72.31
 **415**	-285.109901	74.95	-285.102549	75.81	-285.140685	73.35
 **416** [b]	-285.108441	75.86	-285.101229	76.64	-285.138455	74.75
 **417**	-285.108110	76.07	-285.101596	76.41	-285.137277	75.49
 **418**	-285.070976	99.37	-285.064005	100.00	-285.100643	98.48

 **419**	-285.043661	116.51	-285.037177	116.84	-285.072792	115.96
 **420**	-285.036752	120.85	-285.030302	121.15	-285.065684	120.42

[a]Positional isomer neglected;[b]rotamer neglected.

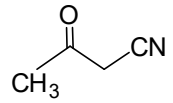
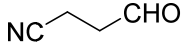
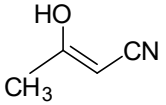
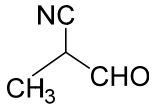
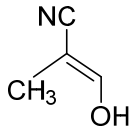
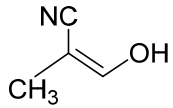
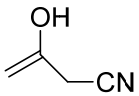
Table S6. Bicyclic compounds C_4H_5NO and their thermodynamic parameters

Structure	E(zpve). a.u.	ΔE(zpve), kcal/mol	H, a.u.	ΔH(kcal/mol)	G(298). a.u.	ΔG(kcal/mol)
 **500** [a]	-285.149514	50.09	-285.142922	50.48	-285.178297	49.75
 **501**	-285.138734	56.85	-285.132420	57.07	-285.167353	56.62
 **502** [a]	-285.114446	72.09	-285.108009	72.39	-285.143278	71.73
 **503** [a]	-285.096723	83.22	-285.090108	83.62	-285.125507	82.88
 **504** [a]	-285.078719	94.51	-285.072219	94.85	-285.107410	94.23
 **505**	-285.053056	110.62	-285.046161	111.20	-285.082466	109.89

 **506**	-285.053587	110.28	-285.047092	110.61	-285.082369	109.95

[a]Positional isomer neglected.

Table S7. Acyclic nitriles C_4H_5NO and their thermodynamic parameters

Structure	E(zpve). a.u.	ΔE(zpve), kcal/mol	H, a.u.	ΔH(kcal/mol)	G(298). a.u.	ΔG(kcal/mol)
 **600**	-285.215399	8.74	-285.208703	9.20	-285.244724	8.07
 **601**	-285.207256	13.85	-285.199916	14.72	-285.237819	12.40
 **602**	-285.202790	16.66	-285.195400	17.55	-285.232649	15.65
 **603**	-285.200916	17.83	-285.193452	18.77	-285.231316	16.48
 **604**	-285.196166	20.81	-285.188543	21.85	-285.226483	19.51
 **605**	-285.193626	22.41	-285.186073	23.40	-285.223717	21.25
 **606**	-285.190455	24.40	-285.183266	25.16	-285.220556	23.23

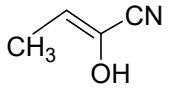
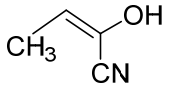
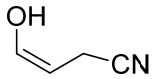
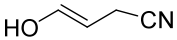
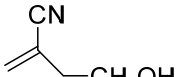
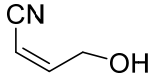
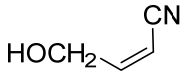
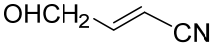
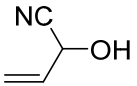
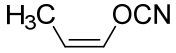
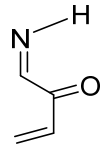
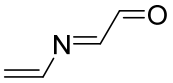
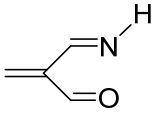
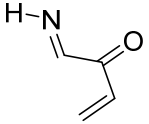
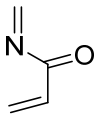
 **607**	-285.189308	25.12	-285.181550	26.24	-285.220307	23.39
 **608**	-285.189493	25.00	-285.181983	25.97	-285.219521	23.88
 **609**	-285.186123	27.12	-285.179431	27.57	-285.215378	26.48
 **610**	-285.184869	27.90	-285.177337	28.88	-285.215382	26.48
 **611**	-285.179658	31.17	-285.172261	32.07	-285.210008	29.85
 **612**	-285.179824	31.07	-285.173129	31.52	-285.209299	30.30
 **613**	-285.179809	31.08	-285.173124	31.53	-285.209275	30.31
 **614**	-285.179809	31.08	-285.171031	32.84	-285.207475	31.44
 **615**	-285.172284	35.80	-285.164814	36.74	-285.202590	34.51
 **616**	-285.161402	42.63	-285.154494	43.22	-285.191744	41.31

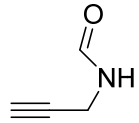
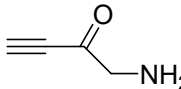
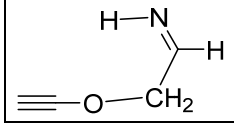
Table S8. Conjugated trienes C_4H_5NO and their thermodynamic parameters

Structure	E(zpve). a.u.	ΔE(zpve), kcal/mol	H, a.u.	ΔH(kcal/mol)	G(298). a.u.	ΔG(kcal/mol)
 **700** [b]	-285.177734	32.38	-285.171310	32.67	-285.206924	31.79

 **701** [b]	-285.171676	36.18	-285.164393	37.01	-285.201694	35.07
 **702** [b]	-285.171283	36.43	-285.164836	36.73	-285.200461	35.84
 **703** [b]	-285.168799	37.99	-285.162215	38.37	-285.198755	36.91
 **704** [b]	-285.162554	41.91	-285.155721	42.45	-285.192477	40.85

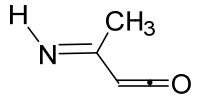
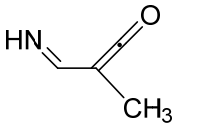
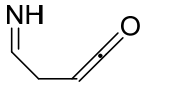
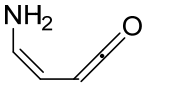
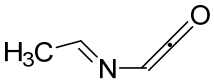
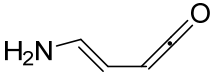
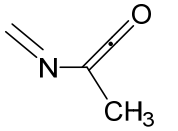
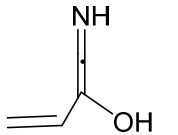
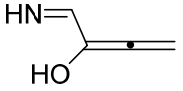
[b]Rotamer neglected.

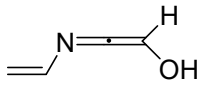
Table S9. Acetylenes C_4H_5NO and their thermodynamic parameters

Structure	E(zpve). a.u.	ΔE(zpve), kcal/mol	H, a.u.	ΔH(kcal/mol)	G(298). a.u.	ΔG(kcal/mol)
 **800**	-285.158760	44.29	-285.151329	45.20	-285.189458	42.75
 **801**	-285.144009	53.54	-285.136338	54.61	-285.174522	52.12
 **802** [b]	-285.101478	80.23	-285.093917	81.23	-285.132200	78.68

[b]Rotamer neglected.

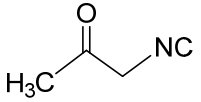
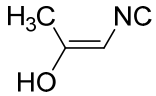
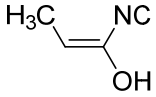
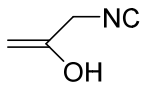
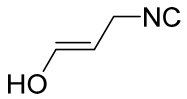
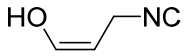
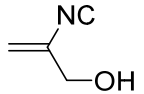
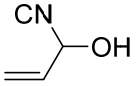
Table S10. Allenes C_4H_5NO. ketenes and their thermodynamic parameters

Structure	E(zpve). a.u.	ΔE(zpve), kcal/mol	H, a.u.	ΔH(kcal/mol)	G(298). a.u.	ΔG(kcal/mol)
 **900** [b]	-285.191324	23.85	-285.183876	24.78	-285.222050	22.30
 **901** [b]	-285.182745	29.24	-285.175883	29.80	-285.212549	28.26
 **902** [b]	-285.174717	34.27	-285.167318	35.17	-285.205666	32.58
 **903** [b]	-285.175228	33.95	-285.168409	34.49	-285.204908	33.05
 **904** [b]	-285.170278	37.06	-285.162663	38.09	-285.201201	35.38
 **905** [b]	-285.167770	38.63	-285.160601	39.39	-285.198776	36.90
 **906** [b]	-285.164811	40.49	-285.157007	41.64	-285.195997	38.64
 **907** [b]	-285.142065	54.76	-285.134612	55.69	-285.172017	53.69
 **908** [b]	-285.136723	58.11	-285.129354	58.99	-285.166697	57.03

 **909** [b]	-285.128969	62.98	-285.121207	64.11	-285.159660	61.45

[b]Rotamer neglected.

Table S11. Acyclic isonitriles C_4H_5NO and their thermodynamic parameters

Structure	E(zpve). a.u.	ΔE(zpve), kcal/mol	H, a.u.	ΔH(kcal/mol)	G(298). a.u.	ΔG(kcal/mol)
 **1000**	-285.177682	32.41	-285.170656	33.08	-285.207548	31.40
 **1001**	-285.164412	40.74	-285.156678	41.85	-285.194667	39.48
 **1002**	-285.161051	42.85	-285.153108	44.09	-285.191707	41.34
 **1003**	-285.154690	46.84	-285.147310	47.73	-285.184717	45.72
 **1004**	-285.150526	49.45	-285.142845	50.53	-285.181105	47.99
 **1005**	-285.103766	78.80	-285.144141	49.72	-285.180427	48.41
 **1006**	-285.149063	50.37	-285.141604	51.31	-285.179255	49.15
 **1007**	-285.145973	52.31	-285.138446	53.29	-285.176215	51.06

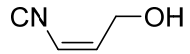
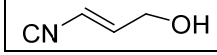
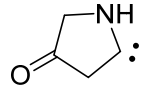
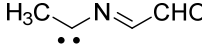
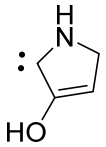
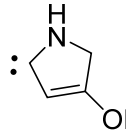
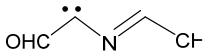
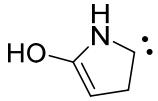
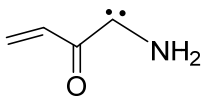
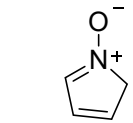
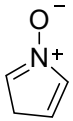
 **1008**	-285.146626	51.90	-285.139782	52.45	-285.176204	51.06
 **1009**	-285.143396	53.93	-285.136367	54.59	-285.173026	53.06

Table S12. Carbenes C_4H_5NO and their thermodynamic parameters

Structure	E(zpve). a.u.	ΔE(zpve), kcal/mol	H, a.u.	ΔH(kcal/mol)	G(298). a.u.	ΔG(kcal/mol)
 **1100** [a]	-285.153903	47.33	-285.147722	47.47	-285.182830	46.91
 **1101** [a.b]	-285.143530	53.84	-285.135770	54.97	-285.174218	52.31
 **1102**	-285.142635	54.41	-285.136711	54.38	-285.170686	54.53
 **1103**	-285.139204	56.56	-285.133209	56.58	-285.167312	56.64
 **1104**	-285.135128	59.12	-285.127340	60.26	-285.166156	57.37
 **1105** [a]	-285.137037	57.92	-285.130872	58.04	-285.165280	57.92
 **1106** [a.b]	-285.105616	77.63	-285.098696	78.23	-285.135632	76.52

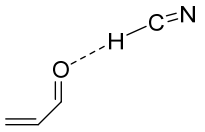
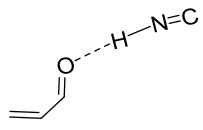
[a]Positional isomer neglected;[b]rotamer neglected.

Table S13. Bipolar compounds C_4H_5NO and their thermodynamic parameters

Structure	E(zpve). a.u.	ΔE(zpve), kcal/mol	H, a.u.	ΔH(kcal/mol)	G(298). a.u.	ΔG(kcal/mol)
 **1200** [a.b]	-285.135776	58.71	-285.130117	58.52	-285.163639	58.95
 **1201** [a.b]	-285.131281	61.53	-285.125617	61.34	-285.159143	61.77

[a]Positional isomer neglected;[b]rotamer neglected.

Table S14. Intermolecular associates C_4H_5NO and their thermodynamic parameters

Structure	E(zpve). a.u.	ΔE(zpve), kcal/mol	H, a.u.	ΔH(kcal/mol)	G(298). a.u.	ΔG(kcal/mol)
 **1300** [b]	-285.167303	38.93	-285.158443	40.74	-285.200968	35.53
 **1301** [b]	-285.164966	40.39	-285.155864	42.36	-285.200403	35.88

[b]Rotamer neglected.

000

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.333766	-0.745002	-0.000015
2	6	0	1.482851	0.582328	-0.000180
3	6	0	0.117755	1.212895	0.000110
4	1	0	2.089388	-1.518311	-0.000113
5	1	0	2.421929	1.114992	0.000177
6	1	0	-0.082120	1.833387	-0.880104
7	1	0	-0.081698	1.833554	0.880273
8	7	0	-0.022118	-1.101158	0.000052
9	1	0	-0.388399	-2.038084	0.000325
10	6	0	-0.837058	0.014504	0.000052
11	8	0	-2.048520	0.011777	-0.000091

001

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.858335	0.022595	-0.000039
2	6	0	0.048654	1.211645	0.000027
3	6	0	1.316366	0.802890	0.000141
4	6	0	1.382013	-0.701431	-0.000037
5	1	0	-0.327802	2.224930	-0.000616
6	1	0	2.205963	1.420024	-0.000171
7	1	0	1.910128	-1.077064	-0.886648
8	1	0	1.910558	-1.077221	0.886365
9	8	0	-2.072644	-0.007890	0.000053
10	7	0	-0.012578	-1.062396	0.000093
11	1	0	-0.361838	-2.004974	-0.000557

002

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.596951	0.095813	-0.000008
2	6	0	1.443174	0.673303	0.000018
3	7	0	0.142707	1.158157	0.000008
4	1	0	2.297543	1.332589	-0.000056
5	6	0	-2.079530	0.001959	0.000044
6	1	0	-2.493566	1.009674	0.000228
7	1	0	-2.435908	-0.533144	-0.884491
8	1	0	-2.435893	-0.533811	0.884096
9	6	0	1.412788	-0.676177	-0.000015
10	1	0	2.152825	-1.458451	0.000103
11	8	0	0.104895	-1.061668	-0.000021

003

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-1.400254	-0.631564	-0.000033
2	6	0	-0.244539	1.130242	-0.000068
3	7	0	-1.547201	0.649041	-0.000106
4	1	0	-0.027440	2.187739	-0.000114
5	6	0	0.625736	0.092967	0.000021
6	8	0	-0.118633	-1.054157	0.000038
7	1	0	-2.164057	-1.394164	-0.000034
8	6	0	2.103528	-0.040332	0.000110
9	1	0	2.452005	-0.581210	0.885036
10	1	0	2.452097	-0.581371	-0.884680
11	1	0	2.560039	0.951090	0.000045

004

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.349363	-0.702304	-0.000051
2	6	0	0.643680	0.017320	0.000025
3	7	0	-0.134954	-1.137597	0.000083
4	6	0	-0.183460	1.088648	0.000080
5	8	0	-1.471688	0.636937	-0.000042
6	1	0	-2.264125	-1.275496	-0.000077
7	6	0	2.133307	-0.040979	-0.000042
8	1	0	2.496313	-0.575547	-0.882319
9	1	0	2.565174	0.962358	0.000184
10	1	0	2.496438	-0.575991	0.881896
11	1	0	-0.040593	2.156250	-0.000001

005

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.868865	0.056411	0.006507
2	6	0	0.011047	1.219074	0.014593
3	6	0	1.289438	0.769444	0.002358
4	1	0	-0.312406	2.248257	0.012782
5	1	0	2.195272	1.364266	0.031867
6	8	0	-2.081683	-0.011281	-0.008768
7	7	0	1.397710	-0.591648	-0.092282
8	1	0	2.202339	-1.065111	0.283499
9	6	0	0.069765	-1.170838	0.018305
10	1	0	-0.162218	-1.836565	-0.817440
11	1	0	-0.061804	-1.723607	0.954831

006

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.685832	0.063888	-0.000095
2	6	0	0.124916	1.171544	-0.000081

3	6	0	1.468297	0.682297	0.000074
4	6	0	1.420511	-0.684394	0.000019
5	1	0	-0.198590	2.202211	-0.000017
6	1	0	2.366206	1.282548	0.000144
7	1	0	2.202670	-1.426489	-0.000316
8	8	0	-2.030590	-0.105906	-0.000089
9	7	0	0.088947	-1.054559	0.000015
10	1	0	-0.275234	-1.991391	0.000424
11	1	0	-2.440314	0.762271	0.000869

007

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.872377	-0.016997	-0.000025
2	6	0	0.087133	-1.200856	-0.000048
3	6	0	1.465562	-0.527535	0.000084
4	1	0	-0.097536	-1.820410	0.881263
5	1	0	2.067827	-0.780009	-0.877463
6	8	0	-2.078459	-0.027922	-0.000048
7	7	0	1.264371	0.931685	0.000043
8	6	0	0.019558	1.193851	-0.000008
9	1	0	-0.362662	2.211414	-0.000032
10	1	0	2.067607	-0.779959	0.877799
11	1	0	-0.097423	-1.820235	-0.881509

008

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.847778	0.019040	-0.000112
2	6	0	-0.080633	1.232501	-0.000062
3	6	0	-1.427700	0.561856	0.000208
4	1	0	0.090719	1.860745	0.880761
5	1	0	-2.363948	1.118028	0.000443
6	8	0	2.052392	0.021500	0.000052
7	7	0	-1.441654	-0.712825	-0.000186
8	6	0	-0.069075	-1.206134	0.000045
9	1	0	0.116594	-1.832812	-0.879171
10	1	0	0.090125	1.860321	-0.881412
11	1	0	0.116722	-1.832085	0.879794

009

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.411011	0.726901	-0.000174
2	6	0	-0.153826	1.188056	0.000158
3	6	0	0.695446	-0.009028	-0.000487
4	7	0	0.066831	-1.128064	0.000125
5	6	0	-1.343167	-0.775258	0.000031
6	1	0	-1.841525	-1.202420	0.879904

7	1	0	0.201621	2.209192	0.000232
8	1	0	-1.841804	-1.203708	-0.878961
9	8	0	2.029623	0.100448	0.000180
10	1	0	2.378310	-0.799910	-0.000445
11	1	0	-2.326059	1.305695	-0.000208

010

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.723696	-0.029358	0.000064
2	6	0	-0.072593	1.148483	-0.000004
3	6	0	-1.386963	0.738567	-0.000051
4	1	0	0.277013	2.171533	0.000079
5	1	0	-2.299617	1.314056	0.000089
6	8	0	2.083806	-0.122768	-0.000058
7	7	0	-1.404947	-0.623344	-0.000097
8	1	0	-2.233388	-1.190605	0.000416
9	6	0	-0.118050	-1.115076	0.000078
10	1	0	0.097331	-2.170693	-0.000164
11	1	0	2.446301	0.765569	0.000202

011

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.723400	0.020352	-0.000003
2	6	0	-0.121122	1.160868	-0.000062
3	6	0	-1.414683	0.694719	0.000059
4	1	0	0.197245	2.191955	-0.000118
5	1	0	-2.351360	1.230514	0.000123
6	8	0	2.083324	0.103605	-0.000114
7	1	0	2.446938	-0.784911	0.001165
8	7	0	-1.379613	-0.668367	-0.000052
9	1	0	-2.183416	-1.269688	0.000032
10	6	0	-0.070775	-1.103421	0.000022
11	1	0	0.180370	-2.153250	-0.000022

012

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.685738	0.105565	-0.000025
2	6	0	-0.166794	1.177205	0.000113
3	6	0	-1.490604	0.642120	-0.000094
4	6	0	-1.399344	-0.721757	0.000224
5	1	0	0.130085	2.214121	0.000224
6	1	0	-2.408954	1.210707	-0.000129
7	1	0	-2.154420	-1.491469	0.000439
8	8	0	2.041677	0.117982	-0.000310
9	7	0	-0.053175	-1.047716	-0.000042
10	1	0	0.312157	-1.984272	-0.000627

11	1	0	2.385962	-0.777730	0.001554

013

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.369643	0.790105	-0.000096
2	6	0	-0.086548	1.168253	-0.000261
3	6	0	0.695331	-0.084738	0.000212
4	7	0	-0.007466	-1.155577	0.000169
5	6	0	-1.388426	-0.712142	-0.000098
6	1	0	-1.912902	-1.108960	0.878902
7	1	0	0.316423	2.174488	-0.000487
8	1	0	-1.912745	-1.109141	-0.879107
9	8	0	2.039500	-0.128624	0.000124
10	1	0	-2.245963	1.425935	-0.000224
11	1	0	2.387168	0.766829	0.000198

014

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.816656	-0.012650	-0.000005
2	6	0	-1.314719	0.809443	-0.000016
3	6	0	-0.041987	1.194135	-0.000006
4	1	0	0.349988	2.202260	0.000000
5	1	0	2.529051	0.738034	0.000049
6	7	0	2.072430	-0.171319	0.000026
7	6	0	-1.362518	-0.688757	0.000006
8	1	0	-1.864854	-1.092158	-0.887756
9	8	0	-0.005510	-1.100827	-0.000017
10	1	0	-1.864818	-1.092118	0.887809
11	1	0	-2.196886	1.436812	-0.000025

015

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.355994	0.751223	-0.000030
2	6	0	-0.106843	1.208502	0.000054
3	6	0	0.813973	0.059774	-0.000196
4	6	0	-1.324926	-0.748575	0.000029
5	1	0	-1.800421	-1.181347	0.888406
6	1	0	0.241707	2.230857	0.000128
7	1	0	-1.800456	-1.181446	-0.888281
8	1	0	-2.272616	1.326822	-0.000030
9	7	0	2.077892	0.100052	0.000050
10	1	0	2.460876	-0.845790	0.000135
11	8	0	0.058551	-1.084375	0.000019

016

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.703576	0.108192	-0.000109
2	6	0	0.134329	1.158971	0.000141
3	6	0	1.210718	-0.885834	0.000154
4	6	0	1.516686	0.583397	-0.000009
5	1	0	2.114006	0.854802	-0.881050
6	7	0	-0.046900	-1.148206	-0.000153
7	8	0	-2.045340	0.103607	-0.000077
8	1	0	-2.318535	-0.820384	0.001011
9	1	0	-0.124553	2.206001	0.000400
10	1	0	1.955753	-1.676090	0.000626
11	1	0	2.115409	0.855903	0.879640

017

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.432296	0.660551	-0.000012
2	6	0	0.710644	0.059451	-0.000129
3	6	0	-0.061608	1.165832	-0.000051
4	1	0	0.244843	2.203425	0.000183
5	6	0	-0.190028	-1.140159	0.000105
6	8	0	2.042001	-0.103798	-0.000291
7	1	0	2.469757	0.758137	0.001778
8	7	0	-1.550328	-0.623165	-0.000107
9	1	0	-2.313913	1.298255	0.000014
10	1	0	-0.022215	-1.771558	-0.880213
11	1	0	-0.022463	-1.769768	0.881840

018

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.704839	0.028517	0.000007
2	6	0	0.062653	1.135862	0.000081
3	6	0	1.266184	-0.828676	-0.000191
4	6	0	1.480798	0.657839	0.000028
5	1	0	2.057384	0.969646	-0.881096
6	7	0	0.031008	-1.178764	-0.000019
7	8	0	-2.039619	-0.124374	-0.000042
8	1	0	-0.258088	2.167700	-0.000522
9	1	0	2.063015	-1.567048	0.000604
10	1	0	2.057332	0.969160	0.881367
11	1	0	-2.448522	0.745625	0.000565

019

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.458181	0.611402	-0.000040
2	6	0	-0.709121	0.111488	-0.000086
3	6	0	0.114114	1.177704	0.000146
4	1	0	-0.154571	2.223898	0.000696
5	6	0	0.141215	-1.131808	0.000237
6	8	0	-2.052674	0.123736	-0.000194
7	1	0	-2.385323	-0.778006	-0.000237
8	7	0	1.522797	-0.677741	-0.000415
9	1	0	2.368875	1.206448	-0.000214
10	1	0	-0.046135	-1.754119	0.885106
11	1	0	-0.047369	-1.756641	-0.882430

020

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.143006	1.130653	-0.000123
2	6	0	-0.731622	-0.049862	0.000015
3	6	0	1.470346	-0.616187	-0.000016
4	8	0	-2.073028	0.097991	0.000071
5	6	0	0.064085	-1.133546	-0.000005
6	1	0	-0.222731	-2.176857	0.000025
7	1	0	2.043980	-0.936190	-0.879059
8	7	0	1.392844	0.841855	0.000022
9	1	0	-0.218971	2.155762	-0.000093
10	1	0	2.043977	-0.936199	0.879025
11	1	0	-2.486828	-0.769776	0.000144

021

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.493792	-0.568411	-0.000109
2	6	0	-0.730866	-0.098254	0.000090
3	6	0	0.112401	-1.143793	0.000022
4	1	0	-0.140173	-2.194252	-0.000083
5	6	0	0.097650	1.117771	0.000240
6	8	0	-2.082153	-0.128323	0.000040
7	7	0	1.359084	0.885570	0.000037
8	1	0	2.081575	-0.863487	0.878368
9	1	0	2.081422	-0.863441	-0.878709
10	1	0	-0.295160	2.134758	-0.000852
11	1	0	-2.421887	0.770136	-0.000762

022

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.309766	0.729739	-0.000034
2	6	0	-0.051952	1.198589	-0.000024

3	6	0	0.835982	0.036377	0.000034
4	1	0	0.246580	2.236228	-0.000046
5	1	0	-2.248161	1.270091	-0.000072
6	7	0	2.102224	-0.105122	0.000053
7	6	0	-0.107866	-1.156313	0.000010
8	1	0	0.014699	-1.776130	0.891435
9	1	0	0.014750	-1.776146	-0.891397
10	8	0	-1.437275	-0.609762	-0.000031
11	1	0	2.556386	0.809558	0.000034

023

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.708894	0.027457	-0.000167
2	6	0	0.058847	1.133283	-0.000034
3	6	0	1.527869	-0.474720	-0.000083
4	8	0	-2.047263	-0.136125	-0.000079
5	1	0	-0.249628	2.170770	-0.000108
6	1	0	2.485895	-0.985451	-0.000782
7	1	0	-2.468407	0.728871	0.000408
8	7	0	1.441811	0.807377	0.000119
9	6	0	0.192460	-1.165914	0.000042
10	1	0	0.047738	-1.799768	-0.882428
11	1	0	0.048140	-1.797693	0.884156

024

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.341997	0.683044	0.000007
2	6	0	-0.108089	1.206430	-0.000050
3	6	0	0.833837	0.092464	0.000034
4	1	0	0.158372	2.251592	-0.000090
5	1	0	-2.305484	1.176011	-0.000012
6	7	0	2.105902	0.170527	0.000059
7	1	0	2.522934	-0.762606	0.000052
8	6	0	-0.057639	-1.147566	0.000013
9	1	0	0.092951	-1.762588	0.892191
10	1	0	0.093042	-1.762600	-0.892144
11	8	0	-1.407474	-0.667466	-0.000054

025

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.123619	1.153893	0.000083
2	6	0	1.392781	-0.612952	0.000077
3	1	0	-0.214004	2.185671	0.000137
4	1	0	1.910129	-0.980256	-0.893239
5	8	0	0.046161	-1.098565	-0.000047
6	6	0	-2.104604	-0.051468	-0.000196

7	1	0	-2.665432	0.874237	-0.000355
8	1	0	-2.643688	-0.989866	0.000135
9	6	0	-0.772368	-0.012324	-0.000084
10	1	0	1.910010	-0.980355	0.893420
11	7	0	1.356733	0.830884	0.000143

026

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.709529	-0.077696	-0.000008
2	6	0	-0.106974	-1.145618	-0.000180
3	6	0	-1.509504	0.524460	-0.000095
4	8	0	2.060764	-0.089702	0.000166
5	1	0	0.163181	-2.191655	-0.000261
6	1	0	-2.443671	1.077487	-0.000110
7	7	0	-1.473373	-0.759138	-0.000247
8	6	0	-0.144890	1.158977	0.000234
9	1	0	0.014664	1.786878	-0.885508
10	1	0	0.014313	1.785875	0.886780
11	1	0	2.390049	0.812257	-0.000203

027

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.616389	0.111584	-0.000170
2	6	0	-0.258788	1.152088	0.000103
3	6	0	-1.526743	0.514358	0.000115
4	8	0	-0.065291	-1.044863	0.000518
5	1	0	-0.035727	2.206844	0.000200
6	1	0	-2.511194	0.961850	0.000140
7	7	0	-1.423096	-0.789207	-0.000512
8	6	0	2.100155	0.014074	-0.000134
9	1	0	2.451914	-0.523794	0.884457
10	1	0	2.451775	-0.525819	-0.883539
11	1	0	2.541153	1.011649	-0.001305

028

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.709395	0.010946	0.388115
2	6	0	1.427298	0.678106	-0.149145
3	8	0	-1.937439	0.017339	-0.274515
4	1	0	2.346392	1.210935	-0.356964
5	6	0	0.214974	1.179374	0.105567
6	7	0	0.086105	-1.197328	0.144305
7	6	0	1.276143	-0.792733	-0.109412
8	1	0	2.084579	-1.498471	-0.288387
9	1	0	-0.941009	0.012232	1.463030

10	1	0	-0.088546	2.216462	0.162275
11	1	0	-1.758752	-0.152727	-1.204719

029

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.631004	0.025081	0.000219
2	7	0	-0.034425	-1.105221	0.000201
3	6	0	2.128706	0.026056	-0.000186
4	1	0	2.515194	-0.489460	0.882153
5	1	0	2.514833	-0.487120	-0.884057
6	1	0	2.511350	1.048139	0.001050
7	6	0	-1.480890	0.571101	-0.000158
8	1	0	-2.486467	0.963421	-0.000506
9	6	0	-0.253111	1.143004	0.000190
10	1	0	-0.000621	2.191262	0.000332
11	8	0	-1.370946	-0.760144	-0.000096

030

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.235663	1.094195	0.000527
2	7	0	1.488293	0.719924	-0.000394
3	6	0	0.183578	-1.067043	0.000436
4	1	0	0.030263	-2.135913	0.000519
5	6	0	-0.666740	-0.009308	-0.000026
6	8	0	1.458839	-0.656317	-0.000211
7	6	0	-2.161764	0.008230	-0.000246
8	1	0	-2.551793	0.523409	0.882554
9	1	0	-2.551654	0.523061	-0.883312
10	1	0	-2.564310	-1.007222	-0.000081
11	1	0	0.004304	2.151284	0.000620

031

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.703019	-0.016181	0.368575
2	6	0	1.419888	0.703337	-0.142227
3	8	0	-1.874548	-0.091990	-0.395357
4	1	0	2.328285	1.257851	-0.340252
5	6	0	0.194872	1.177369	0.101835
6	1	0	-2.483011	0.577868	-0.073317
7	7	0	0.115513	-1.198747	0.130575
8	6	0	1.299480	-0.769452	-0.107170
9	1	0	2.123971	-1.459459	-0.271717
10	1	0	-0.926532	-0.030924	1.451918
11	1	0	-0.122238	2.211381	0.156123

032

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.792418	0.006612	0.000183
2	6	0	-0.161256	-1.158341	0.000381
3	7	0	-1.354703	0.816794	-0.000276
4	6	0	-0.116789	1.149415	0.000477
5	1	0	0.157190	2.196325	0.000156
6	1	0	-0.069464	-1.786226	-0.891691
7	8	0	-1.468656	-0.556588	-0.000365
8	1	0	-0.069824	-1.785576	0.892995
9	6	0	2.124903	0.013644	-0.000297
10	1	0	2.701867	-0.904805	-0.000946
11	1	0	2.676741	0.947446	-0.000129

100

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.418321	-0.221029	0.000452
2	6	0	0.761579	1.132795	-0.000242
3	6	0	-0.559828	1.236862	-0.000164
4	6	0	-0.773118	-1.070905	-0.000199
5	7	0	0.460156	-1.324106	-0.000472
6	1	0	-1.120804	2.162223	-0.000485
7	1	0	2.072414	-0.340065	-0.873224
8	1	0	1.367120	2.031866	-0.001007
9	1	0	-1.513732	-1.866210	-0.000602
10	8	0	-1.397312	0.144342	0.000517
11	1	0	2.070686	-0.340150	0.875408

101

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.991966	-0.948549	-0.056237
2	6	0	-1.278497	0.511328	0.137992
3	6	0	1.081645	0.756685	0.004059
4	6	0	0.275189	-1.360811	-0.038837
5	1	0	-1.821037	-1.634271	-0.188771
6	1	0	-1.579394	0.735477	1.172578
7	1	0	1.863082	1.512768	0.005131
8	1	0	0.545969	-2.403583	-0.165193
9	7	0	1.365322	-0.479642	0.114182
10	8	0	-0.126285	1.316277	-0.172732
11	1	0	-2.073824	0.864973	-0.523028

102

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	0.223335	1.353025	-0.079628
2	6	0	1.312802	0.419561	0.166119
3	6	0	1.016650	-0.879789	-0.018483
4	6	0	-1.241255	-0.372933	0.222823
5	7	0	-1.007828	1.004023	-0.136075
6	1	0	1.747472	-1.679531	-0.085298
7	1	0	2.333034	0.750322	0.302437
8	1	0	-1.304774	-0.455091	1.320685
9	8	0	-0.235503	-1.303517	-0.226281
10	1	0	-2.168097	-0.730003	-0.224725
11	1	0	0.462005	2.395089	-0.295300

103

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.208468	0.614617	0.159055
2	6	0	1.121121	-0.712828	-0.021043
3	6	0	-1.163876	-0.589359	0.265304
4	1	0	1.967741	-1.387747	-0.067816
5	1	0	2.155353	1.099499	0.355601
6	1	0	-1.167514	-0.693985	1.363630
7	8	0	-0.063030	-1.322950	-0.265146
8	1	0	-2.067932	-1.046478	-0.137956
9	6	0	-1.033197	0.866336	-0.111200
10	1	0	-1.914944	1.436049	-0.402021
11	7	0	0.105206	1.443380	-0.106137

104

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.009587	0.644889	1.176075
2	6	0	-0.009587	-0.684184	1.153367
3	6	0	-0.009587	-0.684184	-1.153367
4	1	0	-0.014491	-1.296175	2.044155
5	1	0	-0.025606	1.177217	2.118386
6	8	0	0.036103	-1.442790	-0.000000
7	1	0	-0.014491	-1.296175	-2.044155
8	6	0	-0.009587	0.644889	-1.176075
9	1	0	-0.025606	1.177217	-2.118386
10	7	0	0.084341	1.434667	0.000000
11	1	0	-0.568930	2.209106	0.000000

105

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.881760	-1.008925	0.000061
2	6	0	1.440490	-0.229685	-0.000176

3	1	0	-1.687987	-1.732574	0.000252
4	1	0	2.101901	-0.288496	0.875306
5	6	0	0.735712	1.098294	0.000155
6	1	0	1.332971	2.007725	0.000392
7	7	0	-0.516554	1.338090	0.000063
8	8	0	-1.395331	0.254940	-0.000182
9	6	0	0.409228	-1.317390	0.000111
10	1	0	0.708336	-2.358191	0.000308
11	1	0	2.101281	-0.288377	-0.876150

106

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.276900	-0.305941	0.249975
2	6	0	0.456550	1.327463	-0.078555
3	1	0	-2.240490	-0.569314	-0.189396
4	1	0	0.892134	2.298509	-0.284543
5	6	0	1.335514	0.184099	0.143757
6	1	0	2.390622	0.317957	0.361257
7	7	0	0.975299	-1.042476	0.005198
8	8	0	-0.360005	-1.247969	-0.302728
9	6	0	-0.857312	1.097820	-0.076117
10	1	0	-1.596181	1.866178	-0.277784
11	1	0	-1.340254	-0.452895	1.341539

107

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.562522	1.265783	0.156157
2	1	0	1.005968	2.227845	0.375439
3	6	0	-0.863443	1.105231	-0.090170
4	1	0	-1.482720	1.959508	-0.338434
5	6	0	1.329116	0.177993	0.003661
6	1	0	2.413532	0.160835	0.016060
7	6	0	-1.363290	-0.134895	-0.074984
8	1	0	-2.400440	-0.385267	-0.268408
9	7	0	-0.511274	-1.252222	0.211763
10	1	0	-0.379249	-1.339723	1.224040
11	8	0	0.804049	-1.042789	-0.307378

200

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.937211	1.159926	0.000441
2	6	0	-0.605050	1.335846	-0.000894
3	1	0	1.454625	1.530248	-0.887820
4	1	0	1.452619	1.529585	0.890174
5	1	0	-1.013160	1.821160	-0.891021
6	1	0	-1.014762	1.822603	0.887671

7	6	0	0.745794	-0.370097	0.000089
8	6	0	-0.776222	-0.191109	-0.000064
9	7	0	-1.709593	-1.038105	0.000708
10	1	0	-2.620516	-0.570166	0.000788
11	8	0	1.487243	-1.309260	-0.000273

201

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.030001	1.088275	0.000225
2	6	0	-0.494353	1.399904	-0.000265
3	1	0	1.579951	1.408921	-0.888184
4	1	0	1.579446	1.408896	0.888960
5	1	0	-0.859828	1.918906	-0.889007
6	1	0	-0.860295	1.919376	0.887999
7	6	0	0.700844	-0.413857	0.000116
8	8	0	1.335525	-1.431179	-0.000191
9	6	0	-0.799455	-0.095850	0.000091
10	7	0	-1.871389	-0.759712	0.000099
11	1	0	-1.645972	-1.759517	0.000071

202

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.091167	1.349717	0.054707
2	6	0	-0.693077	0.150622	0.023678
3	1	0	-0.405286	2.382715	0.132791
4	7	0	1.269338	0.900093	-0.160977
5	1	0	1.967019	1.138565	0.541343
6	6	0	-2.066119	-0.410356	-0.011658
7	1	0	-2.812555	0.373910	0.135006
8	1	0	-2.266024	-0.897441	-0.971576
9	1	0	-2.198138	-1.164558	0.769850
10	6	0	0.692968	-0.438689	-0.040365
11	8	0	1.221749	-1.505201	0.045156

204

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.161668	1.061042	-0.000034
2	1	0	-1.728316	1.343843	-0.894125
3	1	0	-1.728420	1.343850	0.893988
4	6	0	0.726094	0.121765	0.000007
5	6	0	0.327671	1.407955	0.000052
6	6	0	-0.652035	-0.396874	0.000000
7	7	0	-1.093827	-1.581644	0.000019
8	1	0	-2.114947	-1.590899	0.000017
9	8	0	1.902757	-0.510854	-0.000018
10	1	0	1.718734	-1.457622	-0.000044

11	1	0	0.847306	2.355850	0.000023

205

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.783341	-1.029991	0.021626
2	1	0	0.816650	-1.593321	0.957524
3	1	0	0.657898	-1.706384	-0.826515
4	6	0	1.048539	0.965817	0.009497
5	6	0	-0.081317	0.213630	0.052391
6	1	0	1.299207	2.021448	0.026688
7	7	0	1.937315	-0.095203	-0.141679
8	1	0	2.758863	-0.175555	0.446226
9	6	0	-1.498716	0.471607	0.003171
10	1	0	-1.772097	1.549456	-0.002276
11	8	0	-2.354101	-0.394450	-0.016250

206

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.728518	-0.166517	0.002355
2	6	0	-1.753900	-1.006698	0.010963
3	1	0	-2.774455	-0.645704	0.019536
4	1	0	-1.570931	-2.073175	0.009809
5	6	0	0.738156	-0.188149	-0.023327
6	6	0	1.728623	-1.068406	0.008741
7	1	0	1.510730	-2.127762	0.061796
8	1	0	2.765320	-0.754445	-0.019646
9	7	0	0.720840	1.248265	-0.117884
10	1	0	1.052409	1.691596	0.740418
11	8	0	-0.741890	1.218781	0.002610

300

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.893547	-0.752746	-0.120184
2	6	0	1.893447	0.752850	-0.120216
3	6	0	0.729084	-0.000016	0.460164
4	1	0	1.724626	-1.252823	-1.066941
5	1	0	2.547471	-1.277213	0.567798
6	1	0	1.724456	1.252866	-1.066992
7	1	0	2.547306	1.277432	0.567740
8	1	0	0.616228	-0.000011	1.540121
9	7	0	-0.491152	-0.000151	-0.266942
10	6	0	-1.673804	-0.000088	-0.047970
11	8	0	-2.846958	0.000100	0.037013

301

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.864036	-1.063583	0.605419
2	6	0	1.150384	0.038827	-0.364598
3	6	0	-0.149086	-0.724171	-0.479088
4	1	0	1.393554	-2.004989	0.511377
5	1	0	0.596902	-0.773071	1.615670
6	1	0	1.875489	-0.157408	-1.153952
7	1	0	-0.248038	-1.415821	-1.309221
8	6	0	-1.380592	-0.078309	-0.101919
9	7	0	-2.384123	0.417033	0.195579
10	8	0	1.050278	1.357524	0.042801
11	1	0	1.760275	1.535287	0.665786

302

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.135908	-0.717515	0.752785
2	6	0	1.135854	-0.717550	-0.752854
3	6	0	0.193952	0.188063	0.000007
4	1	0	0.725031	-1.573914	1.275420
5	1	0	1.945878	-0.201588	1.256213
6	1	0	0.724955	-1.573985	-1.275417
7	1	0	1.945784	-0.201634	-1.256356
8	8	0	0.493939	1.552966	0.000156
9	1	0	-0.322225	2.058004	-0.001201
10	6	0	-1.216769	-0.140417	0.000056
11	7	0	-2.352086	-0.372300	0.000019

303

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.098942	-0.719589	-0.739764
2	6	0	1.081966	-0.701732	0.775216
3	6	0	0.160122	0.187207	-0.015445
4	1	0	1.925825	-0.229296	-1.240314
5	1	0	0.676416	-1.578396	-1.247639
6	1	0	1.904107	-0.205683	1.279221
7	1	0	0.648371	-1.548901	1.294277
8	6	0	-2.363061	-0.382989	0.004036
9	7	0	-1.211063	-0.143324	-0.014242
10	8	0	0.413392	1.539740	-0.106657
11	1	0	0.147776	1.950232	0.723139

304

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-1.797265	-0.757440	-0.004416
2	6	0	-1.796776	0.757932	-0.003331
3	6	0	-0.574645	0.000115	-0.388165
4	1	0	-1.778804	-1.248820	0.961996
5	1	0	-2.331477	-1.289233	-0.783861
6	1	0	-1.777982	1.247925	0.963777
7	1	0	-2.330651	1.291191	-0.782004
8	1	0	-0.209521	0.000739	-1.408758
9	8	0	0.485347	-0.001013	0.583599
10	6	0	1.683858	-0.000161	0.114071
11	7	0	2.779232	0.000517	-0.275556

305

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.929586	-0.356449	-0.156064
2	6	0	1.256670	0.997348	-0.138511
3	6	0	0.611180	-0.180807	0.510780
4	1	0	1.930675	-0.895874	-1.096535
5	1	0	2.793291	-0.528952	0.475872
6	1	0	0.816509	1.345081	-1.066672
7	1	0	1.649193	1.775907	0.505597
8	8	0	-0.469518	-0.803237	-0.180204
9	1	0	0.509495	-0.241040	1.589648
10	7	0	-1.581378	-0.093978	-0.051595
11	6	0	-2.609666	0.478011	0.016277

306

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.891876	-0.753921	-0.121951
2	6	0	1.894466	0.751566	-0.121516
3	6	0	0.730045	0.000716	0.461641
4	1	0	1.719866	-1.254562	-1.067824
5	1	0	2.546832	-1.278729	0.564783
6	1	0	1.724175	1.253362	-1.067103
7	1	0	2.551230	1.273741	0.565489
8	1	0	0.620298	0.000602	1.541885
9	6	0	-1.674070	0.000239	-0.047218
10	8	0	-2.847384	-0.001304	0.034982
11	7	0	-0.491033	0.003488	-0.263260

307

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.704740	-0.071723	0.528643
2	1	0	-0.856555	-0.059506	1.613075

3	6	0	-1.960455	-0.306031	-0.292168
4	1	0	-2.387624	-1.283891	-0.058325
5	1	0	-2.706120	0.463659	-0.080167
6	1	0	-1.734984	-0.280953	-1.361507
7	6	0	0.426019	0.831950	0.087332
8	6	0	0.648699	-0.618946	0.120554
9	8	0	0.784667	1.942729	-0.180310
10	7	0	1.249993	-1.699270	-0.126710
11	1	0	2.200858	-1.497747	-0.449800

308

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.908635	1.257462	-0.158224
2	6	0	0.175321	0.291656	0.464978
3	1	0	-1.357765	1.989125	0.504733
4	1	0	-0.681216	1.583625	-1.167402
5	1	0	0.386732	0.399856	1.529736
6	6	0	-1.188268	-0.171208	0.041790
7	8	0	-1.950883	-1.103730	-0.058035
8	7	0	1.236374	-0.054469	-0.440284
9	6	0	2.386084	-0.345047	0.026377
10	1	0	2.636660	-0.344769	1.093062
11	1	0	3.181020	-0.613881	-0.663387

309

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.692403	0.097676	0.534478
2	1	0	0.835439	0.103715	1.619846
3	6	0	-0.409555	-0.841897	0.079178
4	6	0	-0.687202	0.587580	0.095348
5	6	0	1.947720	0.353677	-0.281278
6	1	0	2.364448	1.338420	-0.054261
7	1	0	2.704506	-0.402026	-0.058412
8	1	0	1.731129	0.312448	-1.352148
9	8	0	-0.713499	-1.972016	-0.173083
10	7	0	-1.457883	1.543552	-0.188365
11	1	0	-0.982548	2.436494	-0.018159

310

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.189216	0.502325	-0.001716
2	6	0	1.029218	1.353735	0.000396
3	6	0	1.065698	-0.154728	0.001218
4	1	0	1.292763	1.880751	0.916771
5	1	0	1.297796	1.878877	-0.915596
6	6	0	1.789303	-1.261898	-0.000231

7	1	0	1.308488	-2.234314	-0.002532
8	1	0	2.873991	-1.226649	0.001297
9	8	0	-1.978990	-0.758375	0.000656
10	1	0	-2.927388	-0.595013	0.000863
11	7	0	-1.454821	0.532392	-0.000579

400

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.697103	-0.071068	0.000158
2	6	0	-0.602129	-0.478360	-0.000255
3	6	0	-0.294058	0.934736	-0.000213
4	8	0	-0.670213	2.087095	0.000162
5	6	0	2.125260	-0.478324	0.000222
6	1	0	2.234585	-1.564439	0.048935
7	1	0	2.622371	-0.118443	-0.905290
8	1	0	2.644402	-0.036930	0.855604
9	7	0	-1.448412	-1.514382	-0.000467
10	1	0	-2.439874	-1.353672	0.002214
11	1	0	-1.117948	-2.464511	0.001041

401

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.854680	-0.111110	-0.000072
2	8	0	1.840150	-0.828251	0.000046
3	6	0	-0.536905	-0.690668	-0.000250
4	6	0	-1.696315	0.030714	0.645478
5	6	0	-1.696391	0.031160	-0.645299
6	1	0	-0.500956	-1.780143	-0.000602
7	7	0	0.937001	1.251246	-0.000224
8	1	0	1.852139	1.668157	0.001085
9	1	0	0.122653	1.839514	0.000996
10	1	0	-2.152007	0.288963	1.586868
11	1	0	-2.152447	0.290220	-1.586293

402

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.598685	0.877387	-0.019883
2	6	0	-1.927019	-0.594685	0.017138
3	6	0	-0.583983	0.069462	0.001984
4	1	0	-2.293897	-1.084774	-0.885916
5	1	0	-2.295282	-1.039521	0.942798
6	1	0	-1.999203	1.877839	-0.053982
7	6	0	0.873967	-0.172871	-0.000750
8	8	0	1.350541	-1.292085	-0.013242
9	7	0	1.623831	0.964953	0.006329
10	1	0	1.205495	1.877574	0.045556

11	1	0	2.626061	0.875135	0.022237

403

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.395827	-0.109857	-0.361379
2	8	0	2.469364	-0.466385	0.065569
3	1	0	1.178373	-0.090432	-1.455373
4	6	0	0.260159	0.351062	0.486136
5	6	0	-0.754646	1.323753	-0.112690
6	6	0	-1.144798	0.097367	0.022578
7	1	0	0.489674	0.358243	1.556317
8	1	0	-0.913198	2.357121	-0.358474
9	7	0	-2.028640	-0.920647	-0.102338
10	1	0	-1.846976	-1.745671	0.445449
11	1	0	-3.001562	-0.677599	-0.203976

404

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.704864	0.011376	-0.643958
2	6	0	-1.704916	0.011382	0.643912
3	6	0	-0.532920	-0.685477	0.000028
4	1	0	-0.489146	-1.777598	0.000058
5	1	0	-2.141364	0.291292	-1.587320
6	1	0	-2.141483	0.291316	1.587238
7	6	0	0.826129	-0.064375	0.000078
8	7	0	1.949640	-0.658169	-0.000025
9	1	0	1.819965	-1.667794	-0.000096
10	8	0	0.786676	1.283226	-0.000015
11	1	0	1.710563	1.566727	0.000059

405

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.616204	-0.865397	-0.000079
2	6	0	0.578569	-0.092723	0.000145
3	6	0	1.904517	0.616186	0.000014
4	1	0	2.263459	1.092429	-0.914765
5	1	0	2.263810	1.092308	0.914711
6	1	0	2.041460	-1.854909	-0.000257
7	6	0	-0.864658	0.098495	0.000041
8	7	0	-1.477931	1.211652	-0.000072
9	1	0	-0.810203	1.979388	0.000004
10	8	0	-1.542732	-1.063483	0.000016
11	1	0	-2.478950	-0.822281	-0.000039

406

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.671219	0.812672	-0.000494
2	6	0	0.583568	0.107283	0.000178
3	6	0	1.860031	-0.683642	0.000375
4	1	0	2.181296	-1.183850	0.915439
5	1	0	2.181068	-1.184961	-0.914162
6	1	0	2.160867	1.772740	-0.001448
7	6	0	-0.875283	0.068177	0.000057
8	7	0	-1.667211	1.063051	0.000278
9	1	0	-1.144855	1.935945	0.000609
10	8	0	-1.353551	-1.188037	-0.000340
11	1	0	-2.316704	-1.103875	-0.000363

407

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.709333	0.022208	-0.644268
2	6	0	-1.709331	0.022218	0.644265
3	6	0	-0.545550	-0.688931	0.000004
4	1	0	-0.494251	-1.777315	0.000015
5	1	0	-2.151744	0.299031	-1.586052
6	1	0	-2.151740	0.299055	1.586046
7	6	0	0.820951	-0.090160	0.000004
8	7	0	1.848543	-0.837022	0.000000
9	1	0	2.719884	-0.303944	-0.000008
10	8	0	0.788345	1.268319	-0.000003
11	1	0	1.690870	1.603767	-0.000005

408

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.628974	0.837043	0.000133
2	6	0	-0.591918	0.061214	-0.000088
3	6	0	-1.912107	-0.645364	-0.000099
4	1	0	-2.262875	-1.127203	-0.914544
5	1	0	-2.262610	-1.127857	0.914093
6	1	0	-2.048793	1.829209	0.000725
7	6	0	0.851515	-0.108279	0.000048
8	7	0	1.365628	-1.270696	0.000116
9	1	0	2.386740	-1.239255	0.000004
10	8	0	1.484914	1.092757	-0.000166
11	1	0	2.437744	0.950234	0.000278

409

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	1.675941	0.831660	-0.000778
2	6	0	0.590877	0.126687	0.000288
3	6	0	1.867324	-0.665036	0.000601
4	1	0	2.191452	-1.166078	0.915022
5	1	0	2.191048	-1.167976	-0.912928
6	1	0	2.154669	1.796518	-0.002429
7	6	0	-0.865089	0.082488	0.000115
8	7	0	-1.546163	1.155624	0.000563
9	1	0	-2.551534	0.974903	0.000270
10	8	0	-1.312595	-1.197973	-0.000542
11	1	0	-2.276049	-1.197743	-0.000894

410

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.638728	-1.183382	0.642563
2	6	0	0.639388	-1.183369	-0.642399
3	6	0	0.365773	0.154430	-0.000145
4	1	0	0.735217	-1.677499	1.593779
5	1	0	0.736579	-1.677733	-1.593430
6	7	0	1.397883	1.162763	0.000304
7	1	0	1.334045	1.757509	-0.819202
8	1	0	1.332358	1.758548	0.818919
9	6	0	-1.059986	0.639494	-0.000277
10	1	0	-1.165444	1.749891	-0.000140
11	8	0	-2.032670	-0.076637	-0.000062

411

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.132155	-0.589141	0.000307
2	6	0	-0.873956	-0.293090	0.000197
3	6	0	-1.805507	0.894656	-0.000245
4	1	0	-1.950296	1.478340	-0.914600
5	1	0	-2.932329	-1.309363	-0.000376
6	1	0	-1.950028	1.478870	0.913805
7	7	0	0.438764	-0.700691	-0.000212
8	6	0	1.289925	0.242409	0.000192
9	1	0	1.021765	1.306620	0.000960
10	8	0	2.595585	-0.043714	-0.000176
11	1	0	3.105024	0.771088	0.000402

412

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.932075	-0.348251	-0.436516
2	6	0	-0.728497	-0.368437	0.040781

3	6	0	-1.519957	0.873044	0.358862
4	1	0	-1.293629	1.813742	-0.151319
5	1	0	-2.704376	-0.780560	-1.049859
6	1	0	-1.904679	1.010591	1.373246
7	7	0	0.453300	-1.042534	0.236588
8	6	0	1.554894	-0.432647	0.114426
9	1	0	2.485208	-0.959306	0.329522
10	8	0	1.674636	0.845986	-0.291011
11	1	0	2.601100	1.103131	-0.294934

413

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.810944	0.851238	-0.126670
2	6	0	0.861217	-0.033592	-0.117592
3	6	0	2.215437	-0.566041	0.235391
4	1	0	2.768280	-1.174709	-0.485683
5	1	0	2.173504	1.838983	-0.355942
6	1	0	2.434744	-0.820079	1.276344
7	7	0	-0.427585	-0.423045	-0.375726
8	6	0	-1.362779	0.195131	0.209306
9	1	0	-1.204544	0.991201	0.947753
10	8	0	-2.638288	-0.120673	-0.055930
11	1	0	-3.221497	0.410880	0.492448

414

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.233153	-0.748741	0.008034
2	6	0	0.748175	0.139254	-0.000638
3	7	0	2.064824	0.479103	-0.076897
4	1	0	2.290759	1.399558	0.266324
5	1	0	2.721081	-0.233480	0.203148
6	8	0	-0.572061	-2.043843	0.001936
7	1	0	-1.532363	-2.099322	-0.003371
8	6	0	-0.616407	0.624268	0.000930
9	6	0	-1.501616	1.626114	0.001786
10	1	0	-1.172606	2.657516	-0.017429
11	1	0	-2.566143	1.427374	0.013454

415

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.056952	1.305516	-0.000226
2	6	0	-0.035398	0.541778	0.000031
3	1	0	1.449040	2.312737	-0.000411
4	6	0	-1.514197	0.471326	0.000316
5	1	0	-1.884051	1.011141	0.886215
6	1	0	-1.884517	1.012138	-0.884776

7	8	0	-1.900951	-0.881631	-0.000327
8	1	0	-2.860560	-0.919015	-0.000145
9	6	0	1.251343	-0.108551	0.000014
10	7	0	2.046792	-1.094732	0.000087
11	1	0	1.507945	-1.961240	0.000310

416

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.485094	1.186485	-0.000013
2	6	0	-0.065320	-0.030260	0.000023
3	1	0	0.357423	2.258256	0.000064
4	8	0	-1.163380	-0.754302	0.000004
5	6	0	-2.369145	0.016710	-0.000009
6	1	0	-2.418934	0.644274	-0.894842
7	1	0	-3.188144	-0.700314	-0.000323
8	1	0	-2.419264	0.643801	0.895142
9	6	0	1.368388	0.046530	-0.000019
10	7	0	2.558495	-0.388610	0.000005
11	1	0	2.552391	-1.408129	-0.000004

417

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.035136	1.305043	-0.000889
2	6	0	-0.039412	0.515455	0.000144
3	1	0	1.399285	2.323073	-0.001674
4	6	0	-1.520156	0.453910	0.001216
5	1	0	-1.877718	1.002189	0.887623
6	1	0	-1.879347	1.006025	-0.882133
7	8	0	-1.932565	-0.887388	-0.001278
8	1	0	-2.892653	-0.905206	-0.000312
9	6	0	1.248232	-0.115221	0.000044
10	7	0	1.921542	-1.188207	0.000537
11	1	0	2.917361	-0.964646	-0.000122

418

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.995401	-0.100655	0.644214
2	6	0	1.995347	-0.100783	-0.644256
3	6	0	0.644745	-0.344907	0.000061
4	1	0	0.226153	-1.348783	0.000175
5	1	0	2.510201	-0.011734	1.586200
6	1	0	2.510070	-0.012054	-1.586302
7	6	0	-0.361658	0.743289	0.000019
8	1	0	0.002835	1.770176	-0.000222
9	7	0	-1.633910	0.644494	-0.000044
10	8	0	-2.055348	-0.686698	0.000036

11	1	0	-3.012118	-0.597136	-0.000060

419

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.906664	0.657980	0.071442
2	6	0	-1.899060	-0.633748	0.087401
3	6	0	-0.646737	0.012339	-0.446793
4	1	0	-2.415460	1.592062	0.242367
5	1	0	-2.395269	-1.570059	0.280999
6	1	0	-0.436095	-0.000771	-1.518365
7	6	0	0.601778	0.027487	0.374267
8	1	0	0.444236	0.069889	1.456991
9	8	0	1.661613	-0.780155	-0.040967
10	7	0	1.751028	0.686211	-0.178959
11	1	0	2.356579	0.962296	0.600558

420

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.871493	0.653020	-0.076377
2	6	0	1.848901	-0.641050	-0.047826
3	6	0	0.599751	0.034937	0.398394
4	1	0	2.384151	1.576417	-0.288935
5	1	0	2.328676	-1.590877	-0.213017
6	1	0	0.308469	0.046254	1.454956
7	8	0	-1.605890	-0.794323	0.052364
8	7	0	-0.529914	0.050686	-0.522625
9	6	0	-1.715854	0.595404	0.045507
10	1	0	-2.431389	1.028739	-0.652979
11	1	0	-1.659129	1.085377	1.021250

500

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.200756	1.224894	0.437886
2	6	0	1.118156	1.070074	-0.288862
3	6	0	0.502221	-0.283213	-0.239742
4	1	0	2.024665	1.193012	0.314806
5	1	0	1.228996	1.551963	-1.262769
6	1	0	-0.367637	1.742344	1.376308
7	6	0	-0.905399	0.117560	-0.115801
8	8	0	-1.990323	-0.433992	-0.122081
9	7	0	1.065829	-1.445296	0.133718
10	1	0	0.458189	-2.189127	0.439901
11	1	0	2.032244	-1.485067	0.411490

501

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.092480	-0.081940	-0.068394
2	6	0	-0.345580	0.059555	-0.041972
3	6	0	-1.626639	-0.174267	-0.739542
4	6	0	-1.515481	-0.341912	0.774463
5	1	0	-1.718046	-1.063448	-1.354377
6	1	0	-2.158414	0.699186	-1.103501
7	7	0	0.601040	1.211848	-0.043698
8	1	0	0.728119	1.782444	0.788571
9	8	0	2.103516	-0.718291	-0.019449
10	1	0	-1.531417	-1.343246	1.192889
11	1	0	-1.984330	0.419844	1.390562

502

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.578770	-0.386175	0.657041
2	1	0	-1.619175	-1.394538	1.057006
3	1	0	-2.172716	0.355616	1.186200
4	6	0	-0.346608	0.082256	0.002617
5	6	0	0.569804	1.306405	0.102830
6	6	0	1.087247	-0.104095	0.001082
7	1	0	0.632285	1.847925	1.045486
8	1	0	0.681034	1.927273	-0.785735
9	7	0	-1.479322	-0.305748	-0.809344
10	1	0	-1.951270	0.534497	-1.139965
11	8	0	2.049382	-0.815110	-0.034876

503

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.914005	0.073069	-0.476763
2	6	0	0.457056	0.147383	0.025952
3	6	0	1.563817	-0.639418	0.461084
4	1	0	2.043504	-1.335404	1.137314
5	8	0	-1.749121	-0.893120	0.079742
6	1	0	-2.640539	-0.533284	0.098040
7	6	0	-0.438883	1.264176	0.393634
8	1	0	-0.317936	2.227617	-0.094819
9	7	0	1.827667	0.017841	-0.583030
10	1	0	-0.814555	1.300603	1.413067
11	1	0	-1.079084	0.289288	-1.533775

504

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-1.000541	0.075141	0.033483
2	6	0	0.445121	0.192313	0.024262
3	6	0	1.664639	-0.285558	0.677884
4	1	0	2.377851	0.412659	1.108769
5	8	0	-2.005224	-0.798794	0.042021
6	1	0	-2.836626	-0.312803	-0.002888
7	6	0	-0.553076	1.305566	-0.002925
8	7	0	1.546386	-0.200290	-0.817792
9	1	0	-0.719098	2.368446	-0.046322
10	1	0	1.398010	-1.129412	-1.206807
11	1	0	1.660100	-1.271278	1.139392

505

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.498501	-0.408027	0.788281
2	7	0	-1.587533	-0.463392	-0.721393
3	1	0	-2.275055	0.267806	-0.931635
4	6	0	-0.520509	0.147303	-0.012955
5	6	0	0.309068	1.334294	0.018696
6	6	0	0.929912	0.167394	-0.024078
7	6	0	2.190998	-0.602834	-0.031632
8	1	0	2.236732	-1.234992	-0.922971
9	1	0	3.062586	0.054586	-0.012231
10	1	0	0.396339	2.409754	0.072726
11	1	0	2.223319	-1.266142	0.837426

506

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.436925	-0.427434	-0.775896
2	7	0	1.527411	-0.459226	0.717868
3	1	0	2.161494	0.321660	0.920203
4	6	0	0.428529	0.084507	0.006591
5	6	0	-0.362267	1.359284	-0.028102
6	6	0	-1.006569	-0.000349	0.028073
7	1	0	-0.408082	1.907031	-0.967783
8	1	0	-0.382884	1.984076	0.863668
9	6	0	-2.121593	-0.704545	0.039611
10	1	0	-2.091989	-1.789166	0.061490
11	1	0	-3.094423	-0.222930	0.027472

600

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.981091	-0.068194	0.000150
2	8	0	-2.061076	-0.606977	-0.001575

3	6	0	0.272365	-0.971695	0.001500
4	1	0	0.209040	-1.620348	0.880734
5	1	0	0.208598	-1.623790	-0.875118
6	6	0	-0.791364	1.424303	0.000706
7	1	0	-0.213512	1.731787	0.878433
8	1	0	-0.212261	1.732109	-0.876084
9	1	0	-1.764687	1.913256	0.000033
10	6	0	1.555368	-0.275992	-0.000053
11	7	0	2.561394	0.296039	-0.001316

601

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.888254	0.434126	-0.000218
2	8	0	-2.325547	-0.690768	0.000067
3	1	0	-2.566608	1.312194	-0.000192
4	6	0	-0.415788	0.761883	0.000078
5	1	0	-0.202876	1.389068	0.874665
6	1	0	-0.202092	1.389932	-0.873565
7	6	0	0.448697	-0.501683	-0.000041
8	1	0	0.219380	-1.114883	-0.876046
9	1	0	0.219251	-1.115390	0.875593
10	6	0	1.876283	-0.183818	0.000084
11	7	0	3.001671	0.086025	-0.000059

602

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.788691	-0.096356	0.000072
2	6	0	0.325247	-0.852339	0.000204
3	1	0	0.246555	-1.932932	0.000317
4	6	0	1.622593	-0.271871	0.000117
5	7	0	2.681657	0.205236	-0.000245
6	8	0	-1.979821	-0.730381	-0.000161
7	1	0	-2.694082	-0.087323	-0.000552
8	6	0	-0.820828	1.400022	0.000075
9	1	0	-1.350264	1.765138	0.887174
10	1	0	0.184958	1.819475	0.000235
11	1	0	-1.350120	1.765304	-0.886981

603

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.335110	-0.214883	0.158067
2	8	0	1.456952	-1.327981	-0.274535
3	1	0	2.213438	0.425896	0.386213
4	6	0	0.004961	0.479385	0.445314
5	1	0	-0.011247	0.679449	1.525799
6	6	0	-0.066493	1.824895	-0.302262

7	1	0	-0.973955	2.364673	-0.027818
8	1	0	0.795957	2.443500	-0.039570
9	1	0	-0.068942	1.665916	-1.382707
10	6	0	-1.137197	-0.381320	0.130228
11	7	0	-2.061307	-1.029148	-0.121959

604

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.199698	0.439986	-0.000001
2	6	0	-1.140566	0.496048	-0.000005
3	1	0	-1.645615	1.460089	-0.000029
4	6	0	0.856569	-0.832580	-0.000001
5	7	0	1.430388	-1.841064	-0.000005
6	6	0	1.065877	1.673743	0.000003
7	1	0	1.711218	1.700211	0.882985
8	1	0	1.711217	1.700225	-0.882979
9	1	0	0.450341	2.577019	0.000010
10	8	0	-1.911299	-0.606431	0.000018
11	1	0	-2.838945	-0.361835	-0.000078

605

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.102448	0.177506	-0.000006
2	6	0	0.852445	-0.765785	-0.000012
3	1	0	0.597807	-1.822722	-0.000005
4	6	0	-1.461210	-0.272068	-0.000005
5	7	0	-2.571347	-0.611589	0.000008
6	8	0	2.161508	-0.445073	-0.000004
7	1	0	2.693952	-1.243317	0.000086
8	6	0	0.165193	1.659486	0.000009
9	1	0	-0.273986	2.132431	0.883087
10	1	0	1.239154	1.848138	0.000299
11	1	0	-0.273450	2.132340	-0.883400

606

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.847958	-0.788030	0.468029
2	6	0	0.899867	-0.025765	-0.074333
3	1	0	2.748747	-0.360598	0.896792
4	1	0	1.739279	-1.863809	0.500517
5	6	0	-0.355094	-0.574689	-0.707315
6	1	0	-0.425090	-0.216098	-1.740192
7	1	0	-0.318863	-1.665902	-0.731212
8	8	0	0.918807	1.326603	-0.159062
9	1	0	1.694135	1.665873	0.298679
10	6	0	-1.569364	-0.157376	0.002113

11	7	0	-2.532696	0.157553	0.559564

607

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.839573	-0.720606	-0.000032
2	6	0	0.139405	0.193517	0.000008
3	1	0	-0.531901	-1.760454	-0.000042
4	6	0	1.518722	-0.225450	-0.000008
5	7	0	2.619484	-0.585847	0.000015
6	8	0	0.022954	1.545983	-0.000004
7	1	0	-0.909131	1.783626	-0.000022
8	6	0	-2.310275	-0.439995	0.000011
9	1	0	-2.786592	-0.881348	-0.881255
10	1	0	-2.786363	-0.880355	0.881922
11	1	0	-2.555715	0.626796	-0.000550

608

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.091761	0.577244	0.000025
2	6	0	-0.245725	0.520098	-0.000169
3	1	0	1.550353	1.565329	0.000222
4	6	0	-0.946521	-0.739981	-0.000086
5	7	0	-1.482945	-1.766681	0.000074
6	8	0	-1.105508	1.573551	0.000092
7	1	0	-0.596860	2.390418	-0.000187
8	6	0	2.013649	-0.601549	0.000024
9	1	0	1.466061	-1.546480	0.000719
10	1	0	2.662537	-0.583271	-0.881774
11	1	0	2.663606	-0.582507	0.881002

609

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.202842	-0.672790	0.157535
2	6	0	1.137758	-0.150930	-0.436514
3	1	0	2.275865	-0.749899	1.239063
4	1	0	3.042595	-1.045436	-0.418661
5	1	0	1.066073	-0.072379	-1.517887
6	6	0	-0.057998	0.369894	0.317286
7	1	0	0.149336	0.336423	1.397094
8	8	0	-0.317212	1.680470	-0.129332
9	1	0	-1.103899	2.010248	0.316235
10	6	0	-1.233323	-0.507411	0.077351
11	7	0	-2.169707	-1.165043	-0.096448

610

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.709756	0.601834	-0.000113
2	6	0	0.384876	0.712569	0.000442
3	1	0	2.358877	1.473701	-0.000320
4	1	0	-0.063678	1.697562	0.000721
5	8	0	2.310926	-0.618742	-0.000362
6	1	0	3.264149	-0.514557	-0.001289
7	6	0	-0.506816	-0.508209	0.000766
8	1	0	-0.304943	-1.135769	0.876858
9	1	0	-0.304143	-1.136781	-0.874413
10	6	0	-1.930324	-0.168329	-0.000056
11	7	0	-3.054661	0.105513	-0.000700

611

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.522936	0.124913	-0.306177
2	6	0	0.444556	0.164115	0.471597
3	1	0	1.530069	0.589497	-1.292107
4	1	0	0.463647	-0.316869	1.444046
5	6	0	-0.820434	0.862453	0.047983
6	1	0	-1.098038	1.645189	0.763682
7	1	0	-0.689340	1.353847	-0.922135
8	6	0	-1.961420	-0.057853	-0.061521
9	7	0	-2.855416	-0.788697	-0.139089
10	8	0	2.668796	-0.484168	0.085971
11	1	0	3.317374	-0.439211	-0.618929

612

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.444687	1.873169	-0.192025
2	6	0	-0.145325	0.600881	0.073865
3	1	0	-1.456932	2.187251	-0.419926
4	1	0	0.329658	2.633245	-0.182230
5	6	0	-1.163877	-0.416829	0.045240
6	7	0	-1.924287	-1.292306	0.037706
7	6	0	1.242836	0.092949	0.421687
8	1	0	1.258223	-0.201108	1.481876
9	1	0	1.958305	0.908583	0.293546
10	8	0	1.663533	-0.955715	-0.414499
11	1	0	1.138812	-1.737135	-0.213818

613

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.869793	1.039594	-0.046035
2	6	0	0.449146	0.879515	0.097399
3	1	0	-1.309533	2.024736	-0.155605
4	1	0	1.090473	1.756704	0.096097
5	6	0	-1.779379	-0.067171	-0.056314
6	7	0	-2.511482	-0.966911	-0.062233
7	6	0	1.151850	-0.426791	0.299602
8	1	0	0.556392	-1.247666	-0.125282
9	1	0	1.229273	-0.609112	1.384704
10	8	0	2.425457	-0.320736	-0.298598
11	1	0	2.899167	-1.141278	-0.143406

614

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.440594	0.857627	0.000033
2	6	0	0.882088	1.050689	0.000108
3	1	0	-1.105517	1.716755	0.000044
4	1	0	1.311527	2.045846	0.000205
5	6	0	-1.114517	-0.482319	-0.000117
6	1	0	-0.787127	-1.052848	0.883527
7	1	0	-0.787087	-1.052653	-0.883866
8	8	0	-2.506696	-0.260108	-0.000107
9	1	0	-2.948602	-1.112191	-0.001105
10	6	0	1.797584	-0.050107	-0.000047
11	7	0	2.517573	-0.959911	0.000312

615

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.314080	-0.125161	0.004575
2	6	0	0.803021	0.606511	-0.003142
3	1	0	-0.262350	-1.210789	0.012236
4	1	0	0.775453	1.693164	-0.011187
5	6	0	2.103806	0.011513	-0.001225
6	7	0	3.165718	-0.454485	0.000145
7	6	0	-1.698551	0.456372	0.004592
8	1	0	-1.820598	1.105199	-0.877149
9	1	0	-1.825414	1.092331	0.895038
10	8	0	-2.611232	-0.616716	-0.005490
11	1	0	-3.502444	-0.260196	-0.004824

616

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.057996	0.369876	0.317302
2	1	0	0.149524	0.336542	1.397092

3	6	0	1.137661	-0.151158	-0.436543
4	6	0	2.202910	-0.672651	0.157515
5	1	0	1.065660	-0.073124	-1.517923
6	1	0	3.042585	-1.045466	-0.418689
7	1	0	2.276246	-0.749241	1.239055
8	8	0	-0.317142	1.680416	-0.129475
9	1	0	-1.103801	2.010320	0.316048
10	6	0	-1.233301	-0.507487	0.077668
11	7	0	-2.169818	-1.164835	-0.096491

617

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.619135	0.649691	0.000026
2	6	0	-0.303205	0.784817	0.000016
3	1	0	-2.187875	1.573749	0.000045
4	1	0	0.250979	1.715175	0.000025
5	6	0	-2.345967	-0.664912	0.000014
6	1	0	-2.083979	-1.259206	0.880700
7	1	0	-3.426165	-0.513973	0.000004
8	1	0	-2.083961	-1.259200	-0.880669
9	8	0	0.495687	-0.372551	-0.000008
10	6	0	1.775335	-0.203650	-0.000022
11	7	0	2.931905	-0.095974	-0.000035

700

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.048779	0.453136	0.000000
2	8	0	-0.625448	1.525335	-0.000006
3	6	0	1.430259	0.393909	0.000009
4	6	0	2.164171	-0.719851	-0.000004
5	1	0	1.905201	1.371116	0.000023
6	1	0	3.247927	-0.667186	-0.000001
7	1	0	1.732886	-1.715064	-0.000023
8	6	0	-0.882748	-0.818477	-0.000006
9	1	0	-0.387033	-1.789414	0.000020
10	7	0	-2.148677	-0.780509	0.000005
11	1	0	-2.432068	0.209132	0.000000

701

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.837926	-0.401130	-0.000077
2	8	0	2.916756	0.144896	0.000074
3	1	0	1.717884	-1.502092	-0.000324
4	6	0	0.556393	0.351519	-0.000003
5	1	0	0.622007	1.447587	-0.000192
6	7	0	-0.533947	-0.311066	0.000070

7	6	0	-1.738602	0.402063	-0.000019
8	6	0	-2.901612	-0.248337	0.000010
9	1	0	-1.696022	1.494552	-0.000092
10	1	0	-3.844257	0.286393	-0.000033
11	1	0	-2.920663	-1.332843	0.000085

702

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.090944	0.744074	-0.000184
2	8	0	-0.633394	1.857244	0.000412
3	1	0	-2.192809	0.578451	-0.000846
4	6	0	-0.323964	-0.539925	-0.000089
5	6	0	-1.040041	-1.671523	-0.000300
6	1	0	-0.568167	-2.649728	-0.000209
7	1	0	-2.126506	-1.653004	-0.000577
8	6	0	1.153873	-0.612544	0.000213
9	1	0	1.535395	-1.644977	0.000756
10	7	0	1.905884	0.410426	-0.000076
11	1	0	2.884513	0.117838	0.000272

703

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.032255	0.498248	0.000003
2	8	0	-0.511649	1.611849	-0.000007
3	6	0	1.445616	0.326736	0.000015
4	6	0	2.119547	-0.824010	-0.000016
5	1	0	1.978307	1.274070	0.000041
6	1	0	3.204795	-0.828107	-0.000013
7	1	0	1.641088	-1.797667	-0.000051
8	6	0	-0.925520	-0.729051	0.000012
9	1	0	-0.437923	-1.709796	0.000098
10	7	0	-2.183643	-0.569505	-0.000018
11	1	0	-2.651905	-1.478292	0.000026

704

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.064886	0.681127	0.000068
2	8	0	-0.056804	1.896227	0.000379
3	6	0	1.406834	0.022228	-0.000909
4	6	0	1.631714	-1.287684	0.000429
5	1	0	2.217473	0.744210	-0.002622
6	1	0	2.641052	-1.684683	-0.000322
7	1	0	0.819910	-2.009563	0.002318
8	7	0	-0.986044	-0.154885	0.001099
9	6	0	-2.000172	-0.870288	-0.000757
10	1	0	-2.470251	-1.202344	-0.935585

11	1	0	-2.471022	-1.205543	0.932507

800

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.575497	-0.074670	-0.345080
2	8	0	-2.556465	-0.647574	0.074411
3	1	0	-1.408696	0.134911	-1.420331
4	7	0	-0.568642	0.409869	0.435859
5	1	0	-0.613087	0.165842	1.415251
6	6	0	0.670833	0.943524	-0.090812
7	1	0	0.945103	1.849126	0.460598
8	1	0	0.490275	1.255106	-1.125436
9	6	0	1.788535	-0.009317	-0.054660
10	6	0	2.701906	-0.792732	-0.009561
11	1	0	3.503957	-1.494306	0.024300

801

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.667090	-0.414271	0.000063
2	6	0	-1.516664	-0.051696	0.000007
3	1	0	-3.690330	-0.716258	0.000103
4	6	0	-0.109446	0.335181	-0.000027
5	8	0	0.235845	1.497305	-0.000020
6	6	0	0.890100	-0.818630	-0.000128
7	1	0	0.672762	-1.447863	0.872485
8	1	0	0.672879	-1.447504	-0.873040
9	7	0	2.279362	-0.427728	0.000078
10	1	0	2.460511	0.162166	-0.806279
11	1	0	2.460485	0.161613	0.806848

802

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.502462	0.764995	0.373558
2	1	0	1.080042	1.670279	0.190425
3	1	0	0.238532	0.706394	1.436247
4	8	0	-0.702332	0.893576	-0.404242
5	6	0	-1.630511	0.023518	-0.120013
6	6	0	-2.495124	-0.775932	0.133251
7	1	0	-3.276341	-1.465328	0.347408
8	6	0	1.292866	-0.448047	-0.037617
9	1	0	0.694257	-1.330668	-0.300717
10	7	0	2.559012	-0.401573	-0.033217
11	1	0	2.950923	-1.305477	-0.301988

900

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.980720	-0.113307	0.000101
2	6	0	0.281380	-0.869088	-0.000079
3	1	0	0.245271	-1.952104	-0.000341
4	7	0	-2.064366	-0.787719	0.000001
5	1	0	-2.867591	-0.157463	-0.000050
6	6	0	1.473124	-0.299954	0.000046
7	8	0	2.524667	0.199413	0.000132
8	6	0	-0.873898	1.395764	-0.000103
9	1	0	-0.330120	1.745478	0.883799
10	1	0	-0.330212	1.745252	-0.884153
11	1	0	-1.863437	1.857077	-0.000110

901

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.819488	-0.700680	0.000667
2	8	0	1.409216	-1.700179	-0.000409
3	6	0	0.166548	0.457297	0.000716
4	6	0	-1.294811	0.382746	0.000136
5	1	0	-1.777748	1.370338	-0.000196
6	7	0	-1.931503	-0.723004	-0.000175
7	1	0	-2.936072	-0.555785	-0.000739
8	6	0	0.920837	1.772227	-0.000303
9	1	0	1.546510	1.897458	0.887706
10	1	0	1.549945	1.894161	-0.886334
11	1	0	0.191787	2.586755	-0.003232

902

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.823409	0.014029	-0.150415
2	6	0	-0.634206	0.483835	-0.454741
3	1	0	-0.505960	0.861621	-1.462795
4	6	0	0.529367	0.490439	0.513840
5	1	0	0.959599	1.492392	0.597275
6	1	0	0.186519	0.191294	1.510969
7	6	0	1.617293	-0.453540	0.069125
8	1	0	1.298931	-1.497580	-0.064550
9	7	0	2.796268	-0.036234	-0.143970
10	1	0	3.397882	-0.807466	-0.439396
11	8	0	-2.880639	-0.399401	0.124929

903

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	1.282785	0.162759	0.000076
2	8	0	2.177635	-0.584221	0.000165
3	6	0	0.426260	1.181137	-0.000270
4	1	0	0.898673	2.156708	-0.000727
5	6	0	-1.021909	1.053173	0.000123
6	6	0	-1.659344	-0.121398	0.000180
7	1	0	-1.590274	1.977893	0.000373
8	1	0	-2.746710	-0.177981	0.000485
9	7	0	-0.866435	-1.309831	-0.000232
10	1	0	-1.041964	-1.884133	0.817945
11	1	0	-1.042515	-1.883936	-0.818429

904

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.701629	0.003973	0.005271
2	6	0	0.827885	1.002366	0.022293
3	1	0	1.231367	2.006661	0.056566
4	7	0	-0.569439	0.853348	-0.036719
5	6	0	-1.129690	-0.286732	0.061206
6	1	0	-0.563000	-1.218638	0.213444
7	6	0	-2.615407	-0.424567	-0.026194
8	1	0	-2.893832	-1.075769	-0.862459
9	1	0	-3.015219	-0.884884	0.884218
10	1	0	-3.074273	0.555398	-0.166268
11	8	0	2.449316	-0.890806	-0.030490

905

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.759530	-0.008851	-0.000008
2	6	0	-0.887862	0.983282	-0.000004
3	1	0	-1.322648	1.976049	0.000071
4	8	0	-2.533370	-0.881271	0.000000
5	6	0	0.567592	0.812235	-0.000006
6	6	0	1.243163	-0.339634	0.000009
7	1	0	1.144273	1.732331	-0.000021
8	1	0	0.707529	-1.294946	0.000031
9	7	0	2.672559	-0.338880	-0.000001
10	1	0	3.024863	-0.836657	0.812382
11	1	0	3.024851	-0.836643	-0.812399

906

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.826106	-0.683325	-0.001919
2	6	0	0.155719	0.462847	0.003733

3	7	0	-1.250990	0.482627	0.051375
4	6	0	-1.969610	-0.564348	-0.028206
5	1	0	-1.583434	-1.584695	-0.151632
6	1	0	-3.049544	-0.447923	0.030446
7	8	0	1.366395	-1.718670	0.012895
8	6	0	0.872870	1.787161	-0.018896
9	1	0	0.589792	2.378083	0.857084
10	1	0	1.958315	1.659323	-0.011676
11	1	0	0.600137	2.352170	-0.915277

907

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.519731	-0.472251	-0.091951
2	1	0	2.986247	-0.601342	0.808668
3	6	0	1.341269	-0.140516	-0.010537
4	6	0	0.059433	0.197180	-0.017112
5	8	0	-0.264308	1.537743	0.077637
6	1	0	-0.734021	1.777144	-0.729327
7	6	0	-1.002039	-0.804952	-0.052689
8	6	0	-2.299298	-0.511566	0.063752
9	1	0	-0.681893	-1.833259	-0.201669
10	1	0	-3.055275	-1.285847	0.009779
11	1	0	-2.634898	0.506238	0.234630

908

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.273394	-0.115014	0.000007
2	6	0	-2.520495	-0.497820	0.000023
3	1	0	-3.063699	-0.666768	0.927924
4	1	0	-3.063687	-0.666651	-0.927917
5	6	0	-0.006952	0.253903	-0.000037
6	6	0	1.051054	-0.774117	-0.000029
7	1	0	0.663840	-1.800235	-0.000114
8	7	0	2.281500	-0.458516	0.000032
9	1	0	2.854837	-1.303241	0.000066
10	8	0	0.433536	1.540197	-0.000001
11	1	0	-0.331354	2.123212	0.000050

909

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.519764	-0.386565	0.051576
2	6	0	1.790835	-0.302105	0.377208
3	1	0	2.169188	-0.860398	1.229789
4	7	0	-0.657746	-0.527909	-0.279555
5	8	0	2.643710	0.569721	-0.273162
6	1	0	3.283076	0.046320	-0.766080

7	6	0	-1.665355	0.315405	0.243777
8	6	0	-2.932193	0.154565	-0.124392
9	1	0	-1.358010	1.087209	0.948975
10	1	0	-3.709574	0.798089	0.270168
11	1	0	-3.208442	-0.621423	-0.829680

1000

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.788207	0.193181	0.000119
2	8	0	-0.577583	1.378647	-0.000036
3	6	0	-2.184000	-0.394806	-0.000006
4	1	0	-2.719703	-0.032709	-0.881139
5	1	0	-2.188670	-1.487423	0.000008
6	1	0	-2.719865	-0.032685	0.881011
7	6	0	0.346735	-0.837708	-0.000022
8	1	0	0.232929	-1.481949	0.880407
9	1	0	0.232860	-1.481695	-0.880649
10	7	0	1.625558	-0.248313	0.000013
11	6	0	2.692839	0.243579	0.000002

1001

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.754971	-0.090057	-0.000007
2	6	0	-0.372679	-0.816601	-0.000003
3	1	0	-0.342427	-1.898927	0.000000
4	8	0	1.931247	-0.765278	0.000006
5	1	0	2.660621	-0.140472	-0.000005
6	6	0	0.822187	1.403508	0.000000
7	1	0	1.358061	1.759284	0.887176
8	1	0	1.358181	1.759283	-0.887104
9	1	0	-0.174132	1.844200	-0.000068
10	7	0	-1.619465	-0.230578	-0.000002
11	6	0	-2.700149	0.238634	0.000005

1002

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.990941	-0.735017	0.000965
2	6	0	-0.313978	-0.462355	-0.000032
3	1	0	1.260333	-1.785300	0.002252
4	7	0	-0.782481	0.842183	-0.000813
5	6	0	-1.154408	1.962029	0.000559
6	8	0	-1.274835	-1.420850	-0.001329
7	1	0	-2.141537	-1.005958	0.007993
8	6	0	2.063264	0.315778	-0.000207
9	1	0	3.051739	-0.145943	0.007161
10	1	0	1.999498	0.957821	-0.885372

11	1	0	1.991107	0.968298	0.876579

1003

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.019454	-0.539323	-0.372232
2	6	0	-0.883354	0.018850	0.034892
3	1	0	-2.109850	-1.615222	-0.449186
4	1	0	-2.878470	0.074042	-0.613756
5	6	0	0.316662	-0.798836	0.463632
6	1	0	0.388996	-0.809517	1.557161
7	1	0	0.221306	-1.828438	0.114324
8	7	0	1.526950	-0.243195	-0.041664
9	6	0	2.527338	0.216081	-0.459326
10	8	0	-0.765384	1.361360	0.190582
11	1	0	0.165286	1.609983	0.156649

1004

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.481192	0.116715	0.308952
2	6	0	0.409939	0.168871	-0.478282
3	1	0	1.468202	0.541483	1.312818
4	1	0	0.440301	-0.273417	-1.468741
5	6	0	-0.860912	0.831070	-0.036145
6	1	0	-0.730458	1.310863	0.939536
7	1	0	-1.164404	1.611325	-0.742628
8	7	0	-1.948581	-0.092399	0.068008
9	8	0	2.642957	-0.452260	-0.092928
10	1	0	3.280648	-0.428341	0.622975
11	6	0	-2.829866	-0.866161	0.139378

1005

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.670307	0.605345	0.000188
2	6	0	-0.345155	0.705959	0.000484
3	1	0	-2.313917	1.481062	0.000223
4	1	0	0.117673	1.684420	0.000768
5	8	0	-2.278998	-0.612629	-0.000166
6	1	0	-3.231503	-0.502362	-0.000429
7	6	0	0.543339	-0.512622	0.000428
8	1	0	0.347079	-1.137889	-0.877825
9	1	0	0.347812	-1.137304	0.879264
10	7	0	1.922198	-0.161038	-0.000236
11	6	0	3.057032	0.141378	-0.000936

1006

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.798536	1.730156	0.199108
2	6	0	0.272029	0.538925	-0.072397
3	1	0	1.850578	1.846628	0.429744
4	1	0	0.170560	2.613004	0.191538
5	7	0	1.054912	-0.609489	-0.051171
6	6	0	1.633022	-1.636634	-0.038025
7	6	0	-1.173007	0.273395	-0.434964
8	1	0	-1.733425	1.206200	-0.346027
9	1	0	-1.216993	-0.048877	-1.486499
10	8	0	-1.786344	-0.659674	0.418399
11	1	0	-1.347826	-1.508194	0.299919

1007

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.114292	-0.455110	-0.311603
2	6	0	-0.959711	-0.742926	0.272217
3	1	0	-2.319259	0.539645	-0.690656
4	1	0	-2.881432	-1.212781	-0.428075
5	1	0	-0.740549	-1.736682	0.652440
6	6	0	0.141663	0.265824	0.478247
7	1	0	0.292438	0.420416	1.557527
8	8	0	-0.174069	1.457269	-0.164564
9	1	0	0.491807	2.113051	0.060786
10	7	0	1.385802	-0.273805	-0.011743
11	6	0	2.407163	-0.711983	-0.397747

1008

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.932647	0.992608	0.000032
2	6	0	-0.391383	0.847774	-0.000276
3	1	0	1.424491	1.957798	-0.000306
4	1	0	-1.016672	1.734557	-0.001080
5	6	0	-1.099536	-0.473302	0.000224
6	1	0	-0.786696	-1.053489	-0.882787
7	1	0	-0.786936	-1.052741	0.883814
8	8	0	-2.486603	-0.218449	-0.000071
9	1	0	-2.947322	-1.060439	-0.000229
10	7	0	1.779111	-0.100861	0.000864
11	6	0	2.483636	-1.045758	-0.000795

1009

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.841284	0.567864	0.000002
2	6	0	0.283004	-0.144638	-0.000007
3	1	0	-0.852925	1.654110	0.000032
4	1	0	0.241834	-1.229929	-0.000037
5	7	0	-2.092260	-0.016756	-0.000027
6	6	0	-3.176586	-0.477813	-0.000051
7	6	0	1.657106	0.464852	0.000022
8	1	0	1.777376	1.107947	-0.886144
9	1	0	1.777342	1.107942	0.886195
10	8	0	2.587116	-0.595192	0.000037
11	1	0	3.471823	-0.222835	0.000053

1100

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.064713	1.272442	0.015189
2	6	0	-1.419830	0.948918	-0.071505
3	6	0	-0.179041	-1.176581	-0.063588
4	1	0	0.375617	1.919562	-0.842989
5	1	0	0.285801	1.841757	0.952947
6	1	0	-0.040988	-1.873777	0.800480
7	1	0	-0.033885	-1.776540	-0.997061
8	7	0	-1.572451	-0.564896	-0.037793
9	1	0	-2.049227	-0.838923	0.797427
10	6	0	0.833009	-0.041484	-0.001146
11	8	0	2.084592	-0.167197	0.035007

1101

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.719845	-0.392737	0.078555
2	8	0	2.911213	-0.249616	-0.116572
3	1	0	1.294012	-1.364592	0.414770
4	6	0	0.732499	0.654130	-0.095276
5	1	0	1.009675	1.658832	-0.389608
6	7	0	-0.523184	0.387641	0.121248
7	6	0	-1.646401	0.147856	0.449311
8	6	0	-2.865029	-0.344849	-0.232179
9	1	0	-3.229646	-1.233614	0.287911
10	1	0	-3.646461	0.413874	-0.142277
11	1	0	-2.700487	-0.577464	-1.289426

1102

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.465917	0.628438	0.000032
2	6	0	0.061049	1.131428	0.000090

3	6	0	-0.752455	0.059017	-0.000241
4	6	0	-0.013166	-1.230155	0.000145
5	1	0	2.037868	0.927011	-0.887516
6	1	0	2.038476	0.927121	0.887162
7	1	0	-0.208392	2.178127	0.000271
8	7	0	1.241836	-0.819811	-0.000085
9	1	0	2.017720	-1.465109	0.000178
10	8	0	-2.098137	0.063037	0.000018
11	1	0	-2.361502	-0.865132	0.000198

1103

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.460920	0.912153	-0.000071
2	6	0	0.011275	1.190797	0.000095
3	6	0	-0.702288	0.045792	-0.000021
4	6	0	0.228229	-1.125862	0.000099
5	7	0	1.503020	-0.424444	-0.000031
6	1	0	2.373352	-0.932414	-0.000497
7	1	0	-0.404074	2.192215	0.000106
8	1	0	0.095990	-1.753146	-0.888658
9	8	0	-2.022484	-0.195715	-0.000147
10	1	0	-2.491385	0.645049	0.000226
11	1	0	0.096032	-1.752161	0.889602

1104

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.953653	-0.233209	0.144131
2	8	0	2.463576	0.865448	0.075619
3	1	0	2.452693	-1.094164	0.636988
4	6	0	0.713638	-0.607580	-0.520679
5	7	0	-0.429198	-0.549648	-0.094531
6	6	0	-1.654393	-0.492226	0.235803
7	1	0	-2.077618	-1.364043	0.727058
8	6	0	-2.498710	0.717149	-0.029338
9	1	0	-3.366620	0.452359	-0.642420
10	1	0	-2.875534	1.142068	0.906909
11	1	0	-1.922264	1.482930	-0.551280

1105

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.387537	0.959964	-0.000049
2	6	0	-1.537532	-0.556947	0.000079
3	6	0	-0.154944	-1.154653	-0.000015
4	6	0	0.683433	-0.115068	0.000042
5	1	0	-2.139138	-0.841717	-0.873552
6	1	0	-2.139207	-0.841555	0.873683

7	1	0	0.104847	-2.203190	-0.000360
8	8	0	2.020445	0.036385	0.000087
9	1	0	2.432571	-0.831938	-0.000348
10	7	0	-0.064517	1.091645	-0.000038
11	1	0	0.408457	1.986028	-0.000189

1106

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.070297	0.334630	-0.000209
2	8	0	0.366639	1.541488	-0.000023
3	6	0	1.085944	-0.766814	-0.000308
4	6	0	2.382043	-0.473477	0.000383
5	1	0	0.728977	-1.795836	-0.000921
6	1	0	3.145548	-1.243547	0.000394
7	1	0	2.689804	0.567750	0.001001
8	6	0	-1.237513	-0.094701	-0.000739
9	7	0	-2.469083	-0.401634	0.000445
10	1	0	-3.009915	-0.523581	-0.856827
11	1	0	-3.008571	-0.523080	0.858662

1200

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.472866	-0.609498	0.000145
2	6	0	1.396886	0.732879	0.000030
3	6	0	0.006480	1.139405	-0.000028
4	1	0	2.362798	-1.222194	-0.000409
5	1	0	2.224262	1.429924	-0.000375
6	1	0	-0.430554	2.125929	0.000465
7	6	0	0.080133	-1.148635	0.000049
8	1	0	-0.182848	-1.730533	-0.887289
9	1	0	-0.183385	-1.730141	0.887466
10	7	0	-0.767135	0.072256	-0.000129
11	8	0	-2.019816	-0.007960	-0.000016

1201

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.312000	0.819740	-0.000316
2	6	0	0.022377	1.141230	0.000002
3	6	0	0.005656	-1.111665	-0.000295
4	1	0	2.147547	1.505240	-0.000636
5	1	0	-0.505429	2.082653	0.000480

6	1	0	-0.410427	-2.106316	-0.000432
7	6	0	1.431297	-0.679420	0.000210
8	1	0	1.980409	-1.040176	-0.879282
9	1	0	1.978704	-1.037634	0.881993
10	7	0	-0.784661	-0.060104	-0.000136
11	8	0	-2.040770	-0.000294	0.000153

1300

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.482800	-1.155266	0.000001
2	6	0	1.292037	-0.554672	0.000017
3	1	0	2.581827	-2.235149	0.000022
4	1	0	3.404069	-0.576976	-0.000035
5	1	0	0.361591	-1.115525	0.000053
6	6	0	1.204143	0.913601	-0.000014
7	1	0	2.177044	1.445591	0.000007
8	8	0	0.164355	1.542999	-0.000004
9	1	0	-1.611433	0.638443	0.000014
10	6	0	-2.457517	-0.036679	0.000002
11	7	0	-3.336674	-0.786040	-0.000010

1301

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.409629	-1.089566	-0.000009
2	6	0	1.196060	-0.535300	-0.000027
3	1	0	2.548641	-2.165015	-0.000023
4	1	0	3.308771	-0.477470	0.000031
5	1	0	0.285859	-1.128309	-0.000064
6	6	0	1.059168	0.926661	0.000022
7	1	0	2.008813	1.496098	0.000013
8	8	0	-0.002304	1.524585	-0.000038
9	1	0	-1.525319	0.586146	-0.000107
10	6	0	-3.107127	-0.934096	0.000103
11	7	0	-2.279245	-0.102047	-0.000010