crystals

Supplementary Materials

Table S1. Energies at B3LYP/6-31+G(2d,p) (hartrees), Number of Imaginary Frequencies, Zero-point Energies (kcal.mol^{-1}), Heat Capacity Corrections (kcal/mol), Entropies (cal.mol^{-1}.K^{-1}), Solvation Free Energies (kcal.mol^{-1}), and Free Energies Relative to the Appropriate Reference[1].

Notation	E	NIF	ZPE	Cp corr	S	ΔG(solv)[2]	ΔG(aq,298K)
OH(-)	-75.827789	0	5.45	2.07	41.16	-94.76	
H_2O	-76.459496	0	13.20	2.37	45.12	-2.05[3]	
H_2BOH	-101.951780	0	21.93	2.52	55.13	-3.82	
OBOH	-176.053459	0	12.49	2.72	58.01	-14.65	
$B(OH)_3$	-252.593740	0	30.16	3.39	67.08	-11.63	
1,2-$C_2B_8H_{10}$ (o)	-281.178680	0	90.78	5.06	80.00	-0.50	0.0
1,6-$C_2B_8H_{10}$ (m)	-281.208391	0	90.99	5.02	79.80	2.69	-15.2
1,10-$C_2B_8H_{10}$ (p)	-281.241954	0	91.57	4.95	76.71	3.89	-33.7
oTS1-O	-357.044168	1	96.91	6.54	90.03	-53.74	27.2
oA-O	-357.113410	0	98.37	6.60	92.00	-46.19	2.0
oTS2O	-357.108792	1	98.61	5.75	85.07	-42.58	10.0
oB-O	-357.120746	0	100.03	5.69	84.53	-44.80	1.8
oTS3-O	-357.102381	1	96.25	5.54	83.75	-39.89	14.5
oP1-O	-357.157614	0	98.75	5.95	86.83	-40.16	-18.4
4,5-$C_2B_6H_{11}^-$	-232.091516	0	90.10	5.11	80.09	-39.67	-50.7
oC-O	-433.633394	0	113.93	8.01	104.68	-41.59	-18.2
oTS4-O	-433.570180	1	112.24	6.80	92.82	-45.21	18.5
oD-O	-433.602552	0	114.79	7.25	95.60	-47.70	-2.2
oTS5-O	-433.580785	1	113.04	7.32	95.86	-48.36	9.1
oE-O	-433.599801	0	114.98	7.15	94.88	-47.59	0.0
oTS6-O	-433.598519	1	114.29	6.99	93.98	-47.61	0.2
oF-O	-433.606445	0	115.38	7.02	93.98	-45.17	-1.2
oTS7-O	-433.588877	1	112.00	6.67	91.60	-43.15	8.8
oP2-O	-433.631286	0	113.90	7.27	96.67	-45.07	-18.8
oTS8-O	-433.566481	1	112.57	7.63	101.00	-58.47	6.2
oG-O	-433.565108	0	113.16	7.98	104.20	-63.94	1.61
oG'-O	-433.565580	0	113.19	7.94	103.47	-63.85	1.6
oTS9-O	-433.576085	1	111.84	7.75	100.98	-50.19	7.9
oH-O	-433.576130	0	112.28	8.14	104.08	-53.32	4.6
oTS10-O	-433.575937	1	111.65	7.93	102.66	-51.94	5.7
oI-O	-408.084176	0	103.63	7.65	99.69	-66.84	0.1
oJ-O	-484.556906	0	119.24	8.95	110.14	-60.59	-1.1
oTS11-O	-484.556404	1	116.26	8.31	105.64	-58.96	-1.5
oK-O	-408.139092	0	104.38	7.30	97.08	-48.64	-27.9
oK'-O	-408.144534	0	104.56	7.14	96.58	-44.34	-26.8
oTS12-O	-408.127154	1	101.63	6.87	94.28	-45.37	-19.5
oL-O	-408.132091	1	103.64	6.87	94.25	-51.68	-26.9
oM-O	-484.601206	0	118.40	9.69	121.84	-56.47	-28.4
oM'-O	-484.608526	0	118.46	9.43	116.84	-53.96	-29.2
oTS13-O	-484.563436	1	117.50	8.77	108.62	-58.13	-4.2
4,5-$C_2B_6H_{11}^-$	-232.074923	0	88.66	5.29	81.08	-39.43	-41.7
mTS1-O	-357.069023	1	97.21	6.47	90.64	-57.64	7.9
mA-O	-357.155856	0	99.37	5.77	85.21	-37.08	-22.9
mTS2-O	-357.133179	1	97.99	5.96	86.52	-37.77	-11.0
mB-O	-357.146068	0	98.35	6.53	91.57	-39.37	-21.2
mTS3-O	-357.128638	1	97.67	6.18	88.53	-41.79	-12.9
mC-O	-357.137111	0	98.22	6.57	91.66	-43.31	-19.7
mTS4-O	-357.126256	1	97.93	6.12	88.68	-44.67	-14.1
mD-O	-357.147793	0	98.67	6.37	90.42	-42.12	-24.6
mTS5-O	-357.136498	1	97.71	6.14	88.14	-41.38	-17.3

mE-O	-357.164882	0	99.10	6.14	87.97	-42.72	-35.0
mTS6-O	-357.118801	1	97.74	6.14	87.87	-44.75	-9.4
mP3-O	-357.157720	0	98.45	6.37	89.39	-46.54	-35.1
pTS1-O	-357.099402	1	97.77	6.36	89.90	-53.13	3.6
pA-O	-357.144750	0	98.65	6.52	91.75	-42.45	-13.6
pA'-O	-357.135302	0	98.48	6.61	92.04	-43.87	-9.3
pTS2-O	-357.130282	1	98.20	5.93	86.29	-41.14	-2.7
pB-O	-357.151051	0	100.22	5.61	83.99	-41.84	-14.0
pTS3-O	-357.129196	1	98.12	5.98	86.72	-41.09	-2.1
pC-O	-357.135300	0	98.48	6.61	92.04	-43.87	-9.3
pTS4-O	-357.127514	1	97.72	6.34	91.17	-41.65	-3.0
pD-O	-357.150209	0	98.44	6.57	92.27	-37.76	-12.7
pTS5-O	-357.111403	1	96.38	5.52	83.52	-37.78	11.1
pP1-O	-357.165123	0	97.84	6.18	87.90	-38.46	-22.4
NH_3	-56.583838	0	21.48	2.39	45.98	-3.67	
H_2BNH_2	-82.076329	0	30.06	2.62	54.56	-1.24	
1,2-$C_2B_8H_{10}$	-281.178620	0	90.68	5.09	80.17	-0.43	0.0
1,6-$C_2B_8H_{10}$	-281.208341	0	91.08	5.02	79.83	2.73	-15.1
1,10-$C_2B_8H_{10}$	-281.241927	0	91.79	4.93	75.27	3.91	-33.0
oTS1-N	-337.728083	1	113.91	6.71	92.06	-4.70	32.1
oA-N	-337.748345	0	116.24	6.45	89.90	-11.06	15.8
oTS2-N	-337.702560	1	111.12	6.30	88.33	-0.43	50.3
oP1-N	-337.789680	0	116.94	5.65	84.29	-3.75	-1.3
oTS3-N	-337.714651	1	112.54	6.42	89.26	-0.64	43.8
oB-N	-337.747392	0	113.50	6.78	92.60	-0.39	23.8
oTS4-N	-337.731204	1	113.14	6.48	90.72	-1.46	32.8
oC-N	-337.745594	0	113.30	6.91	94.22	-0.34	24.4
oTS5-N	-337.730128	1	111.25	6.99	94.89	-0.01	32.3
oD-N	-337.734569	0	112.87	7.15	96.24	0.27	31.2
oTS6-N	-337.720140	1	111.32	7.05	94.81	0.81	39.5
P2-N	-337.774463	0	116.04	5.98	86.52	-3.48	7.3
oTS7-N	-337.722391	1	112.42	6.46	89.70	-1.01	38.3
oE-N	-337.735445	0	112.25	7.06	94.69	-0.55	29.5
oTS8-N	-337.728785	1	112.92	6.43	89.29	0.49	36.4
oP3-N	-337.768806	0	116.11	6.00	86.82	-3.20	11.1
oTS9-N	-337.732496	1	114.42	6.16	88.21	-3.06	32.1
oF-N	-337.734214	0	114.04	6.78	92.53	-3.30	29.7
oTS10-N	-337.728282	1	113.44	6.51	91.01	-6.51	29.8
oG-N	-337.745683	0	114.73	6.33	88.75	-2.08	25.1
oTS11-N	-337.727340	1	114.00	6.23	89.17	-2.74	35.0
oH-N	-337.742838	0	114.85	6.28	88.12	-2.77	26.5
oTS12-N	-337.721880	1	113.70	6.13	87.34	-2.22	39.1
oI-N	-337.733182	0	113.67	6.49	89.57	-1.85	32.0
oTS13-N	-337.732694	1	113.72	6.00	86.33	-1.97	32.8
oP4-N	-337.797561	0	116.33	5.77	85.06	-2.27	-5.5
mTS1-N	-337.751378	1	113.96	6.73	92.38	-2.67	19.5
mA-N	-337.766264	0	115.98	6.47	89.91	-10.03	5.3
mTS2-N	-337.724750	1	111.43	6.34	89.22	0.01	36.9
mB-N	-337.781499	0	116.00	6.05	86.70	-4.04	2.3
mTS3-N	-337.762538	1	114.34	6.18	87.85	-4.56	11.8
mC-N	-337.776235	0	115.52	6.27	88.29	-4.43	4.5
mTS4-N	-337.749568	1	113.40	6.22	87.87	-2.04	21.5
mD-N	-337.751105	0	113.42	6.65	90.53	-0.68	21.6
mTS5-N	-337.748912	1	112.99	6.33	88.56	-1.63	21.9
mE-N	-337.760716	0	114.37	6.30	88.46	-2.86	14.6
mTS6-N	-337.757016	1	114.26	6.02	86.82	-4.78	15.1
mTS7-N	-337.758327	1	113.82	6.29	88.89	1.15	19.4
mF-N	-337.789236	0	115.60	6.11	87.57	-3.11	-2.2

mTS8-N	-337.753630	1	112.93	6.73	92.62	-0.69	19.0
$C_2B_7H_9$	-255.728589	0	81.50	4.97	79.53	2.05	-24.6
pTS1-N	-337.739932	1	112.15	6.17	87.99	0.54	28.8
pP1-N	-337.789158	0	115.72	5.97	86.26	-2.17	-0.9
pTS2-N	-337.759626	1	113.62	6.24	88.10	0.95	18.4
pA-N	-337.766452	0	113.41	6.98	94.68	-0.18	11.5
pTS3-N	-337.765698	1	112.29	6.74	92.68	1.02	12.4
pB-N	-337.774289	0	113.54	6.77	92.75	0.75	8.0
pB'-N	-337.779402	0	113.88	6.79	94.96	0.40	4.2
pTS4-N	-337.746010	1	112.66	6.58	90.99	1.39	25.9
pC-N	-337.747121	0	113.05	7.12	96.28	0.98	24.1
pTS5-N	-337.744393	1	112.28	6.97	95.70	-0.80	23.3
pD-N	-255.701238	0	80.77	5.18	81.39	2.64	-7.9
pTS6-N	-255.660290	1	79.40	4.98	79.29	2.44	16.6
pP2-N	-255.728589	0	81.50	4.97	79.53	2.05	-24.6

[1]The last column tabulate free energies in aqueous solution at 298K relative to 1,2-$C_2B_8H_{10}$+OH^- or 1,2-$C_2B_8H_{10}$+NH_3. In some cases, H_2NBH_2 is added for mass balance. In the formation of $C_2B_6H_{11}^-$, the comparison is with respect to 1,2-$C_2B_8H_{10}$ + OH^- + $3H_2O$. [2]For reactions with OH^-, optimization and frequencies were calculated at the SMD(water)/B3LYP/6-311+G(2d,p) level of theory. For reactions with NH_3, optimization and frequencies were calculated at the B3LYP/6-311+G(2d,p) level of theory. Solvation free energies are the difference in energy between B3LYP/6-311+G(2d,p) and SMD(warter)/B3LYP/6-311+G(2d,p). There are two separate entries for 1,2-$C_2B_8H_{10}$, 1,6-$C_2B_8H_{10}$, and 1,10-$C_2B_8H_{10}$; one optimized with SMD (OH^- reactions) and one optimized in the gas phase (NH_3 reactions). [3]The solvation free energy of liquid water is set to the experimental value of -2.05 kcal.mol^{-1}.

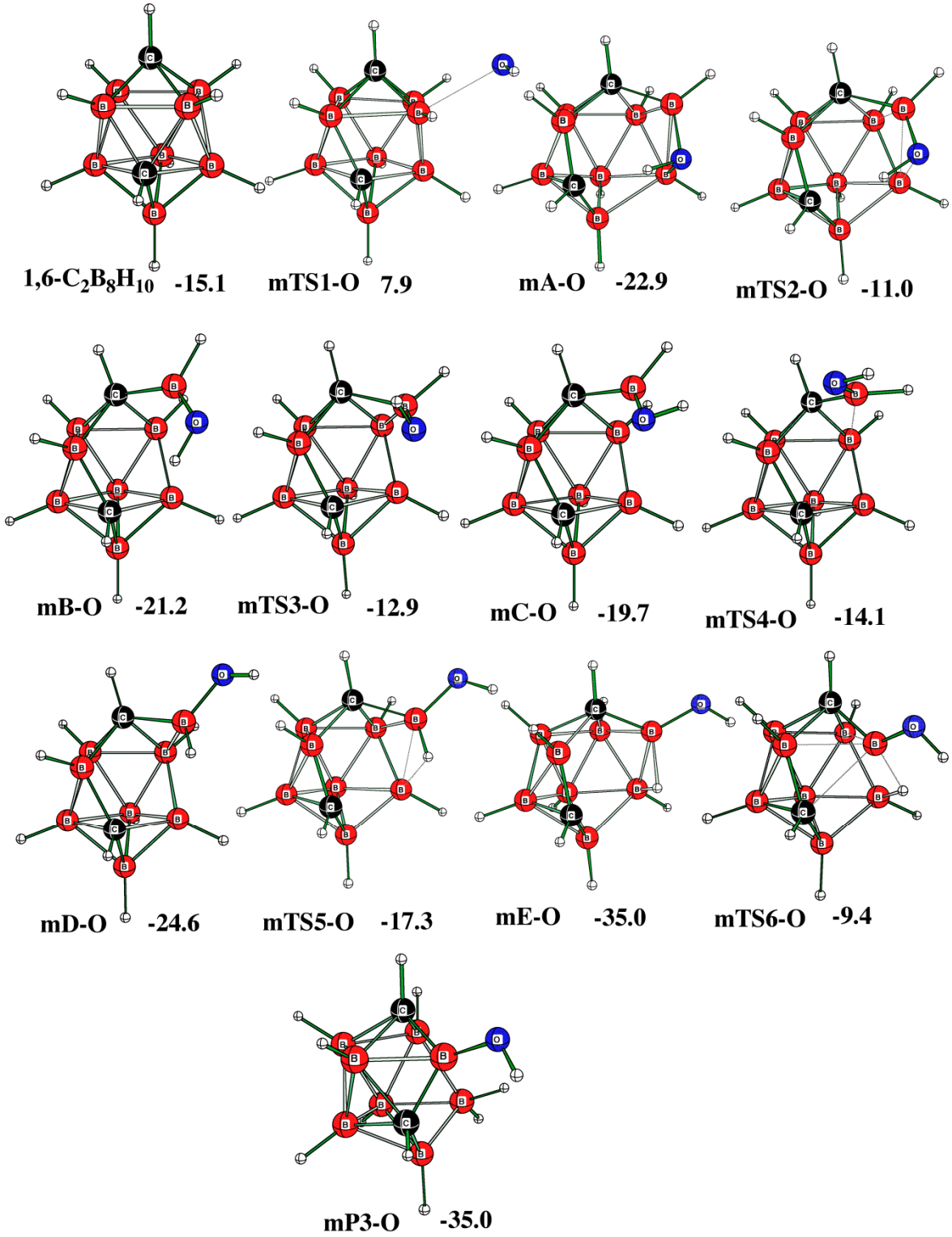

Figure S1. Individual stationary points as detected in the reaction pathway of the reaction of *closo*-1,6-$C_2B_8H_{10}$ with $OH^{(-)}$.

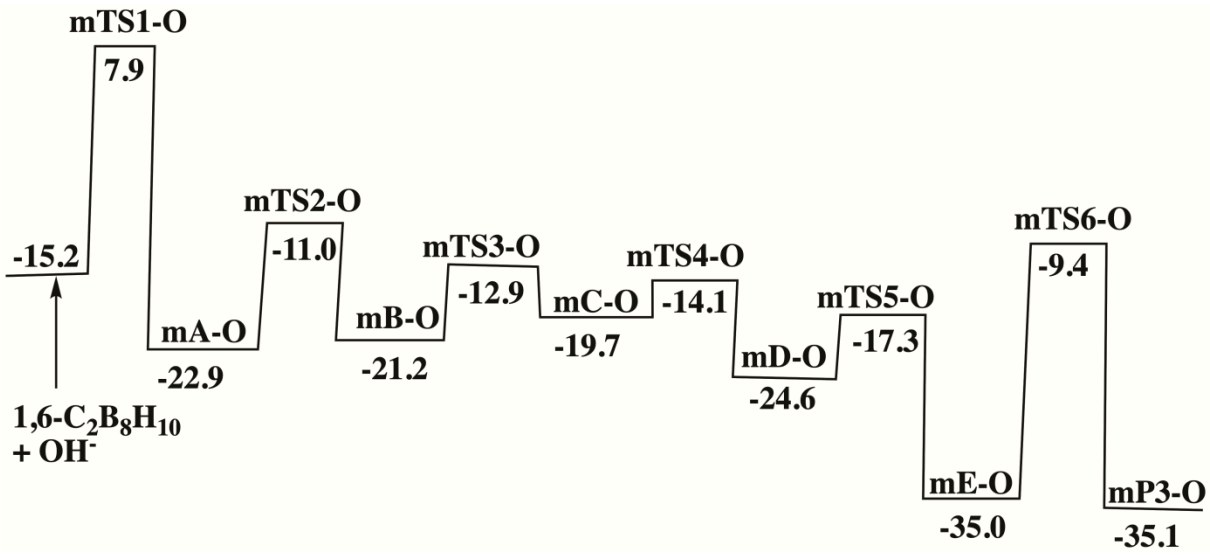

Figure S2. Relative free energies (kcal.mol^{-1}) of the individual stationary points on the PES of the reaction of *closo*-1,6-$C_2B_8H_{10}$ with $OH^{(-)}$.

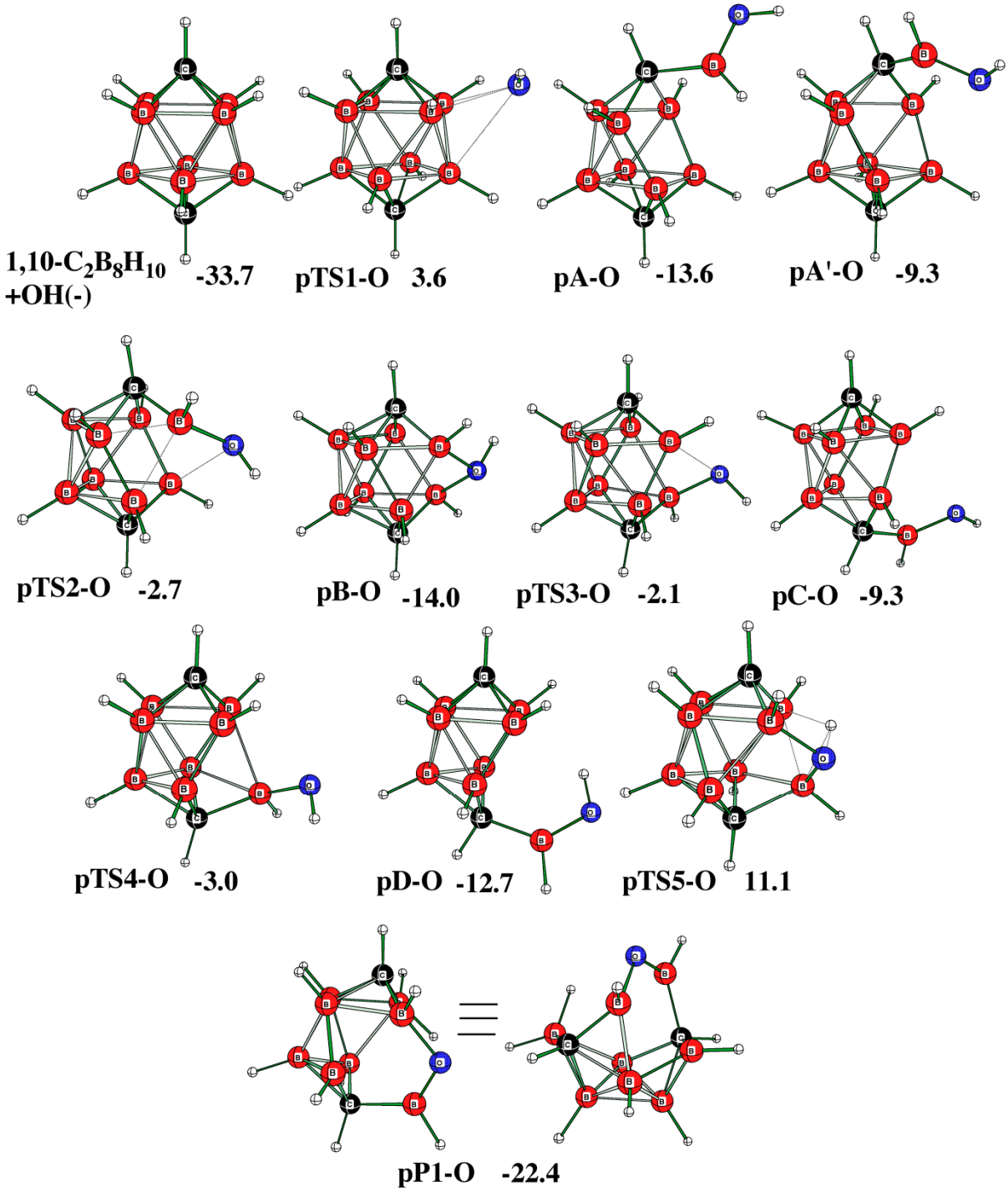

Figure S3. Individual stationary points as detected in the reaction pathway of the reaction of *closo*-1,10-$C_2B_8H_{10}$ with $OH^{(-)}$.

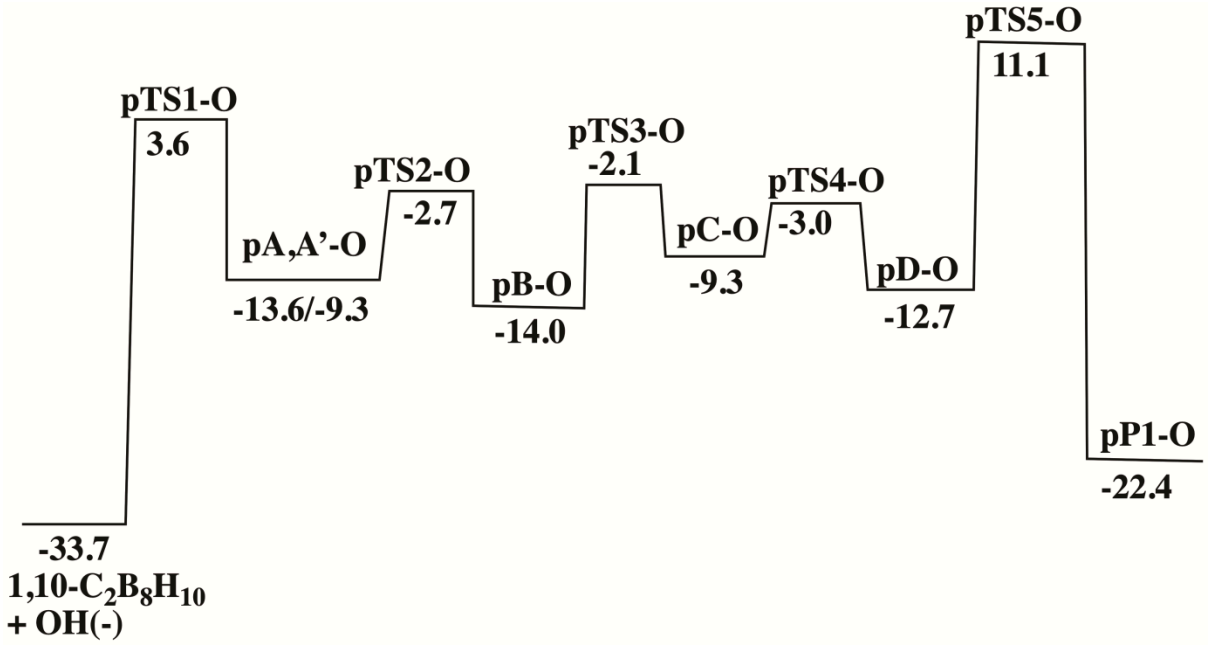

Figure S4. Relative free energies (kcal.mol^{-1}) of the individual stationary points on the PES of the reaction of *closo*-1,10-$C_2B_8H_{10}$ with $OH^{(-)}$.

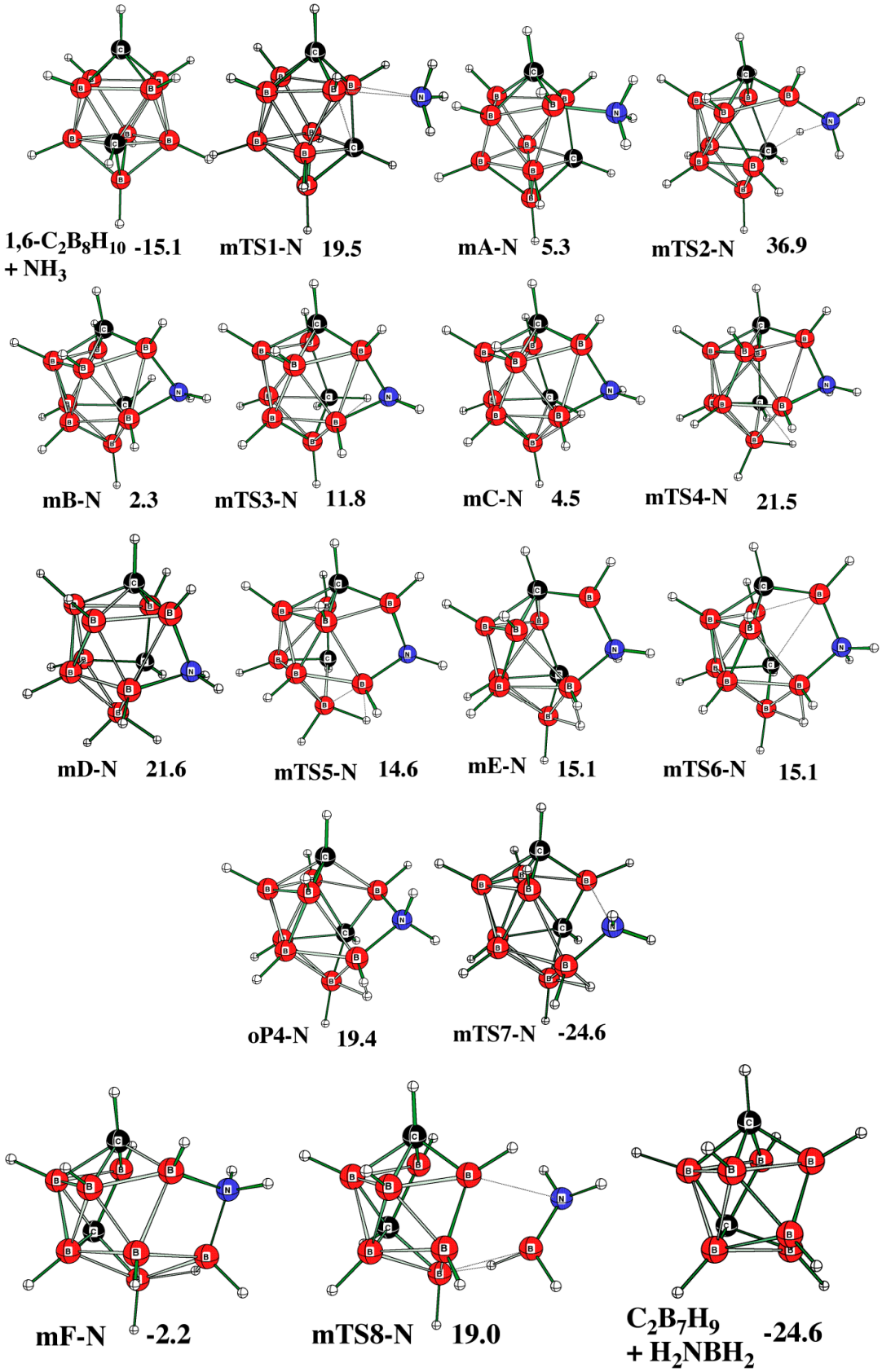

Figure S5. Individual stationary points as detected in the reaction pathway of the reaction of *closo*-1,6-$C_2B_8H_{10}$ with NH_3.

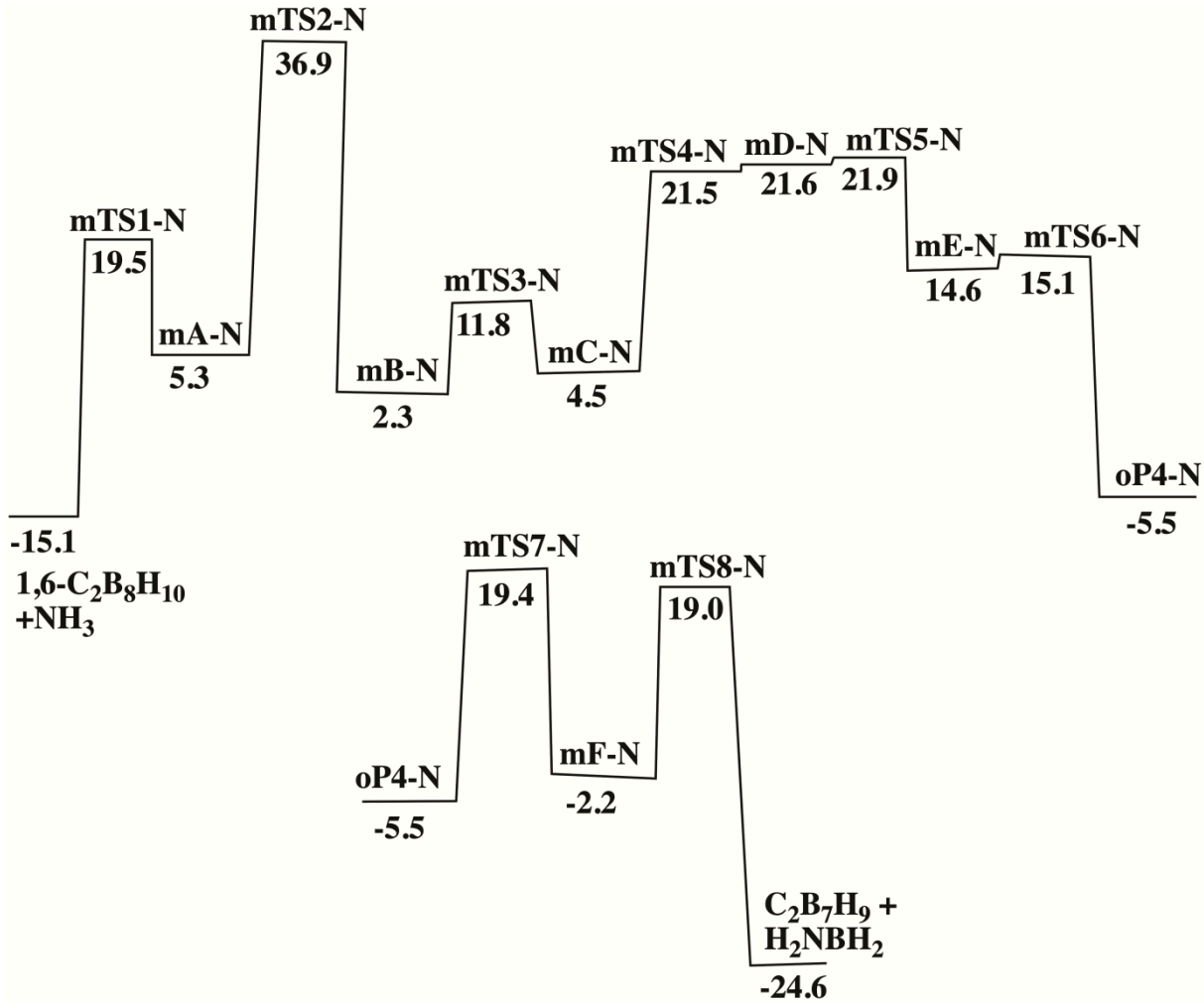

Figure S6. Relative free energies (kcal.mol^{-1}) of the individual stationary points on the PES of the reaction of *closo*-1,6-$C_2B_8H_{10}$ with NH_3.

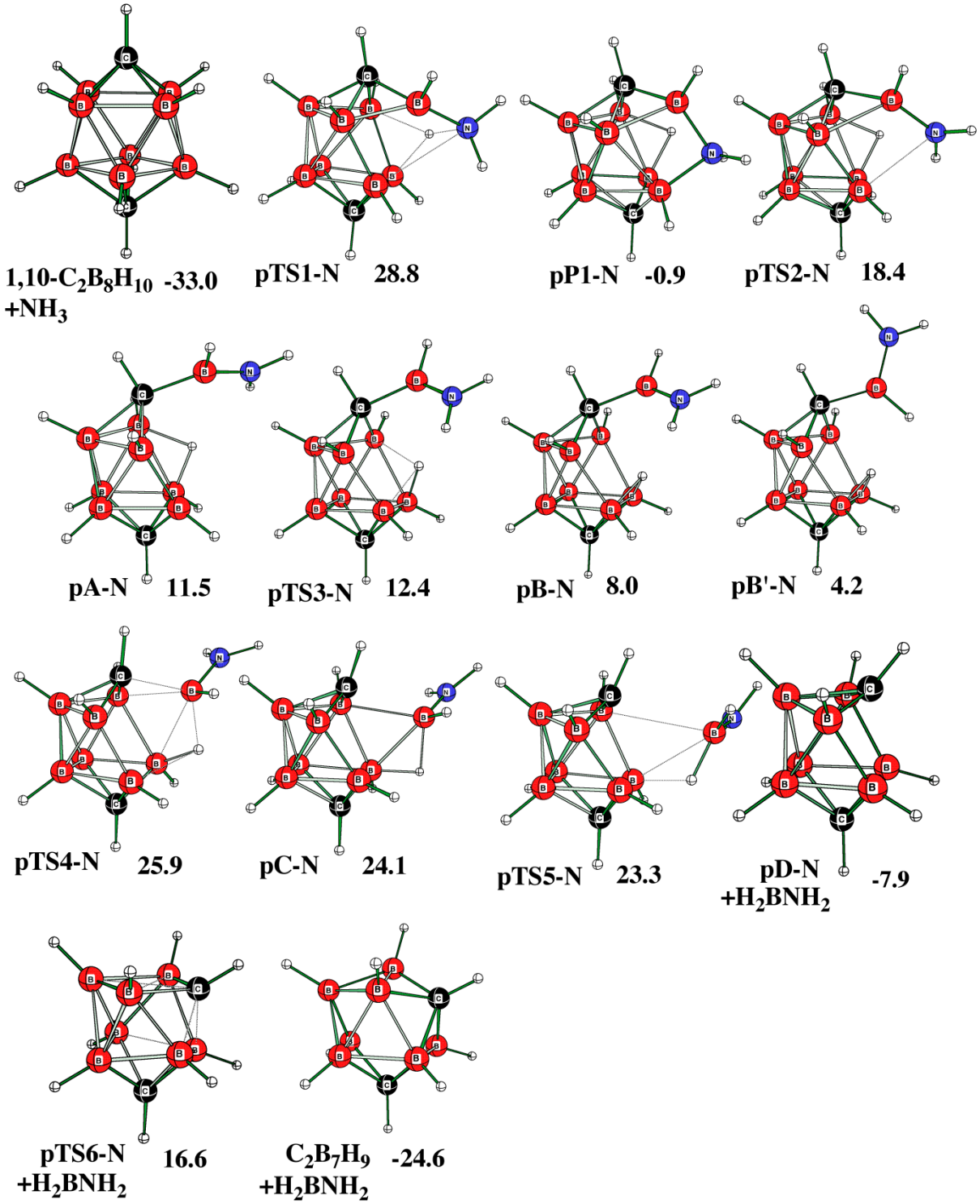

Figure S7. Individual stationary points as detected in the reaction pathway of the reaction of *closo*-1,10-$C_2B_8H_{10}$ with NH_3.

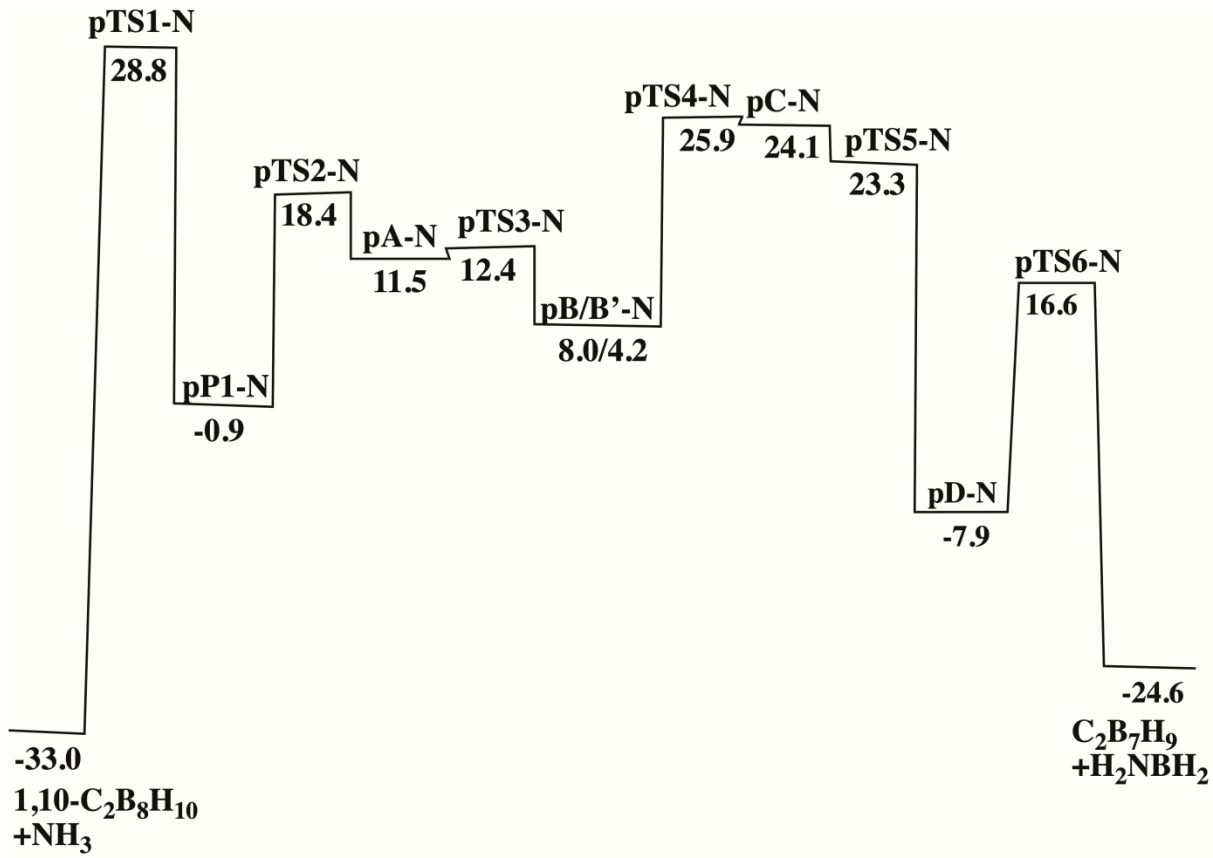

Figure S8. Relative free energies (kcal.mol^{-1}) of the individual stationary points on the PES of the reaction of *closo*-1,10-$C_2B_8H_{10}$ with NH_3.

Table S2. Cartesian coordinates of all species in Table S1.

OH(-)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.107158
2	1	0	0.000000	0.000000	-0.857263

H2O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	8	0	-0.000000	0.000000	0.118471
2	1	0	-0.000000	0.763205	-0.473882
3	1	0	-0.000000	-0.763205	-0.473882

H2BOH

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	0.111798	-0.000000
2	8	0	0.057563	-1.193700	0.000000
3	1	0	-0.778041	-1.685822	0.000000
4	8	0	0.039692	1.334554	-0.000000

OBOH

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	0.111798	-0.000000
2	8	0	0.057563	-1.193700	0.000000
3	1	0	-0.778041	-1.685822	0.000000
4	8	0	0.039692	1.334554	-0.000000

B(OH)3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.000000	0.000464	0.000000
2	8	0	0.389750	1.314399	0.000000
3	1	0	-0.357691	1.926397	0.000000
4	8	0	-1.332884	-0.320433	-0.000000
5	1	0	-1.488386	-1.274137	-0.000000
6	8	0	0.943092	-0.994323	-0.000000
7	1	0	1.846408	-0.651718	-0.000000

1,2-C2B8H10 (o)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.876615	1.385490	-0.000000
2	5	0	0.721764	1.330360	-0.000000
3	5	0	-0.356657	0.633999	1.313028
4	5	0	-0.356657	0.633999	-1.313028
5	5	0	1.195824	-0.151059	0.923656
6	5	0	-0.356657	-1.140951	0.914308
7	5	0	-0.356657	-1.140951	-0.914308
8	5	0	1.195824	-0.151059	-0.923656
9	1	0	-1.570496	2.208513	-0.000000
10	1	0	1.328341	2.339683	-0.000000
11	1	0	-0.747775	0.992288	2.362161
12	1	0	-2.401495	-0.220803	-0.000000
13	1	0	-0.747775	0.992288	-2.362161
14	1	0	2.071849	-0.076543	1.716276
15	1	0	-0.906120	-1.848338	1.683077
16	1	0	-0.906120	-1.848338	-1.683077
17	1	0	2.071849	-0.076543	-1.716276
18	1	0	1.621343	-2.569699	0.000000
19	6	0	-1.331917	-0.074951	-0.000000
20	5	0	1.000732	-1.565486	0.000000

1,6-C2B8H10 (m)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.874510	-1.416702	0.000000
2	5	0	-1.188738	-0.141182	0.919300
3	5	0	-1.188738	-0.141182	-0.919300
4	5	0	0.371860	-1.099251	0.932770
5	5	0	-0.707698	1.355427	-0.000000
6	5	0	0.371860	0.646902	-1.299721
7	5	0	0.371860	0.646902	1.299721
8	1	0	-1.423063	-2.343548	0.000000

9	1	0	-2.087821	-0.157316	1.681558
10	1	0	-2.087821	-0.157316	-1.681558
11	1	0	0.858977	-1.881114	-1.663289
12	1	0	0.858977	-1.881114	1.663289
13	1	0	-1.424858	2.295781	-0.000000
14	1	0	0.744570	0.946208	-2.378812
15	1	0	2.403639	-0.243637	-0.000000
16	1	0	0.744570	0.946208	2.378812
17	1	0	1.723003	2.459720	-0.000000
18	5	0	0.969541	1.555615	-0.000000
19	6	0	1.346309	-0.017261	-0.000000
20	5	0	0.371860	-1.099251	-0.932770

1,10-C2B8H10 (p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.670652
2	5	0	0.000000	1.306671	0.754072
3	5	0	-1.306671	0.000000	0.754072
4	5	0	1.306671	-0.000000	0.754072
5	5	0	-0.924237	0.924237	-0.754161
6	5	0	-0.924237	-0.924237	-0.754161
7	5	0	0.924237	0.924237	-0.754161
8	1	0	0.000000	0.000000	2.748438
9	1	0	0.000000	2.378882	1.245107
10	1	0	-2.378882	0.000000	1.245107
11	1	0	-0.000000	-2.378882	1.245107
12	1	0	2.378882	-0.000000	1.245107
13	1	0	-1.682335	1.682335	-1.245327
14	1	0	-1.682335	-1.682335	-1.245327
15	1	0	1.682335	-1.682335	-1.245327
16	1	0	1.682335	1.682335	-1.245327
17	1	0	0.000000	0.000000	-2.748087
18	5	0	-0.000000	-1.306671	0.754072
19	6	0	0.000000	0.000000	-1.670268
20	5	0	0.924237	-0.924237	-0.754161

oTS1-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.564487	1.334234	-0.053777
2	5	0	-0.583843	1.117836	1.049347
3	5	0	-0.921112	1.266031	-0.710283
4	5	0	1.005894	0.057555	0.815617
5	5	0	-1.927633	0.190502	0.305271
6	5	0	-1.144022	-0.455847	-1.234147
7	5	0	0.142585	-1.282991	-0.247482
8	5	0	-0.639591	-0.652212	1.309081
9	1	0	1.186797	2.191050	-0.252320
10	1	0	-0.733692	1.943616	1.880508
11	1	0	-1.258119	2.163894	-1.393111
12	1	0	1.035459	0.243345	-1.926122
13	1	0	1.715571	0.088044	1.761831
14	1	0	-3.041980	0.509869	0.558478
15	1	0	-1.494905	-0.670491	-2.343677
16	1	0	0.813674	-2.210427	-0.535808
17	1	0	-0.672722	-1.082287	2.414621
18	1	0	-2.184904	-2.413632	0.122276
19	6	0	0.404410	0.194298	-1.053570
20	5	0	-1.508918	-1.443033	0.091377
21	8	0	2.903892	-0.461532	-0.142234
22	1	0	3.473513	-0.231127	0.601381

oA-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.831879	1.071096	-0.300881
2	5	0	0.019933	0.766159	1.209439
3	5	0	-0.827109	1.401390	-0.227537
4	5	0	2.069204	0.337017	0.317849
5	5	0	-1.707700	0.342784	0.873986
6	5	0	-1.715343	0.007777	-0.899117
7	5	0	-0.390108	-1.209758	-0.782646
8	5	0	-0.433732	-0.864760	1.249412

9	1	0	1.128420	2.078677	-0.608984
10	1	0	0.324208	1.480314	2.112765
11	1	0	-1.105037	2.508282	-0.535016
12	1	0	0.141488	0.469070	-2.327458
13	1	0	2.759280	0.929457	1.092351
14	1	0	-2.588046	0.814429	1.525128
15	1	0	-2.521115	0.218534	-1.746617
16	1	0	-0.112052	-2.156676	-1.453321
17	1	0	-0.245577	-1.583490	2.188306
18	1	0	-2.504439	-2.149984	0.367767
19	6	0	-0.024304	0.248991	-1.278808
20	5	0	-1.713548	-1.268020	0.243962
21	8	0	2.507220	-0.866152	-0.167357
22	1	0	3.311671	-1.162871	0.275335

oTS2O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.481117	-1.338001	-0.464011
2	5	0	0.117934	-1.060971	1.123122
3	5	0	1.188585	-1.149893	-0.313745
4	5	0	-1.531743	-0.547477	0.454653
5	5	0	1.505229	0.043075	0.976027
6	5	0	1.553270	0.534959	-0.708169
7	5	0	-0.177192	1.161899	-0.943193
8	5	0	-0.106883	0.581147	1.481692
9	1	0	-0.654787	-2.337435	-0.844336
10	1	0	0.010961	-1.968921	1.879842
11	1	0	1.870001	-2.056400	-0.646951
12	1	0	0.268566	-0.609240	-2.445513
13	1	0	-2.337520	-1.183621	1.077857
14	1	0	2.478936	-0.061334	1.653167
15	1	0	2.465465	0.780756	-1.428227
16	1	0	-0.551390	1.988417	-1.708567
17	1	0	-0.485664	0.982812	2.540353
18	1	0	1.175952	2.657713	0.708671
19	6	0	0.190875	-0.312211	-1.408533
20	5	0	0.782431	1.565795	0.420483
21	8	0	-2.096386	0.595268	-0.288040

22	1	0	-2.386126	1.303708	0.298930

oB-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.717493	-1.071076	0.767162
2	6	0	0.717493	-1.071076	-0.767162
3	5	0	-0.787475	-0.612478	1.208582
4	5	0	-0.787475	-0.612478	-1.208582
5	5	0	0.646470	0.520996	1.390748
6	5	0	0.646470	0.520996	-1.390748
7	5	0	-0.787475	1.278858	-0.839826
8	5	0	-0.787475	1.278858	0.839826
9	1	0	-1.237671	-1.011802	2.239805
10	1	0	-1.237671	-1.011802	-2.239805
11	1	0	1.092741	0.636169	-2.486094
12	1	0	1.092741	0.636169	2.486094
13	1	0	1.293312	-1.831542	1.275472
14	1	0	1.293312	-1.831542	-1.275472
15	1	0	-1.312536	2.069535	-1.573370
16	1	0	-1.312536	2.069535	1.573370
17	5	0	1.681981	0.075773	0.000000
18	1	0	2.858094	-0.046229	0.000000
19	1	0	1.362807	2.621220	0.000000
20	5	0	0.751392	1.597576	0.000000
21	8	0	-1.611914	-1.122133	-0.000000
22	1	0	-2.489254	-0.710242	-0.000000

oTS3-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.711591	-1.136642	0.770964
2	5	0	-0.776131	-0.731753	1.220633
3	5	0	1.654524	0.030597	0.000000
4	5	0	-0.776131	1.333565	0.846705

5	5	0	0.606531	0.462410	1.388880
6	5	0	0.606531	0.462410	-1.388880
7	5	0	-0.776131	-0.731753	-1.220633
8	5	0	-0.776131	1.333565	-0.846705
9	1	0	1.327028	-1.858997	1.289009
10	1	0	-1.246335	-1.106278	2.248318
11	1	0	2.832226	-0.065748	0.000000
12	1	0	1.327028	-1.858997	-1.289009
13	1	0	-1.295993	2.113717	1.584219
14	1	0	1.062617	0.606477	2.474999
15	1	0	1.062617	0.606477	-2.474999
16	1	0	-1.246335	-1.106278	-2.248318
17	1	0	-1.295993	2.113717	-1.584219
18	1	0	1.427178	2.552287	0.000000
19	6	0	0.711591	-1.136642	-0.770964
20	5	0	0.752226	1.569943	0.000000
21	8	0	-1.663400	-0.908736	0.000000
22	1	0	-1.762368	0.268295	0.000000

oP1-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.016550	0.851993	0.774927
2	5	0	1.016550	-0.701249	1.161149
3	5	0	-0.279008	1.599391	0.000000
4	5	0	-1.370649	-0.907537	0.878795
5	5	0	-0.537825	0.479605	1.389587
6	5	0	-0.537825	0.479605	-1.389587
7	5	0	1.016550	-0.701249	-1.161149
8	5	0	-1.370649	-0.907537	-0.878795
9	1	0	1.597590	1.596165	1.302831
10	1	0	1.349732	-1.112618	2.229433
11	1	0	-0.338019	2.779914	0.000000
12	1	0	1.597590	1.596165	-1.302831
13	1	0	-2.118025	-1.516751	1.574473
14	1	0	-0.746816	0.924763	2.471102
15	1	0	-0.746816	0.924763	-2.471102
16	1	0	1.349732	-1.112618	-2.229433
17	1	0	-2.118025	-1.516751	-1.574473

18	1	0	-2.741051	1.135167	0.000000
19	6	0	1.016550	0.851993	-0.774927
20	5	0	-1.699863	0.556245	0.000000
21	8	0	1.299900	-1.459377	0.000000
22	1	0	-0.870110	-1.733469	0.000000

4,5-C2B6H11-

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.405921	0.871584	-0.410571
2	5	0	-0.187178	1.376913	0.136706
3	5	0	0.734991	0.005711	0.838626
4	5	0	-1.015895	-0.054382	0.905043
5	5	0	-1.521997	-0.768062	-0.611414
6	1	0	-0.200445	2.455447	0.650037
7	1	0	1.350316	0.082358	1.851300
8	1	0	-1.612490	-0.054860	1.934129
9	1	0	-2.471342	-1.438620	-0.865048
10	1	0	2.716087	-1.164906	0.195585
11	1	0	-0.100699	-2.519357	0.713292
12	5	0	-0.090199	-1.419676	0.263585
13	1	0	2.182696	1.550703	-0.078038
14	1	0	-2.352593	1.315006	-0.577298
15	1	0	-0.420432	-1.416143	-0.997692
16	6	0	-1.428365	0.744119	-0.528185
17	1	0	1.166811	1.010343	-1.455536
18	5	0	1.734107	-0.790871	-0.385221
19	1	0	1.607610	-1.262354	-1.474825

oC-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.225562	-1.087777	0.774428
2	5	0	-0.811606	0.410018	1.167590
3	5	0	-0.162844	-2.139019	0.000000

4	5	0	1.518975	0.019818	0.880215
5	5	0	0.368802	-1.120405	1.388177
6	5	0	0.368802	-1.120405	-1.388177
7	5	0	-0.811606	0.410018	-1.167590
8	5	0	1.518975	0.019818	-0.880215
9	1	0	-1.980044	-1.654991	1.302334
10	1	0	-1.038329	0.896279	2.231101
11	1	0	-0.398601	-3.296833	0.000000
12	1	0	-1.980044	-1.654991	-1.302334
13	1	0	2.392341	0.419493	1.579987
14	1	0	0.463327	-1.598001	2.471271
15	1	0	0.463327	-1.598001	-2.471271
16	1	0	2.392341	0.419493	-1.579987
17	1	0	2.340308	-2.297844	0.000000
18	6	0	-1.225562	-1.087777	-0.774428
19	5	0	1.475596	-1.479479	0.000000
20	8	0	-0.908341	1.216614	0.000000
21	1	0	1.253679	0.946419	0.000000
22	1	0	-1.038329	0.896279	-2.231101
23	8	0	0.116602	3.786542	0.000000
24	1	0	1.076458	3.682944	0.000000
25	1	0	-0.231251	2.866009	0.000000

oTS4-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.193054	-0.037357	1.365847
2	5	0	-0.393242	1.344427	0.579180
3	5	0	1.088680	-1.050176	1.013039
4	5	0	1.597923	1.297838	-0.504299
5	5	0	1.289387	0.738223	1.080807
6	5	0	0.972255	-1.373823	-0.731917
7	5	0	-1.478367	-0.418717	-0.754810
8	5	0	1.523430	-0.074407	-1.610731
9	1	0	-0.514776	-0.188322	2.387377
10	1	0	-0.616692	2.367901	1.150812
11	1	0	1.350722	-1.860410	1.836116
12	1	0	-0.872193	-2.073849	0.689374
13	1	0	2.182548	2.313667	-0.708076

14	1	0	1.731720	1.312810	2.020634
15	1	0	1.194667	-2.514365	-1.016606
16	1	0	2.098886	-0.034318	-2.655586
17	1	0	3.395491	-0.502074	0.152538
18	6	0	-0.477541	-1.149491	0.272466
19	5	0	2.242864	-0.259900	-0.029637
20	8	0	-1.263704	1.091792	-0.588660
21	1	0	0.789872	1.013507	-1.496776
22	1	0	-1.590817	-0.805686	-1.879984
23	8	0	-2.971891	-0.246185	-0.171460
24	1	0	-3.041793	-0.533781	0.751386
25	1	0	-2.413962	0.843831	-0.188282

oD-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.194142	-0.075614	1.359244
2	5	0	-0.265697	1.356439	0.684639
3	5	0	1.001422	-1.163255	0.934727
4	5	0	1.722618	1.229033	-0.422455
5	5	0	1.356754	0.593441	1.123991
6	5	0	0.838246	-1.347394	-0.829332
7	5	0	-1.689846	-0.284132	-0.701072
8	5	0	1.515530	-0.049762	-1.618863
9	1	0	-0.528124	-0.262190	2.370982
10	1	0	-0.461811	2.358547	1.293224
11	1	0	1.198797	-2.042058	1.703855
12	1	0	-1.005753	-2.009255	0.584712
13	1	0	2.392498	2.203737	-0.549013
14	1	0	1.843492	1.060514	2.100800
15	1	0	0.973291	-2.479673	-1.196278
16	1	0	2.097067	0.008987	-2.660047
17	1	0	3.345706	-0.758077	0.104048
18	6	0	-0.566246	-1.090094	0.199945
19	5	0	2.218708	-0.404593	-0.057471
20	8	0	-1.118327	1.213404	-0.540814
21	1	0	0.896080	1.094165	-1.430752
22	1	0	-1.730564	-0.534234	-1.880198
23	8	0	-3.023317	-0.333181	-0.153210

24	1	0	-3.020318	-0.238005	0.808070
25	1	0	-1.793557	1.901125	-0.623167

oTS5-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.173717	-0.034061	-1.361335
2	5	0	0.178798	1.389819	-0.606481
3	5	0	-0.983971	-1.155950	-0.988173
4	5	0	-1.732644	1.229292	0.422327
5	5	0	-1.385972	0.620929	-1.114947
6	5	0	-0.822648	-1.379644	0.774474
7	5	0	1.684176	-0.279127	0.685228
8	5	0	-1.504988	0.007093	1.633502
9	1	0	0.541016	-0.167471	-2.369695
10	1	0	0.384893	2.401277	-1.199627
11	1	0	-1.182343	-2.014259	-1.778290
12	1	0	1.033417	-1.972756	-0.654373
13	1	0	-2.433515	2.191973	0.496105
14	1	0	-1.839103	1.097136	-2.104374
15	1	0	-0.890877	-2.500144	1.177374
16	1	0	-2.175953	-0.105881	2.622518
17	1	0	-3.287571	-0.816292	0.054919
18	6	0	0.548246	-1.085419	-0.254227
19	5	0	-2.160323	-0.434813	0.097307
20	8	0	1.118829	1.214550	0.563893
21	1	0	-0.394395	0.413767	1.784481
22	1	0	1.715170	-0.577521	1.850186
23	8	0	3.005629	-0.331181	0.130703
24	1	0	3.010705	-0.160724	-0.820185
25	1	0	1.828966	1.872826	0.561377

oE-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.139788	-0.141773	-1.346821
2	5	0	0.077746	1.333169	-0.630433
3	5	0	-0.985494	-1.236502	-0.864328
4	5	0	-1.648687	1.285967	0.289234
5	5	0	-1.446260	0.450089	-1.180866
6	5	0	-0.780639	-1.253536	0.942430
7	5	0	1.715785	-0.216505	0.669734
8	5	0	-1.517521	0.268247	1.584931
9	1	0	0.540297	-0.325755	-2.333853
10	1	0	0.286376	2.299819	-1.300145
11	1	0	-1.176864	-2.211398	-1.504530
12	1	0	1.033167	-2.015364	-0.505203
13	1	0	-2.432661	2.192318	0.237548
14	1	0	-1.931168	0.791325	-2.210380
15	1	0	-0.821397	-2.288348	1.524286
16	1	0	-2.074680	0.257170	2.641248
17	1	0	-3.294127	-0.878054	0.098758
18	6	0	0.572161	-1.089405	-0.170808
19	5	0	-2.180892	-0.456473	0.145181
20	8	0	1.125344	1.246393	0.500905
21	1	0	-0.380555	-0.303555	1.796820
22	1	0	1.795767	-0.463970	1.848682
23	8	0	3.022727	-0.278506	0.070316
24	1	0	2.987502	-0.162765	-0.888107
25	1	0	1.841887	1.880279	0.351472

oTS6-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.136533	-0.160377	-1.349135
2	5	0	0.060541	1.328468	-0.678336
3	5	0	-0.966708	-1.261402	-0.833382
4	5	0	-1.685633	1.271825	0.268909
5	5	0	-1.463111	0.410134	-1.180695
6	5	0	-0.747848	-1.233559	0.970902
7	5	0	1.737147	-0.170553	0.663364
8	5	0	-1.519289	0.286276	1.584725
9	1	0	0.528119	-0.360483	-2.336575
10	1	0	0.241318	2.286704	-1.368595

11	1	0	-1.144625	-2.251773	-1.453643
12	1	0	1.063605	-2.005084	-0.478205
13	1	0	-2.491622	2.157546	0.195400
14	1	0	-1.958158	0.716301	-2.216720
15	1	0	-0.765556	-2.253095	1.580628
16	1	0	-2.067047	0.277183	2.646286
17	1	0	-3.274318	-0.940237	0.133379
18	6	0	0.596952	-1.077871	-0.155993
19	5	0	-2.172329	-0.487818	0.166015
20	8	0	1.104921	1.233495	0.420962
21	1	0	-0.362015	-0.246892	1.790113
22	1	0	1.812525	-0.376636	1.850916
23	8	0	3.052504	-0.257108	0.079293
24	1	0	3.026673	-0.140218	-0.879190
25	1	0	1.516935	2.038222	0.757425

oF-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.160243	-0.341987	-1.316675
2	5	0	0.056438	1.226111	-0.856790
3	5	0	-0.944451	-1.373635	-0.660126
4	5	0	-1.653574	1.289232	0.082158
5	5	0	-1.442004	0.228199	-1.238860
6	5	0	-0.742326	-1.108146	1.122104
7	5	0	1.721548	-0.065408	0.677677
8	5	0	-1.504971	0.486181	1.524629
9	1	0	0.558295	-0.674549	-2.264962
10	1	0	0.228647	2.066775	-1.690270
11	1	0	-1.120807	-2.437652	-1.142974
12	1	0	1.085177	-2.052855	-0.200877
13	1	0	-2.457314	2.159150	-0.106704
14	1	0	-1.938763	0.393238	-2.304844
15	1	0	-0.766034	-2.041925	1.855407
16	1	0	-2.065717	0.629421	2.568777
17	1	0	-3.262230	-0.903688	0.238750
18	6	0	0.607131	-1.095656	-0.010336
19	5	0	-2.155740	-0.463577	0.216412
20	8	0	1.123506	1.341086	0.247608

21	1	0	-0.364319	-0.034951	1.829508
22	1	0	1.791000	-0.080713	1.881500
23	8	0	3.030881	-0.221786	0.103846
24	1	0	2.999787	-0.284315	-0.859282
25	1	0	0.798327	1.838728	1.010390

oTS7-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.228307	0.621827	1.247123
2	5	0	0.252581	-0.989769	1.130451
3	5	0	-0.953959	1.454107	0.462987
4	5	0	-1.564082	-1.313224	0.164854
5	5	0	-1.329539	-0.072985	1.302057
6	5	0	-0.767193	0.958416	-1.255615
7	5	0	1.651190	-0.096350	-0.715795
8	5	0	-1.414244	-0.741781	-1.417134
9	1	0	0.597089	1.166143	2.105480
10	1	0	0.497398	-1.656758	2.088666
11	1	0	-1.213171	2.564462	0.770357
12	1	0	1.066893	2.111658	-0.214257
13	1	0	-2.269341	-2.240161	0.409176
14	1	0	-1.838671	-0.086493	2.372489
15	1	0	-0.901289	1.777078	-2.102775
16	1	0	-1.993900	-1.166292	-2.363721
17	1	0	-3.256250	0.707856	-0.309051
18	6	0	0.579920	1.141825	-0.200015
19	5	0	-2.128776	0.336167	-0.241371
20	8	0	0.975533	-1.337350	-0.141406
21	1	0	-0.388033	-0.156714	-1.915400
22	1	0	1.727613	-0.181639	-1.922621
23	8	0	2.974028	0.112469	-0.168754
24	1	0	2.956249	0.173748	0.794799
25	1	0	-0.160332	-1.468659	-0.666681

oP2-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.168153	0.840816	1.063556
2	5	0	-0.676275	1.610403	-0.219969
3	5	0	0.968695	-0.292770	1.436130
4	5	0	2.006910	0.764252	-0.975150
5	5	0	1.496141	1.152619	0.549165
6	5	0	0.735247	-1.529797	0.129718
7	5	0	-1.722288	-0.511317	-0.507172
8	5	0	1.645890	-0.921049	-1.323937
9	1	0	-0.454969	1.270201	2.019714
10	1	0	-0.579582	2.791209	-0.359901
11	1	0	1.132090	-0.567150	2.574278
12	1	0	-1.055399	-1.167855	1.621510
13	1	0	2.884400	1.261972	-1.605029
14	1	0	2.029991	1.989961	1.206818
15	1	0	0.767121	-2.695717	0.340718
16	1	0	2.197164	-1.597119	-2.124404
17	1	0	3.279304	-0.884635	0.634550
18	6	0	-0.568681	-0.676593	0.785066
19	5	0	2.223124	-0.501355	0.246819
20	8	0	-1.413779	0.850134	-1.058353
21	1	0	1.160910	0.212080	-1.827388
22	1	0	0.459943	-1.417774	-1.183032
23	8	0	-3.079824	-0.575244	0.013528
24	1	0	-3.242425	0.141927	0.640059
25	1	0	-1.595933	-1.376485	-1.349044

oTS8-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.273454	-1.049058	0.689296
2	5	0	1.238304	-1.795735	-0.465425
3	5	0	-0.941082	-0.124133	1.376858
4	5	0	-2.042007	-0.740336	-1.120639
5	5	0	-1.374321	-1.393070	0.238009
6	5	0	-0.975163	1.411892	0.405774
7	5	0	1.366770	1.084178	-0.451977

8	5	0	-1.918852	1.001311	-1.106066
9	1	0	0.616589	-1.526006	1.608714
10	1	0	0.653844	-2.377422	-1.356487
11	1	0	-0.995062	-0.093152	2.556267
12	1	0	0.997782	0.855320	1.688928
13	1	0	-2.903835	-1.158042	-1.827061
14	1	0	-1.801407	-2.385202	0.748933
15	1	0	-1.074245	2.472146	0.919177
16	1	0	-2.565530	1.770421	-1.729912
17	1	0	-3.348217	0.389420	0.902792
18	6	0	0.526749	0.532805	0.762125
19	5	0	-2.302302	0.208044	0.369430
20	8	0	2.522393	-1.754350	-0.329293
21	1	0	-1.289978	0.084808	-1.839778
22	1	0	-0.787148	1.657677	-0.878028
23	8	0	2.328145	2.021973	-0.272612
24	1	0	2.456256	2.286544	0.649669
25	1	0	1.178688	0.719276	-1.566318

oG-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.542767	-0.837861	0.736577
2	5	0	-1.183158	-1.693132	-0.519127
3	5	0	-0.267217	0.659112	1.410804
4	5	0	-1.555476	1.350416	-0.981518
5	5	0	-1.691721	0.456151	0.402807
6	5	0	0.976207	1.430519	0.324957
7	5	0	1.864156	-0.733387	-0.546193
8	5	0	0.037469	2.055997	-1.110071
9	1	0	-0.724409	-1.419783	1.637208
10	1	0	-0.678172	-1.470292	-1.596626
11	1	0	-0.161765	0.724258	2.584359
12	1	0	1.510002	-0.570717	1.580733
13	1	0	-2.395513	1.908795	-1.611009
14	1	0	-2.707284	0.347359	1.015608
15	1	0	1.902433	2.028416	0.750564
16	1	0	0.347640	2.989134	-1.766710
17	1	0	-0.998830	3.020976	1.005818

18	6	0	0.958331	-0.317018	0.676408
19	5	0	-0.706130	2.021305	0.436320
20	8	0	-2.108740	-2.583720	-0.307529
21	1	0	-0.545765	1.070742	-1.795059
22	1	0	1.160729	1.364848	-0.985695
23	8	0	3.170342	-1.043506	-0.354016
24	1	0	3.463053	-0.998980	0.567904
25	1	0	1.471032	-0.782568	-1.662539

oG'-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.517816	0.851205	0.741669
2	5	0	1.093234	1.746618	-0.516700
3	5	0	0.321284	-0.661257	1.407889
4	5	0	1.593753	-1.277220	-1.013493
5	5	0	1.716560	-0.385751	0.374062
6	5	0	-0.903555	-1.484236	0.341453
7	5	0	-1.899753	0.649260	-0.498426
8	5	0	0.033665	-2.058185	-1.113962
9	1	0	0.688837	1.432502	1.644835
10	1	0	0.573475	1.514124	-1.585397
11	1	0	0.242410	-0.739247	2.582837
12	1	0	-1.511910	0.485547	1.611998
13	1	0	2.446091	-1.791317	-1.663933
14	1	0	2.738603	-0.234752	0.966880
15	1	0	-1.791886	-2.126317	0.783286
16	1	0	-0.243858	-3.001700	-1.770512
17	1	0	1.157756	-2.983701	0.973809
18	6	0	-0.957914	0.259640	0.703022
19	5	0	0.806509	-1.996042	0.416428
20	8	0	1.985027	2.673493	-0.315956
21	1	0	0.555201	-1.041196	-1.803770
22	1	0	-1.119292	-1.422590	-0.964090
23	8	0	-3.188323	0.918331	-0.167732
24	1	0	-3.734589	1.140394	-0.933693
25	1	0	-1.542375	0.702656	-1.627144

oTS9-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.388799	0.466601	1.079990
2	5	0	-1.029158	1.335763	-0.017179
3	5	0	0.987161	-0.412453	1.371499
4	5	0	1.823819	1.066694	-0.871470
5	5	0	1.235055	1.189272	0.668470
6	5	0	1.065851	-1.543146	-0.038617
7	5	0	-1.501427	-1.012535	-0.686481
8	5	0	1.842476	-0.606751	-1.392709
9	1	0	-0.765894	0.703864	2.071874
10	1	0	-1.223622	0.096887	-1.215924
11	1	0	1.155101	-0.756329	2.488011
12	1	0	-0.808789	-1.725424	1.389519
13	1	0	2.569174	1.803752	-1.431202
14	1	0	1.547479	2.039077	1.438496
15	1	0	1.341528	-2.688018	0.084888
16	1	0	2.534064	-1.058503	-2.239567
17	1	0	3.385933	-0.423668	0.639888
18	6	0	-0.420934	-1.057749	0.626358
19	5	0	2.285203	-0.238464	0.235814
20	8	0	-1.597518	2.360273	-0.425327
21	1	0	1.111324	0.433464	-1.788725
22	1	0	0.798982	-1.383312	-1.339157
23	8	0	-2.882299	-0.943798	-0.222752
24	1	0	-3.206459	-1.824055	-0.001599
25	1	0	-1.286783	-1.894555	-1.496588

oH-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.276292	0.508526	1.127950
2	5	0	0.006047	1.622939	0.084219
3	5	0	0.736317	-0.771117	1.369293
4	5	0	1.934106	0.653680	-0.770529

5	5	0	1.488197	0.735887	0.839953
6	5	0	0.482752	-1.707049	-0.169333
7	5	0	-1.949295	-0.737317	-0.728628
8	5	0	1.484544	-0.913619	-1.454691
9	1	0	-0.673951	0.829578	2.084079
10	1	0	-1.459094	-0.028548	-1.582286
11	1	0	0.826051	-1.261540	2.437220
12	1	0	-1.318738	-1.424606	1.322465
13	1	0	2.820931	1.276628	-1.246634
14	1	0	2.053085	1.395569	1.644192
15	1	0	0.434031	-2.888664	-0.166417
16	1	0	2.050070	-1.424762	-2.357361
17	1	0	3.058757	-1.352795	0.503284
18	6	0	-0.764641	-0.874672	0.565884
19	5	0	2.046663	-0.831519	0.175409
20	8	0	-0.373833	2.666666	-0.497076
21	1	0	1.097019	0.338378	-1.736395
22	1	0	0.277868	-1.341650	-1.470360
23	8	0	-3.158624	-0.110972	-0.191698
24	1	0	-3.679805	-0.747779	0.309463
25	1	0	-2.127621	-1.877908	-1.122526

oTS10-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.167165	0.509642	1.166348
2	5	0	0.228754	1.570016	0.066786
3	5	0	0.786553	-0.840579	1.403221
4	5	0	1.910910	0.598385	-0.809342
5	5	0	1.579797	0.627205	0.838508
6	5	0	0.344669	-1.687661	-0.190132
7	5	0	-2.204020	-0.621232	-0.782412
8	5	0	1.344732	-0.948620	-1.522801
9	1	0	-0.550163	0.870659	2.114091
10	1	0	-1.598689	0.061980	-1.558074
11	1	0	0.957733	-1.309488	2.473157
12	1	0	-1.377043	-1.334148	1.343269
13	1	0	2.812740	1.198560	-1.288353
14	1	0	2.232699	1.269113	1.588640

15	1	0	0.224845	-2.865567	-0.242342
16	1	0	1.924863	-1.476079	-2.410090
17	1	0	3.012395	-1.503905	0.301716
18	6	0	-0.693240	-0.846047	0.660389
19	5	0	2.005729	-0.919051	0.075899
20	8	0	-0.192221	2.638770	-0.470917
21	1	0	1.049345	0.342468	-1.766527
22	1	0	0.137560	-1.261027	-1.573374
23	8	0	-3.240775	0.046429	-0.110474
24	1	0	-3.824741	-0.564653	0.353839
25	1	0	-2.360767	-1.783381	-1.043878

oI-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.536359	-1.000538	-0.251435
2	5	0	1.582983	-0.058190	0.424268
3	5	0	-1.111621	-1.210683	-0.832854
4	5	0	-0.750353	1.670552	-0.592087
5	5	0	-0.181394	0.285040	-1.275688
6	5	0	-1.803779	-0.587941	0.856328
7	5	0	-1.823510	1.253034	0.787465
8	1	0	1.034658	-1.793372	-0.818382
9	1	0	-1.350859	-2.006184	-1.687710
10	1	0	-0.536161	-2.540586	1.008131
11	1	0	-0.893576	2.744216	-1.095518
12	1	0	0.146739	0.253443	-2.427863
13	1	0	-2.795286	-1.026515	1.354213
14	1	0	-2.733664	1.948867	1.115071
15	1	0	-2.908302	0.483359	-1.378153
16	6	0	-0.608952	-1.530080	0.628264
17	5	0	-1.916403	0.384578	-0.719396
18	8	0	1.786881	0.433632	1.582900
19	1	0	-1.447435	0.575408	1.764127
20	1	0	-0.623041	1.856500	0.705812
21	8	0	2.792869	0.169788	-0.601660
22	1	0	2.571713	0.257156	-1.545372
23	1	0	3.353154	0.922115	-0.345424

oJ-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.304146	-1.268591	0.008781
2	5	0	-1.042879	-0.532234	-0.286998
3	5	0	2.002292	-1.110641	0.424329
4	5	0	0.831347	1.488656	1.021895
5	5	0	0.764779	-0.129874	1.316975
6	5	0	2.273837	0.098188	-1.050012
7	5	0	1.791982	1.781711	-0.468462
8	1	0	0.121078	-2.291858	0.351666
9	1	0	2.564947	-1.986832	1.004055
10	1	0	1.583764	-2.035885	-1.686503
11	1	0	0.735577	2.388628	1.801389
12	1	0	0.608111	-0.550521	2.427741
13	1	0	3.275228	0.119575	-1.698150
14	1	0	2.423697	2.779838	-0.626238
15	1	0	3.316156	0.849509	1.338504
16	6	0	1.420572	-1.181407	-1.043062
17	5	0	2.314762	0.626940	0.726417
18	8	0	-1.500049	0.162834	-1.272546
19	1	0	1.495501	1.298380	-1.577230
20	1	0	0.491864	1.951713	-0.162313
21	8	0	-2.116033	-0.896090	0.788478
22	1	0	-1.822655	-0.939360	1.713371
23	1	0	-2.909425	-0.275679	0.693258
24	8	0	-3.793373	0.864508	-0.084899
25	1	0	-4.575708	0.464832	-0.488763
26	1	0	-3.061400	0.763907	-0.754081

oTS11-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.262300	-1.270990	0.042102
2	5	0	-1.092390	-0.522974	-0.209433

3	5	0	1.969232	-1.134629	0.411536
4	5	0	0.854390	1.485136	1.023193
5	5	0	0.768297	-0.130989	1.328300
6	5	0	2.224779	0.058693	-1.073386
7	5	0	1.783281	1.757480	-0.492422
8	1	0	0.075904	-2.290404	0.395201
9	1	0	2.535309	-2.016304	0.979544
10	1	0	1.483440	-2.063293	-1.684473
11	1	0	0.795375	2.388279	1.803025
12	1	0	0.635244	-0.541324	2.445985
13	1	0	3.208768	0.062093	-1.748248
14	1	0	2.429991	2.744135	-0.664099
15	1	0	3.336670	0.809849	1.279982
16	6	0	1.348560	-1.203296	-1.041633
17	5	0	2.316592	0.599001	0.694813
18	8	0	-1.507465	0.170135	-1.244550
19	1	0	1.449422	1.282361	-1.591707
20	1	0	0.492749	1.950008	-0.152078
21	8	0	-2.148483	-0.782027	0.816752
22	1	0	-1.862990	-0.843776	1.739482
23	1	0	-3.012737	-0.024883	0.573040
24	8	0	-3.611225	0.826557	-0.129387
25	1	0	-4.405135	0.425311	-0.511908
26	1	0	-2.810698	0.687760	-0.822083

oK-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.559855	-1.065299	0.131739
2	5	0	-1.662033	-0.002093	-0.175778
3	5	0	1.109800	-1.355562	0.567921
4	5	0	0.742485	1.510940	0.910479
5	5	0	0.208840	0.014231	1.344300
6	5	0	1.719700	-0.417824	-0.991624
7	5	0	1.753308	1.381527	-0.571613
8	1	0	-1.019333	-1.963087	0.557854
9	1	0	1.399909	-2.303971	1.228090
10	1	0	0.438590	-2.302890	-1.466969
11	1	0	0.910071	2.463902	1.611253

12	1	0	-0.056767	-0.238220	2.483531
13	1	0	2.681912	-0.747991	-1.614665
14	1	0	2.652250	2.133804	-0.787982
15	1	0	2.934774	0.210998	1.348363
16	6	0	0.526373	-1.382807	-0.904187
17	5	0	1.913016	0.234839	0.729554
18	8	0	-1.652144	0.699876	-1.360622
19	1	0	1.332014	0.916618	-1.644890
20	1	0	0.558846	1.949445	-0.315516
21	8	0	-2.776802	0.150439	0.630139
22	1	0	-2.735111	-0.384220	1.432937
23	1	0	-2.390280	1.321440	-1.419644

oK'-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.643886	-0.698997	0.605434
2	5	0	-1.786635	0.224721	0.026210
3	5	0	0.985767	-1.389113	0.685945
4	5	0	1.340684	1.504889	0.530998
5	5	0	0.570433	0.279503	1.342725
6	5	0	1.369502	-0.846825	-1.117653
7	5	0	1.932421	0.893503	-1.059594
8	1	0	-1.133237	-1.421419	1.268298
9	1	0	1.196121	-2.279596	1.448386
10	1	0	-0.397184	-2.369855	-0.933417
11	1	0	1.903533	2.454439	0.987697
12	1	0	0.579416	0.282269	2.542260
13	1	0	2.041914	-1.510688	-1.845573
14	1	0	2.902611	1.323772	-1.598963
15	1	0	3.221000	-0.234611	0.795543
16	6	0	0.059301	-1.455091	-0.580574
17	5	0	2.112741	-0.052289	0.389179
18	8	0	-2.993604	-0.388570	-0.224014
19	1	0	1.155601	0.415017	-1.912958
20	1	0	1.022495	1.817276	-0.710426
21	8	0	-1.656029	1.554040	-0.234916
22	1	0	-0.763636	1.827983	0.078161
23	1	0	-3.648632	0.224235	-0.585774

oTS12-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.649536	-0.749244	0.585823
2	5	0	-1.771424	0.261005	-0.024657
3	5	0	0.980712	-1.314755	0.809397
4	5	0	1.176430	1.581228	0.353665
5	5	0	0.454525	0.353765	1.278827
6	5	0	1.429073	-0.957995	-0.998169
7	5	0	1.906088	0.819025	-1.129799
8	1	0	-1.183431	-1.412570	1.270899
9	1	0	1.212670	-2.106555	1.662738
10	1	0	-0.264138	-2.532167	-0.756960
11	1	0	1.634011	2.591773	0.782463
12	1	0	0.355560	0.571914	2.445585
13	1	0	2.182794	-1.643625	-1.614008
14	1	0	2.912774	1.232824	-1.606106
15	1	0	3.120849	0.017817	0.931587
16	6	0	0.112455	-1.553038	-0.494735
17	5	0	2.034539	0.066850	0.445906
18	8	0	-2.952967	-0.399301	-0.344963
19	1	0	1.204634	0.253532	-1.971077
20	1	0	1.005013	1.766707	-0.947792
21	8	0	-1.556731	1.556136	-0.160983
22	1	0	-0.319761	1.558336	0.324943
23	1	0	-3.610615	0.215408	-0.697091

oL-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.658728	-0.698236	0.567805
2	5	0	-1.782247	0.396006	-0.031507
3	5	0	0.878488	-1.484994	0.557201
4	5	0	1.501807	1.439845	0.656107

5	5	0	0.530627	0.126715	1.369060
6	5	0	1.293615	-0.880794	-1.135755
7	5	0	1.948032	0.907593	-1.034874
8	1	0	-1.241709	-1.392326	1.170804
9	1	0	1.046331	-2.417554	1.264977
10	1	0	-0.610707	-2.212765	-1.119936
11	1	0	2.138974	2.193873	1.307942
12	1	0	0.526608	0.138841	2.554544
13	1	0	1.938366	-1.467923	-1.942177
14	1	0	3.023008	1.255257	-1.402884
15	1	0	3.143643	-0.427234	0.769458
16	6	0	-0.068568	-1.373647	-0.707957
17	5	0	2.049886	-0.175017	0.380759
18	8	0	-3.021329	-0.281091	-0.037543
19	1	0	1.145429	0.779713	-1.926764
20	1	0	1.281694	1.953631	-0.521949
21	8	0	-1.566845	1.608756	-0.422732
22	1	0	0.277244	1.456335	0.964441
23	1	0	-3.700754	0.303356	-0.400298

oM-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.344489	-0.544064	-0.191108
2	5	0	-1.014834	0.976913	-0.361889
3	5	0	0.939303	-1.663549	0.041957
4	5	0	1.893046	0.839452	1.402670
5	5	0	0.542689	-0.328352	1.224171
6	5	0	2.067905	-0.733919	-1.089640
7	5	0	2.874452	0.723175	-0.138261
8	1	0	-1.210955	-1.198878	-0.097760
9	1	0	0.695230	-2.769389	0.382289
10	1	0	0.161798	-1.463633	-2.179209
11	1	0	2.334760	1.158056	2.452307
12	1	0	0.056990	-0.651682	2.253999
13	1	0	2.897026	-1.207879	-1.795632
14	1	0	4.043539	0.859174	0.024329
15	1	0	3.067061	-1.345379	1.331560
16	6	0	0.595923	-0.943431	-1.336633

17	5	0	2.260414	-0.709632	0.735516
18	8	0	-2.227036	0.995553	0.372213
19	1	0	2.483258	1.090012	-1.215955
20	1	0	2.208897	1.713528	0.491778
21	8	0	-0.538370	1.942194	-1.075441
22	1	0	0.662683	1.090811	1.340768
23	1	0	-2.658961	1.854506	0.263973
24	8	0	-4.257129	-0.948192	0.149325
25	1	0	-3.527002	-0.302535	0.246092
26	1	0	-4.357516	-1.338622	1.026518

oM'-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.022207	0.923299	0.897233
2	5	0	-1.304992	1.083286	-0.093659
3	5	0	1.572344	0.328219	1.354441
4	5	0	1.621719	0.269638	-1.649633
5	5	0	1.268443	1.254526	-0.191540
6	5	0	1.179327	-1.382333	0.754293
7	5	0	1.461126	-1.475576	-1.130210
8	1	0	-0.132664	1.688623	1.658530
9	1	0	2.186984	0.888817	2.195069
10	1	0	-0.256238	-0.695895	2.435432
11	1	0	2.315677	0.639323	-2.532669
12	1	0	1.695537	2.356945	-0.247298
13	1	0	1.576028	-2.394621	1.232293
14	1	0	2.220861	-2.216669	-1.663233
15	1	0	3.492339	-0.313257	-0.127629
16	6	0	0.212389	-0.483899	1.484604
17	5	0	2.307154	-0.244808	-0.152757
18	8	0	-1.652548	2.444900	-0.151896
19	1	0	0.419664	-1.988978	-0.806527
20	1	0	0.852498	-0.703991	-2.051407
21	8	0	-1.939701	0.109349	-0.674133
22	1	0	0.666025	1.068578	-1.473950
23	1	0	-2.444067	2.555740	-0.696114
24	8	0	-2.511625	-2.395039	0.047900
25	1	0	-3.428463	-2.497050	-0.235092

26	1	0	-2.266354	-1.462410	-0.208066

oTS13-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.309341	0.254635	-0.919255
2	5	0	-1.405949	-0.510444	-0.012123
3	5	0	1.274707	0.873172	-1.310564
4	5	0	1.831070	-1.526730	0.405276
5	5	0	0.946321	-0.907543	-1.021088
6	5	0	1.566566	1.386712	0.493935
7	5	0	2.197362	-0.075667	1.421310
8	1	0	-0.807490	0.430667	-1.873925
9	1	0	1.510645	1.162289	-2.433601
10	1	0	-0.219879	2.479603	-0.515404
11	1	0	2.462323	-2.524957	0.425078
12	1	0	0.976556	-1.621214	-1.964220
13	1	0	2.204888	2.339131	0.804659
14	1	0	3.194950	-0.093204	2.059491
15	1	0	3.516701	-0.107166	-0.754357
16	6	0	0.280851	1.546525	-0.303535
17	5	0	2.408245	-0.085988	-0.331392
18	8	0	-2.140620	-1.440708	-0.716198
19	1	0	1.325999	0.640094	1.894600
20	1	0	1.492634	-1.187855	1.635279
21	8	0	-1.392020	-0.501494	1.378049
22	1	0	0.641404	-1.771986	0.047553
23	1	0	-2.755077	-1.911795	-0.136695
24	8	0	-2.929453	1.257116	0.354736
25	1	0	-3.773690	0.797080	0.269130
26	1	0	-1.993896	0.275482	1.519685

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.246655	-1.473330	0.721594
2	5	0	1.357193	-0.403527	-0.000000
3	5	0	-1.175689	1.183460	0.970820
4	5	0	0.246655	-0.093070	1.363885
5	5	0	0.246655	-0.093070	-1.363885
6	5	0	-1.175689	1.183460	-0.970820
7	1	0	0.548871	-2.381751	1.233908
8	1	0	2.540238	-0.462838	-0.000000
9	1	0	0.548871	-2.381751	-1.233908
10	1	0	-1.156816	2.267077	1.474293
11	1	0	0.582475	0.108503	2.488701
12	1	0	0.582475	0.108503	-2.488701
13	1	0	-1.156816	2.267077	-1.474293
14	1	0	0.950913	2.073770	-0.000000
15	6	0	0.246655	-1.473330	-0.721594
16	5	0	0.367581	1.036359	-0.000000
17	1	0	-1.837040	0.389489	-1.578161
18	1	0	-2.059515	1.234333	0.000000
19	1	0	-1.837040	0.389489	1.578161

mTS1-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.634518	1.297739	0.101172
2	5	0	-0.616773	1.038570	1.067707
3	5	0	-0.768906	1.323893	-0.720737
4	5	0	1.060941	-0.114863	0.661758
5	5	0	-1.976690	0.341780	0.128834
6	5	0	-1.103084	-0.363369	-1.317190
7	5	0	0.033607	-1.294197	-0.200532
8	1	0	1.263632	2.172551	0.133155
9	1	0	-0.836128	1.739090	1.992468
10	1	0	-1.057044	2.299063	-1.321247
11	1	0	1.342834	0.187691	-1.979778
12	1	0	1.591432	-0.387264	1.675241
13	1	0	-3.078180	0.686044	0.388463
14	1	0	-1.461268	-0.560911	-2.429125
15	1	0	0.482560	-2.388141	-0.251070
16	1	0	-1.028473	-0.997962	2.119952

17	1	0	-2.383133	-2.267059	0.019781
18	5	0	-1.678815	-1.323901	-0.045217
19	8	0	3.194092	-0.372790	-0.115178
20	1	0	3.551122	-0.655370	0.734846
21	5	0	0.591220	0.184338	-1.073650
22	6	0	-0.909115	-0.598850	1.121141

mA-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.766368	0.208954	-0.502925
2	5	0	0.603557	1.430130	0.507354
3	5	0	0.842012	0.748872	-1.188057
4	5	0	0.483158	-0.132035	1.440392
5	5	0	-0.981733	-0.972140	0.804824
6	1	0	-0.961885	2.284323	-0.908482
7	1	0	-2.916025	0.438564	-0.698034
8	1	0	0.907732	2.507088	0.906863
9	1	0	-1.603768	1.473781	1.737690
10	1	0	1.983964	-1.188158	-1.686822
11	1	0	1.347508	1.430368	-2.028999
12	1	0	0.635708	-0.231087	2.617507
13	1	0	-1.597216	-1.679918	1.531651
14	1	0	1.479131	-2.414625	0.777891
15	1	0	2.943901	0.419427	0.557904
16	5	0	1.807326	0.199743	0.283431
17	8	0	-1.357912	-1.201854	-0.696653
18	1	0	-0.479201	-1.230685	-1.179119
19	6	0	-0.625222	1.298256	-0.609656
20	5	0	-0.976750	0.806196	0.981008
21	6	0	1.271170	-0.754816	-0.991118
22	5	0	1.038349	-1.380696	0.383937

mTS2-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	5	0	-1.842234	0.270781	-0.136432
2	5	0	0.862313	1.415002	-0.144998
3	5	0	0.482422	0.208024	-1.486252
4	5	0	1.080811	0.316863	1.260848
5	5	0	-0.482789	-0.488065	1.418958
6	1	0	-0.990679	2.083113	-1.180100
7	1	0	-2.886143	0.808116	0.088841
8	1	0	1.311285	2.507405	-0.256124
9	1	0	-0.914382	2.060818	1.595662
10	1	0	1.152971	-1.989870	-1.518326
11	1	0	0.716048	0.465312	-2.628270
12	1	0	1.614376	0.565803	2.295451
13	1	0	-1.086773	-1.128418	2.201064
14	1	0	1.547655	-2.232766	1.185899
15	1	0	3.031034	0.006144	-0.467282
16	5	0	1.861625	-0.027150	-0.262084
17	8	0	-1.950187	-1.135410	-0.278901
18	1	0	-1.145444	-1.492696	-0.700090
19	6	0	-0.665692	1.146202	-0.739320
20	5	0	-0.506309	1.145705	0.958318
21	6	0	0.806275	-1.187307	-0.872644
22	5	0	1.025771	-1.305771	0.648895

mB-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	2.150858	0.303052	-0.186771
2	5	0	-0.728488	1.458645	0.275821
3	5	0	0.040931	0.194806	1.356567
4	5	0	-1.621260	0.449577	-0.918487
5	5	0	-0.361572	-0.818932	-1.127666
6	1	0	1.284063	2.095004	0.585691
7	1	0	3.033129	0.944046	-0.677428
8	1	0	-0.994990	2.587522	0.520223
9	1	0	0.429606	1.509528	-2.088921
10	1	0	-0.455264	-2.058805	1.197102
11	1	0	0.252611	0.241041	2.528512
12	1	0	-2.417391	0.952715	-1.646968

13	1	0	-0.080769	-1.641435	-1.945016
14	1	0	-2.628520	-1.975242	-0.426754
15	1	0	-2.539342	0.170222	1.717716
16	5	0	-1.699258	0.099677	0.881686
17	8	0	2.459634	-1.015518	0.000443
18	1	0	1.718687	-1.514756	0.379755
19	6	0	0.904336	1.105042	0.330078
20	5	0	0.138858	0.827902	-1.155431
21	6	0	-0.538609	-1.130862	0.638556
22	5	0	-1.814721	-1.120882	-0.317570

mTS3-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.752425	0.264974	-0.454321
2	5	0	-0.867284	1.410055	0.347810
3	5	0	0.012452	0.191096	1.391024
4	5	0	-1.556850	0.331719	-0.952141
5	5	0	-0.096603	-0.764482	-1.089941
6	1	0	1.197204	2.177846	0.735328
7	1	0	2.469298	0.826858	-1.249000
8	1	0	-1.295930	2.491537	0.577068
9	1	0	0.335450	1.704940	-1.980321
10	1	0	-0.209976	-2.087000	1.153714
11	1	0	0.175854	0.204318	2.570740
12	1	0	-2.354292	0.761884	-1.721984
13	1	0	0.253554	-1.535509	-1.925928
14	1	0	-2.286179	-2.193616	-0.637461
15	1	0	-2.614440	-0.127520	1.596298
16	5	0	-1.705587	-0.058177	0.835753
17	8	0	2.375496	-0.917173	0.087394
18	1	0	2.921396	-0.676839	0.846496
19	6	0	0.776942	1.224068	0.431929
20	5	0	0.117081	0.969731	-1.075739
21	6	0	-0.414693	-1.167881	0.616314
22	5	0	-1.609515	-1.254243	-0.393158

mC-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	2.080556	0.322403	-0.248953
2	5	0	-0.766558	1.433637	0.317980
3	5	0	0.022816	0.140126	1.361034
4	5	0	-1.640373	0.441820	-0.912634
5	5	0	-0.350285	-0.799418	-1.138110
6	1	0	1.244883	2.081951	0.658363
7	1	0	2.854564	0.946289	-0.917644
8	1	0	-1.051949	2.553183	0.584970
9	1	0	0.394151	1.573476	-2.035549
10	1	0	-0.434258	-2.102555	1.132393
11	1	0	0.225913	0.148472	2.536501
12	1	0	-2.438267	0.957688	-1.630791
13	1	0	-0.062889	-1.596147	-1.979210
14	1	0	-2.617691	-2.004030	-0.496247
15	1	0	-2.574487	0.083969	1.708008
16	5	0	-1.722259	0.049419	0.881168
17	8	0	2.460140	-0.945878	0.122076
18	1	0	3.278245	-1.208461	-0.317112
19	6	0	0.867658	1.097473	0.374230
20	5	0	0.110065	0.858122	-1.125917
21	6	0	-0.547982	-1.162185	0.602347
22	5	0	-1.817440	-1.141817	-0.350518

mTS4-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-2.031408	0.280134	0.503837
2	5	0	0.670964	1.069140	-0.997742
3	5	0	-0.275614	-0.475877	-1.066319
4	5	0	1.886566	0.730426	0.283032
5	5	0	0.771590	-0.146115	1.404154
6	1	0	-1.414361	1.635071	-1.043457
7	1	0	-2.238621	0.658629	1.617302
8	1	0	0.781903	1.884491	-1.851615

9	1	0	0.168327	2.412107	1.226483
10	1	0	0.310923	-2.382541	0.105894
11	1	0	-0.784727	-0.987994	-2.013152
12	1	0	2.835145	1.435469	0.441437
13	1	0	0.757860	-0.418016	2.567976
14	1	0	2.843377	-1.698649	0.870103
15	1	0	2.108206	-0.935530	-1.974356
16	5	0	1.516483	-0.496334	-1.042013
17	8	0	-2.906801	-0.624220	-0.022567
18	1	0	-3.600568	-0.866155	0.605584
19	6	0	-0.903198	0.898000	-0.413039
20	5	0	0.242137	1.336855	0.710146
21	6	0	0.511458	-1.316443	0.066641
22	5	0	1.986758	-0.944721	0.546250

mD-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.780655	-0.234345	-0.482821
2	5	0	0.519883	1.246641	0.789342
3	5	0	0.365541	1.044814	-1.027631
4	5	0	1.312413	-0.318326	1.256088
5	5	0	0.374924	-1.374413	0.119739
6	1	0	-1.517678	1.858430	0.229249
7	1	0	-1.562212	-0.839005	-1.483065
8	1	0	0.567924	2.226611	1.455733
9	1	0	-1.136634	-0.358542	2.054655
10	1	0	1.328998	-0.686691	-2.198945
11	1	0	0.431629	1.880831	-1.874161
12	1	0	1.739675	-0.451035	2.358800
13	1	0	0.141255	-2.542010	0.071285
14	1	0	2.972410	-1.724572	-0.269002
15	1	0	2.893503	1.318491	-0.376929
16	5	0	1.913042	0.686236	-0.155820
17	8	0	-3.070981	-0.316023	0.044301
18	1	0	-3.618253	-0.930168	-0.459237
19	6	0	-0.897906	1.003397	-0.028435
20	5	0	-0.486357	-0.200954	1.072560
21	6	0	1.071695	-0.399537	-1.184316

22	5	0	2.038107	-1.019115	-0.088714

mTS5-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.580540	0.099265	-0.469307
2	5	0	-0.621792	-1.025168	1.039117
3	5	0	-0.672007	-1.288336	-0.774683
4	5	0	-1.087179	0.725623	1.145491
5	5	0	0.141005	1.471677	0.066831
6	1	0	1.301046	-2.002666	0.411118
7	1	0	1.216064	0.631423	-1.482748
8	1	0	-0.750213	-1.822691	1.908405
9	1	0	1.379534	0.323388	2.033505
10	1	0	-1.806842	-0.020126	-2.302789
11	1	0	-0.873935	-2.359025	-1.262582
12	1	0	-1.465799	1.271039	2.132529
13	1	0	0.535277	2.567503	-0.142184
14	1	0	-2.323552	2.108275	-0.682327
15	1	0	-3.123578	-0.754784	0.345243
16	5	0	-2.005835	-0.398361	0.158563
17	8	0	2.984950	0.133486	-0.224870
18	1	0	3.434594	0.675700	-0.881967
19	6	0	0.738765	-1.132921	0.085961
20	5	0	0.647715	0.216912	1.105659
21	6	0	-1.309842	0.004317	-1.335694
22	5	0	-1.577594	1.215528	-0.427439

mE-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.517562	-0.002022	-0.238992
2	5	0	-0.740762	-0.876352	1.126518
3	5	0	-0.851366	-1.323821	-0.653120
4	5	0	-0.891260	0.937020	1.008450

5	5	0	0.571987	1.435552	0.108206
6	1	0	1.114348	-2.105300	0.476237
7	1	0	0.824179	0.941981	-1.023326
8	1	0	-0.990823	-1.590773	2.042619
9	1	0	1.291589	0.144173	2.314885
10	1	0	-2.111632	-0.232289	-2.226589
11	1	0	-1.139543	-2.453334	-0.917121
12	1	0	-1.257800	1.670543	1.872140
13	1	0	1.049467	2.518002	0.206879
14	1	0	-1.792980	2.264125	-1.010607
15	1	0	-3.147736	-0.274908	0.504570
16	5	0	-2.010955	-0.155588	0.169991
17	8	0	2.844095	-0.118451	-0.633190
18	1	0	3.277847	0.736400	-0.749648
19	6	0	0.622074	-1.177524	0.206117
20	5	0	0.675438	0.146976	1.301326
21	6	0	-1.432513	-0.102397	-1.388725
22	5	0	-1.272052	1.239939	-0.688152

mTS6-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.319740	-0.065396	0.155205
2	5	0	-1.014704	-0.821009	-1.081315
3	5	0	0.075543	0.625673	-1.314366
4	5	0	-1.583998	-0.538318	0.590997
5	5	0	-0.110872	-0.538064	1.597486
6	1	0	1.180879	-1.460879	-1.663917
7	1	0	0.991744	0.065330	1.463873
8	1	0	-1.525907	-1.426759	-1.963813
9	1	0	-0.358553	-2.863396	0.323378
10	1	0	-0.064419	2.655203	-0.294946
11	1	0	0.418897	1.027930	-2.378336
12	1	0	-2.554561	-1.002713	1.103121
13	1	0	-0.021501	-0.922405	2.722054
14	1	0	-1.593237	1.723005	1.884490
15	1	0	-2.508881	1.309250	-1.085051
16	5	0	-1.558831	0.807202	-0.576131
17	8	0	2.654403	0.255345	0.151932

18	1	0	2.959362	0.721753	0.941013
19	6	0	0.627317	-0.928655	-0.902190
20	5	0	-0.281402	-1.677116	0.266196
21	6	0	-0.197377	1.595907	-0.102728
22	5	0	-0.993213	1.032511	1.114365

mP3-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.297809	0.086702	-0.047298
2	5	0	1.010617	-1.140610	-0.769857
3	5	0	-0.413590	-1.522655	0.156006
4	5	0	1.780046	0.275333	0.006153
5	5	0	0.903850	1.785753	-0.187708
6	1	0	-0.963519	-0.926725	-2.109799
7	1	0	-0.223939	2.176954	-0.247343
8	1	0	1.542892	-2.016614	-1.365024
9	1	0	1.193539	0.623857	-2.564514
10	1	0	-1.065597	-0.437712	2.202966
11	1	0	-0.969707	-2.558974	0.261057
12	1	0	2.962256	0.407149	0.016924
13	1	0	1.711607	2.677004	-0.269728
14	1	0	1.079532	1.184153	2.403530
15	1	0	1.465327	-1.658913	1.838281
16	5	0	0.967668	-0.938392	1.039431
17	8	0	-2.535410	0.648929	-0.190583
18	1	0	-2.917575	0.932410	0.650775
19	6	0	-0.479865	-0.544570	-1.220054
20	5	0	0.812922	0.496859	-1.440199
21	6	0	-0.537896	-0.261555	1.274124
22	5	0	0.751302	0.805556	1.320096

pTS1-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	5	0	1.067639	0.058034	0.697990
2	5	0	-0.930517	1.265029	-0.728805
3	5	0	-0.653890	1.111421	1.044827
4	5	0	-1.069054	-0.454240	-1.266718
5	5	0	0.206735	-1.273419	-0.240646
6	1	0	1.068172	2.336768	-0.034688
7	1	0	1.669169	0.093149	1.722486
8	1	0	-1.363246	2.182334	-1.335311
9	1	0	1.234971	0.386066	-2.086283
10	1	0	-0.730164	-1.168451	2.361992
11	1	0	-0.901717	1.897555	1.895955
12	1	0	-1.502691	-0.798628	-2.311018
13	1	0	0.762925	-2.293479	-0.453108
14	1	0	-1.951446	-2.233091	0.049657
15	1	0	-3.085772	0.315646	0.475684
16	5	0	-1.934898	0.152520	0.255814
17	8	0	2.939414	-0.412965	-0.113447
18	1	0	3.459319	-0.305842	0.691886
19	6	0	0.519055	1.408248	0.004656
20	6	0	-1.364494	-1.328952	0.048519
21	5	0	0.544178	0.288485	-1.135125
22	5	0	-0.650633	-0.664645	1.294917

pA-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.911325	-0.144482	0.536055
2	5	0	-0.475696	1.050452	-0.997095
3	5	0	-0.294968	1.272048	0.809525
4	5	0	-1.393294	-0.476063	-1.147831
5	5	0	-0.548391	-1.477043	0.084645
6	1	0	1.572530	1.606988	-0.691787
7	1	0	1.691469	-0.643634	1.591293
8	1	0	-0.460008	1.874758	-1.849955
9	1	0	1.037155	-0.917947	-1.912062
10	1	0	-1.477804	-0.250549	2.553564
11	1	0	-0.250871	2.343699	1.341364
12	1	0	-1.969531	-0.800194	-2.132335
13	1	0	-0.500110	-2.660976	0.209867

14	1	0	-2.890538	-1.350061	0.495053
15	1	0	-2.868178	1.454411	0.035755
16	5	0	-1.881426	0.794842	0.054987
17	8	0	3.181195	-0.279169	0.003088
18	1	0	3.752299	-0.815569	0.566406
19	6	0	0.954977	0.868627	-0.175792
20	6	0	-1.975852	-0.802560	0.317518
21	5	0	0.400511	-0.522813	-0.985231
22	5	0	-1.110206	-0.097738	1.428503

pA'-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-2.149793	0.325074	-0.236636
2	5	0	0.739776	1.434045	0.278157
3	5	0	-0.087647	0.755052	-1.175880
4	5	0	1.704466	0.092094	0.914626
5	5	0	0.514857	-1.259886	0.783539
6	1	0	-1.251088	2.105448	0.479790
7	1	0	-2.934442	0.954173	-0.889792
8	1	0	0.998587	2.573229	0.482932
9	1	0	-0.260366	0.449630	2.563733
10	1	0	0.376468	-1.632590	-2.110936
11	1	0	-0.380462	1.418081	-2.124590
12	1	0	2.635328	0.205541	1.642759
13	1	0	0.480026	-2.315193	1.339437
14	1	0	2.504661	-1.761481	-0.397912
15	1	0	2.544995	0.839465	-1.544176
16	5	0	1.658464	0.431122	-0.869656
17	8	0	-2.521108	-0.943330	0.124351
18	1	0	-3.362977	-1.190966	-0.277720
19	6	0	-0.894209	1.086567	0.291691
20	6	0	1.702089	-1.056549	-0.232811
21	5	0	-0.043418	0.230716	1.406215
22	5	0	0.457466	-0.863977	-1.202688

pTS2-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.560591	0.524582	0.381568
2	5	0	-1.172655	1.206827	-0.294277
3	5	0	-0.050273	1.060893	1.111952
4	5	0	-1.600890	-0.431183	-0.699559
5	5	0	0.031321	-1.218484	-0.973759
6	1	0	0.705957	2.406575	-0.740401
7	1	0	2.364757	1.144144	1.033884
8	1	0	-1.872219	2.149469	-0.463410
9	1	0	-0.341943	0.713636	-2.689855
10	1	0	0.513953	-1.134983	2.398090
11	1	0	0.081746	1.902276	1.938458
12	1	0	-2.584296	-0.829105	-1.230405
13	1	0	0.383148	-2.179605	-1.570592
14	1	0	-1.166394	-2.368747	0.679584
15	1	0	-2.389816	-0.051380	1.738614
16	5	0	-1.459562	-0.015970	1.005841
17	8	0	2.163295	-0.610681	-0.336909
18	1	0	2.603146	-1.216855	0.272128
19	6	0	0.488013	1.378158	-0.467049
20	6	0	-0.779073	-1.407076	0.368144
21	5	0	-0.237688	0.369854	-1.551420
22	5	0	0.157548	-0.591812	1.404177

pB-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.990099	1.013144	0.671318
2	5	0	-1.503633	0.555587	-0.627129
3	5	0	-0.814758	1.005071	0.966909
4	5	0	-0.833322	-1.045353	-0.910242
5	5	0	0.985147	-0.940389	-0.763910
6	1	0	-0.197706	2.525984	-0.751487
7	1	0	1.594783	1.859026	1.259688
8	1	0	-2.518313	1.016805	-1.034026
9	1	0	-0.083298	0.577561	-2.774966

10	1	0	0.138323	-0.576533	2.766890
11	1	0	-1.249564	1.855453	1.673636
12	1	0	-1.273570	-1.914780	-1.589668
13	1	0	1.590467	-1.769313	-1.375393
14	1	0	-0.022677	-2.529347	0.747206
15	1	0	-2.405213	-1.125864	1.190343
16	5	0	-1.436692	-0.623624	0.722856
17	8	0	1.949826	0.079885	-0.108427
18	1	0	2.557509	-0.380054	0.495667
19	6	0	-0.095166	1.482529	-0.477863
20	6	0	0.002214	-1.480416	0.475982
21	5	0	-0.070827	0.336751	-1.607314
22	5	0	0.049660	-0.339325	1.601674

pTS3-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.001041	-1.244265	0.954100
2	5	0	1.459417	0.021513	-0.998663
3	5	0	1.610125	-0.421074	0.702104
4	5	0	0.038233	1.085540	-1.082433
5	5	0	-1.550750	0.489186	-0.404359
6	1	0	1.218890	-2.336669	-0.721064
7	1	0	-0.343384	-2.221552	1.529891
8	1	0	2.384722	0.015367	-1.737929
9	1	0	-0.482238	-1.096416	-2.416410
10	1	0	0.308998	0.659485	2.705413
11	1	0	2.600287	-0.812440	1.225048
12	1	0	-0.096242	1.937841	-1.896542
13	1	0	-2.362001	1.140932	-1.017456
14	1	0	-0.744872	2.378046	0.784100
15	1	0	1.851658	2.165201	0.513172
16	5	0	1.159955	1.219661	0.328222
17	8	0	-2.156599	-0.723605	0.182017
18	1	0	-2.932792	-0.466198	0.700303
19	6	0	0.811284	-1.391151	-0.387276
20	6	0	-0.497757	1.361706	0.491663
21	5	0	-0.145694	-0.571363	-1.407002
22	5	0	0.223476	0.341184	1.557836

pC-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.515036	-1.259244	0.784506
2	5	0	1.658373	0.430468	-0.870184
3	5	0	1.704438	0.093243	0.914467
4	5	0	-0.087870	0.753516	-1.176474
5	5	0	-2.149761	0.324901	-0.236943
6	1	0	2.505076	-1.761492	-0.396183
7	1	0	0.480496	-2.313988	1.341476
8	1	0	2.544731	0.838277	-1.545212
9	1	0	0.377484	-1.634429	-2.109705
10	1	0	-0.259784	0.451918	2.563685
11	1	0	2.635274	0.207387	1.642500
12	1	0	-0.381447	1.415308	-2.125769
13	1	0	-2.934453	0.953804	-0.890189
14	1	0	-1.251155	2.105419	0.478971
15	1	0	0.998301	2.573881	0.479955
16	5	0	0.739554	1.434477	0.276453
17	8	0	-2.521421	-0.943219	0.124821
18	1	0	-3.363303	-1.191081	-0.277048
19	6	0	1.702381	-1.056564	-0.231775
20	6	0	-0.894181	1.086486	0.291491
21	5	0	0.457756	-0.865166	-1.201957
22	5	0	-0.043335	0.232049	1.406265

pTS4-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.173247	-1.264427	-0.882150
2	5	0	-1.529451	0.160683	0.942682
3	5	0	-1.663171	-0.229591	-0.794918
4	5	0	0.013246	1.018809	1.099281
5	5	0	1.625376	0.336583	0.465565

6	1	0	-1.686970	-2.191087	0.641831
7	1	0	0.132555	-2.280904	-1.411860
8	1	0	-2.453414	0.301693	1.669594
9	1	0	0.272764	-1.320892	2.267678
10	1	0	-0.032307	0.603880	-2.666418
11	1	0	-2.665588	-0.436524	-1.393518
12	1	0	0.194371	1.800810	1.972036
13	1	0	2.342565	0.914638	1.254151
14	1	0	0.997347	2.299092	-0.684673
15	1	0	-1.561946	2.356562	-0.547943
16	5	0	-1.008843	1.327793	-0.344821
17	8	0	2.337058	-0.801501	-0.127937
18	1	0	2.764493	-0.513796	-0.945047
19	6	0	-1.141084	-1.310934	0.330863
20	6	0	0.658858	1.300269	-0.421841
21	5	0	-0.000994	-0.685257	1.303683
22	5	0	-0.084312	0.323914	-1.506614

pD-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.454401	-0.926288	-1.135437
2	5	0	-1.660033	0.175838	0.920985
3	5	0	-1.631951	0.416281	-0.884987
4	5	0	0.088332	0.335749	1.376771
5	5	0	2.234148	0.288841	-0.139631
6	1	0	-2.518541	-1.726895	-0.270150
7	1	0	-0.384033	-1.751862	-1.992490
8	1	0	-2.569913	0.348974	1.662441
9	1	0	-0.484539	-2.212236	1.473435
10	1	0	0.402917	1.281628	-2.226375
11	1	0	-2.513576	0.791665	-1.584239
12	1	0	0.329656	0.622363	2.512439
13	1	0	3.185635	0.915640	-0.502715
14	1	0	1.304050	2.134091	0.322714
15	1	0	-0.935754	2.623131	0.331100
16	5	0	-0.693838	1.471545	0.186929
17	8	0	2.450833	-1.044167	0.010456
18	1	0	1.614687	-1.475469	0.281893

19	6	0	-1.701466	-1.028081	-0.163479
20	6	0	0.941201	1.111887	0.191874
21	5	0	-0.497530	-1.194830	0.849893
22	5	0	0.120140	0.692757	-1.226939

pTS5-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.799187	-1.176290	0.682841
2	5	0	1.645511	-0.247407	-0.474037
3	5	0	0.952647	-0.695666	1.093395
4	5	0	0.586195	1.063065	-1.038008
5	5	0	-1.181768	0.628209	-0.884660
6	1	0	0.866764	-2.491376	-0.413932
7	1	0	-1.221392	-2.108134	1.290536
8	1	0	2.782097	-0.451965	-0.741387
9	1	0	0.368186	-0.899870	-2.683573
10	1	0	-0.400103	0.804860	2.696743
11	1	0	1.539174	-1.309393	1.921271
12	1	0	0.857286	1.936794	-1.793607
13	1	0	-1.881616	1.238891	-1.637559
14	1	0	-0.574861	2.556197	0.411784
15	1	0	1.924413	1.766483	1.169957
16	5	0	1.140112	1.020266	0.686379
17	8	0	-1.870897	-0.477721	-0.175631
18	1	0	-1.679490	-0.006885	0.983148
19	6	0	0.526812	-1.468731	-0.309323
20	6	0	-0.380423	1.498687	0.284950
21	5	0	0.266164	-0.531994	-1.557625
22	5	0	-0.307996	0.461103	1.561295

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pP1-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.677782	0.291769	-0.769318

2	5	0	0.724678	1.375751	0.704011
3	5	0	0.704582	1.093408	-1.053122
4	5	0	0.634598	-0.267782	1.399788
5	5	0	-0.655045	-1.324484	0.636138
6	1	0	-1.103155	2.385316	-0.346164
7	1	0	-2.491171	0.680797	-1.551836
8	1	0	1.146624	2.388755	1.148556
9	1	0	-1.460648	1.077436	2.144756
10	1	0	1.980101	-1.107477	-2.064798
11	1	0	1.061725	1.902271	-1.844169
12	1	0	1.063499	-0.595248	2.456953
13	1	0	-1.010812	-2.171837	1.403765
14	1	0	1.511883	-2.181401	0.430157
15	1	0	2.882643	0.117489	0.037395
16	5	0	1.699082	0.099400	-0.038454
17	8	0	-1.675931	-0.994608	-0.376691
18	1	0	0.021007	-0.713927	-2.043243
19	6	0	-0.676450	1.397852	-0.205274
20	6	0	0.867838	-1.370849	0.110426
21	5	0	-0.737969	0.692926	1.290973
22	5	0	1.039341	-0.758453	-1.407768

NH3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.116642
2	1	0	0.000000	0.939810	-0.272164
3	1	0	0.813899	-0.469905	-0.272164
4	1	0	-0.813899	-0.469905	-0.272164

H2BNH2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	-0.000000	-0.777939

2	7	0	-0.000000	0.000000	0.610392
3	1	0	0.000000	1.042824	-1.355341
4	1	0	-0.000000	-1.042824	-1.355341
5	1	0	0.000000	-0.842716	1.163816
6	1	0	0.000000	0.842716	1.163816

1,2-C2B8H10

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.883154	1.383431	0.000000
2	5	0	0.719585	1.331678	0.000000
3	5	0	-0.354290	0.634711	1.314632
4	5	0	-0.354290	0.634711	-1.314632
5	5	0	1.195816	-0.145483	0.924850
6	5	0	-0.354290	-1.143280	0.913649
7	5	0	-0.354290	-1.143280	-0.913649
8	5	0	1.195816	-0.145483	-0.924850
9	1	0	-1.577628	2.205172	0.000000
10	1	0	1.315360	2.348409	0.000000
11	1	0	-0.753551	0.991800	2.363115
12	1	0	-2.401178	-0.235352	0.000000
13	1	0	-0.753551	0.991800	-2.363115
14	1	0	2.068990	-0.070215	1.718874
15	1	0	-0.906781	-1.851829	1.680099
16	1	0	-0.906781	-1.851829	-1.680099
17	1	0	2.068990	-0.070215	-1.718874
18	1	0	1.631045	-2.564067	-0.000000
19	6	0	-1.332799	-0.081955	0.000000
20	5	0	1.008103	-1.564080	-0.000000

1,6-C2B8H10

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.872854	-1.418872	0.000000
2	5	0	-1.189437	-0.141669	0.919511

3	5	0	-1.189437	-0.141669	-0.919511
4	5	0	0.371049	-1.096961	0.935384
5	5	0	-0.708770	1.355432	-0.000000
6	5	0	0.371049	0.647004	-1.300984
7	5	0	0.371049	0.647004	1.300984
8	1	0	-1.419788	-2.345683	0.000000
9	1	0	-2.086701	-0.159698	1.684193
10	1	0	-2.086701	-0.159698	-1.684193
11	1	0	0.860290	-1.883187	-1.662668
12	1	0	0.860290	-1.883187	1.662668
13	1	0	-1.424687	2.295299	-0.000000
14	1	0	0.749878	0.943584	-2.378910
15	1	0	2.404208	-0.242966	0.000000
16	1	0	0.749878	0.943584	2.378910
17	1	0	1.726014	2.458391	-0.000000
18	5	0	0.967910	1.558623	-0.000000
19	6	0	1.347023	-0.017869	0.000000
20	5	0	0.371049	-1.096961	-0.935384

1,10-C2B8H10

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.669032
2	5	0	0.000000	1.308292	0.753306
3	5	0	-1.308292	0.000000	0.753306
4	5	0	1.308292	-0.000000	0.753306
5	5	0	-0.925102	0.925102	-0.753306
6	5	0	-0.925102	-0.925102	-0.753306
7	5	0	0.925102	0.925102	-0.753306
8	1	0	0.000000	0.000000	2.745969
9	1	0	0.000000	2.380689	1.244939
10	1	0	-2.380689	0.000000	1.244939
11	1	0	-0.000000	-2.380689	1.244939
12	1	0	2.380689	-0.000000	1.244939
13	1	0	-1.683402	1.683402	-1.244939
14	1	0	-1.683402	-1.683402	-1.244939
15	1	0	1.683402	-1.683402	-1.244939
16	1	0	1.683402	1.683402	-1.244939
17	1	0	0.000000	0.000000	-2.745969

18	5	0	-0.000000	-1.308292	0.753306
19	6	0	0.000000	0.000000	-1.669032
20	5	0	0.925102	-0.925102	-0.753306

oTS1-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.366010	-1.403732	-0.219307
2	5	0	-1.023153	-0.397015	0.839029
3	5	0	1.200732	-1.144266	-0.663161
4	5	0	0.353240	0.623214	1.335380
5	5	0	0.671399	-1.133715	1.027103
6	5	0	1.328825	0.604627	-1.122069
7	5	0	-0.210912	1.208319	-0.408778
8	5	0	1.278787	1.591156	0.251079
9	1	0	-0.774416	-2.350316	-0.539205
10	1	0	-1.782809	-0.712904	1.690447
11	1	0	1.730390	-1.990263	-1.289691
12	1	0	-0.572866	-0.374757	-2.191759
13	1	0	0.242213	1.071545	2.427443
14	1	0	0.796230	-1.982394	1.838048
15	1	0	1.841413	0.876884	-2.153657
16	1	0	-0.979434	2.033503	-0.772104
17	1	0	1.795242	2.631458	0.458699
18	1	0	2.986832	-0.133132	0.969098
19	6	0	-0.152110	-0.240605	-1.204945
20	5	0	1.897503	0.018771	0.531554
21	1	0	-2.915692	0.654325	-1.031808
22	7	0	-2.867666	0.355513	-0.061761
23	1	0	-3.097076	1.158177	0.517541
24	1	0	-3.569747	-0.360143	0.104097

oA-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.511938	-1.314581	-0.415939
2	5	0	-1.459129	-0.457157	0.577747
3	5	0	1.168246	-1.244021	-0.335412
4	5	0	-0.038436	0.697629	1.231217
5	5	0	0.177163	-1.053078	1.112441
6	5	0	1.702547	0.398158	-0.797226
7	5	0	0.119421	1.221810	-0.784245
8	5	0	1.223286	1.528008	0.395038
9	1	0	-0.775417	-2.288611	-0.810795
10	1	0	-2.170919	-1.022384	1.355623
11	1	0	1.748328	-2.206495	-0.692845
12	1	0	0.130862	-0.497919	-2.397636
13	1	0	-0.416502	1.284789	2.195509
14	1	0	0.016167	-1.863904	1.953380
15	1	0	2.594121	0.479250	-1.570929
16	1	0	-0.415088	2.084590	-1.414851
17	1	0	1.699745	2.556223	0.730256
18	1	0	2.497437	-0.279726	1.699632
19	6	0	0.171847	-0.279995	-1.337969
20	5	0	1.606179	-0.063708	0.951051
21	1	0	-2.043307	1.002744	-0.996215
22	7	0	-2.465883	0.549431	-0.181571
23	1	0	-2.755389	1.290531	0.455864
24	1	0	-3.304696	0.044146	-0.465614

oTS2-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.305391	-1.150743	-0.868747
2	5	0	-1.586048	-0.738726	0.016070
3	5	0	1.296386	-1.084095	-0.288645
4	5	0	-0.448329	0.113841	1.568527
5	5	0	-0.071814	-1.342806	0.831782
6	5	0	1.733681	0.619583	-0.217467
7	5	0	0.295429	1.424578	-0.886122
8	5	0	0.556622	1.449077	0.790015
9	1	0	-0.354506	-2.039497	-1.485971
10	1	0	-2.402886	-1.588153	0.191420
11	1	0	2.056914	-1.928803	-0.599603

12	1	0	0.976463	-0.172506	-2.428116
13	1	0	-1.111347	0.436405	2.491379
14	1	0	-0.223401	-2.414943	1.304059
15	1	0	2.812013	0.968188	-0.551267
16	1	0	0.037855	2.350724	-1.574128
17	1	0	0.716568	2.445955	1.408894
18	1	0	1.986421	-0.296624	2.145820
19	6	0	0.625552	-0.018655	-1.416653
20	5	0	1.220019	-0.147151	1.255460
21	1	0	-0.913653	1.295981	0.091872
22	7	0	-2.150585	0.680398	-0.266524
23	1	0	-2.833448	0.993397	0.417942
24	1	0	-2.593589	0.731975	-1.182343

oP1-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.765117	1.087599	0.767406
2	5	0	0.750129	0.665849	1.266687
3	5	0	-1.698009	-0.091927	0.000000
4	5	0	0.750129	-1.335378	0.913782
5	5	0	-0.646834	-0.466556	1.382294
6	5	0	-0.646834	-0.466556	-1.382294
7	5	0	0.750129	0.665849	-1.266687
8	5	0	0.750129	-1.335378	-0.913782
9	1	0	-1.368586	1.816117	1.288885
10	1	0	1.164129	1.058500	2.308136
11	1	0	-2.874596	-0.033244	0.000000
12	1	0	-1.368586	1.816117	-1.288885
13	1	0	1.247144	-2.133761	1.631974
14	1	0	-1.055499	-0.648514	2.475232
15	1	0	-1.055499	-0.648514	-2.475232
16	1	0	1.164129	1.058500	-2.308136
17	1	0	1.247144	-2.133761	-1.631974
18	1	0	-1.344595	-2.613984	0.000000
19	6	0	-0.765117	1.087599	-0.767406
20	5	0	-0.733810	-1.601672	0.000000
21	1	0	1.652470	-1.109967	0.000000
22	7	0	1.595616	1.076889	0.000000

23	1	0	1.681517	2.094826	0.000000
24	1	0	2.547771	0.717114	0.000000

oTS3-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.346169	-1.369967	-0.738759
2	5	0	1.837773	-0.005486	-0.750753
3	5	0	-1.708850	-0.487423	-0.648386
4	5	0	0.718479	1.346441	-0.717827
5	5	0	-0.117802	-0.060597	-1.497745
6	5	0	-1.515601	0.338344	0.866759
7	5	0	0.002443	-0.266982	1.588040
8	5	0	-0.200961	1.441489	0.958161
9	1	0	-0.326237	-2.361024	-1.168117
10	1	0	2.345215	-0.479463	-1.715306
11	1	0	-2.776337	-0.837359	-1.009473
12	1	0	-1.349456	-2.100000	1.095323
13	1	0	1.031498	2.361962	-1.247571
14	1	0	-0.013663	-0.058376	-2.676505
15	1	0	-2.370812	0.504666	1.667272
16	1	0	0.486332	-0.557454	2.620013
17	1	0	-0.304152	2.415178	1.622968
18	1	0	-1.732712	2.061837	-1.068279
19	6	0	-0.857481	-1.236215	0.666910
20	5	0	-1.061377	1.213846	-0.592002
21	1	0	1.029867	1.370749	0.591126
22	7	0	2.297988	-0.458052	0.537484
23	1	0	2.937833	-1.237978	0.599894
24	1	0	2.408088	0.162561	1.326127

oB-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.278544	-1.194294	-0.341632

2	5	0	2.291264	0.293436	-0.357119
3	5	0	-1.351613	-0.118991	-1.242918
4	5	0	0.866734	1.339611	0.138421
5	5	0	0.448466	0.123749	-1.022827
6	5	0	-1.954192	0.430688	0.413032
7	5	0	-0.848183	-0.787122	1.183407
8	5	0	-0.503638	1.003121	1.258582
9	1	0	0.018478	-2.181048	-0.671644
10	1	0	3.047823	0.862697	-1.070498
11	1	0	-1.788172	-0.257239	-2.328570
12	1	0	-2.497099	-1.887959	-0.175290
13	1	0	1.441525	2.377156	0.146174
14	1	0	0.969394	0.030155	-2.093264
15	1	0	-3.005116	0.846777	0.750416
16	1	0	-0.921944	-1.496808	2.127067
17	1	0	-0.751848	1.744593	2.149404
18	1	0	-1.027338	2.424707	-1.018421
19	6	0	-1.795944	-1.079606	-0.061195
20	5	0	-0.727771	1.396794	-0.516250
21	1	0	0.791733	0.793454	1.327823
22	7	0	2.743810	-0.794860	0.380895
23	1	0	3.700008	-1.112000	0.342840
24	1	0	2.157485	-1.343498	0.993018

oTS4-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.289398	-1.248414	-0.018117
2	5	0	-2.398622	0.484517	-0.145900
3	5	0	1.364302	-0.526678	1.155540
4	5	0	-0.866577	1.332480	0.237173
5	5	0	-0.418694	-0.193003	0.997400
6	5	0	1.999964	0.509778	-0.231459
7	5	0	0.903037	-0.359310	-1.378260
8	5	0	0.598283	1.350219	-0.887609
9	1	0	-0.005158	-2.290127	-0.020120
10	1	0	-3.174603	1.307669	-0.525320
11	1	0	1.800272	-1.012571	2.136597
12	1	0	2.473435	-1.896592	-0.422548

13	1	0	-1.255653	2.392113	0.601316
14	1	0	-1.034006	-0.589426	1.929966
15	1	0	3.070554	0.977486	-0.392184
16	1	0	0.964265	-0.757167	-2.489439
17	1	0	0.902070	2.331590	-1.478836
18	1	0	1.021213	1.971565	1.716795
19	6	0	1.794043	-1.073730	-0.277882
20	5	0	0.748220	1.141678	0.921156
21	1	0	-0.697835	1.203539	-1.070899
22	7	0	-2.864658	-0.820476	-0.171943
23	1	0	-3.798865	-1.026105	-0.492485
24	1	0	-2.363291	-1.634183	0.146550

oC-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.560808	-1.267290	-0.240477
2	5	0	-2.088905	-0.221628	-0.527367
3	5	0	1.280501	-0.573267	1.198507
4	5	0	-0.975291	1.075936	0.094281
5	5	0	-0.484195	-0.464160	0.742650
6	5	0	1.990534	0.706757	0.074532
7	5	0	1.247902	-0.159223	-1.334628
8	5	0	0.598965	1.427276	-0.740301
9	1	0	0.415386	-2.325351	-0.411040
10	1	0	-1.873881	-0.739298	-1.577609
11	1	0	1.590627	-1.110967	2.199953
12	1	0	2.867050	-1.562285	-0.249808
13	1	0	-1.708865	1.943628	0.433494
14	1	0	-1.117766	-1.059629	1.550826
15	1	0	2.984562	1.335321	0.165605
16	1	0	1.573654	-0.379166	-2.449143
17	1	0	0.827613	2.501696	-1.186351
18	1	0	0.497768	1.763042	1.961037
19	6	0	2.050161	-0.867012	-0.159211
20	5	0	0.479412	1.027601	1.035017
21	1	0	-0.616250	1.130056	-1.166538
22	7	0	-3.370112	-0.301193	0.000357
23	1	0	-4.118574	-0.783624	-0.471880

24	1	0	-3.640961	0.104279	0.883631

oTS5-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.449148	-1.480808	0.296596
2	5	0	2.070077	0.094826	0.576512
3	5	0	-1.450200	-0.919441	-0.907545
4	5	0	0.985099	0.887235	-0.512481
5	5	0	0.394109	-0.820646	-0.778009
6	5	0	-1.983926	0.588459	-0.210996
7	5	0	-1.255293	0.632846	1.403572
8	5	0	-0.658821	1.658671	0.168308
9	1	0	-0.385264	-2.519394	0.590514
10	1	0	1.787018	-0.153319	1.713134
11	1	0	-2.155963	-1.580517	-1.582168
12	1	0	-2.485999	-1.346563	1.197774
13	1	0	1.561393	1.666959	-1.204983
14	1	0	1.089949	-1.475121	-1.481260
15	1	0	-3.082834	0.991878	-0.366703
16	1	0	-1.409109	0.866479	2.548683
17	1	0	-0.704107	2.839063	0.207722
18	1	0	-0.676146	1.092786	-2.380041
19	6	0	-1.693658	-0.757485	0.757217
20	5	0	-0.565606	0.626800	-1.299443
21	1	0	0.213727	1.172895	0.949117
22	7	0	3.377460	-0.180692	0.178525
23	1	0	4.062351	-0.597201	0.789559
24	1	0	3.722415	-0.007093	-0.753487

oD-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.631140	-1.407832	-0.590747
2	5	0	-2.125995	0.157313	-0.532186

3	5	0	1.589507	-0.969616	0.727658
4	5	0	-1.098005	0.535842	0.782604
5	5	0	-0.239861	-1.119105	0.598863
6	5	0	1.930399	0.698359	0.329534
7	5	0	1.242055	1.008139	-1.246859
8	5	0	0.415539	1.603554	0.127305
9	1	0	0.681821	-2.361124	-1.100526
10	1	0	-1.793208	0.131950	-1.683540
11	1	0	2.382917	-1.645802	1.278039
12	1	0	2.633930	-0.856359	-1.404009
13	1	0	-1.683279	0.924382	1.745692
14	1	0	-0.879197	-1.971836	1.121908
15	1	0	2.979418	1.145890	0.634077
16	1	0	1.578776	1.560145	-2.233131
17	1	0	0.217600	2.764968	0.232558
18	1	0	0.623919	0.601861	2.532846
19	6	0	1.776720	-0.473330	-0.867901
20	5	0	0.507373	0.327242	1.388482
21	1	0	-0.047714	1.209409	-1.025250
22	7	0	-3.465590	-0.131246	-0.270878
23	1	0	-4.130836	-0.380120	-0.986778
24	1	0	-3.857239	-0.126309	0.659149

oTS6-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.724896	-1.178247	-0.940804
2	5	0	-2.286398	0.401381	0.268940
3	5	0	1.853455	-0.766037	0.295368
4	5	0	-0.946847	-0.151202	1.203428
5	5	0	0.227456	-1.501498	0.438871
6	5	0	1.551876	0.969897	0.282691
7	5	0	0.533585	1.492522	-1.007832
8	5	0	-0.153827	1.286557	0.678378
9	1	0	0.860138	-1.931218	-1.709539
10	1	0	-2.952453	1.313081	0.640179
11	1	0	2.918818	-1.230819	0.488284
12	1	0	2.242816	0.119956	-1.879178
13	1	0	-1.599401	-0.562025	2.115038

14	1	0	-0.069692	-2.591733	0.795881
15	1	0	2.462401	1.677481	0.534997
16	1	0	0.927067	2.480490	-1.530321
17	1	0	-0.609653	2.294917	1.094863
18	1	0	1.054663	-0.211309	2.619693
19	6	0	1.464318	0.078037	-1.128246
20	5	0	0.709255	-0.121902	1.490284
21	1	0	-0.630695	1.261077	-1.159155
22	7	0	-2.754518	-0.383131	-0.780857
23	1	0	-3.639915	-0.204890	-1.229913
24	1	0	-2.260536	-1.180423	-1.151171

P2-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.052523	-0.881177	-1.077916
2	5	0	-1.711368	0.765742	-0.409586
3	5	0	1.844570	-0.453147	0.329785
4	5	0	-1.212297	-0.734142	0.804901
5	5	0	0.488438	-1.599496	0.125744
6	5	0	1.076821	1.080172	0.672819
7	5	0	-0.083984	1.553025	-0.620123
8	5	0	-0.645529	1.009632	0.996525
9	1	0	1.556498	-1.368260	-1.904083
10	1	0	-2.703414	1.411819	-0.430394
11	1	0	2.987012	-0.613545	0.573081
12	1	0	2.047121	1.030696	-1.537616
13	1	0	-1.930586	-1.176988	1.638729
14	1	0	0.472182	-2.778750	0.245493
15	1	0	1.736806	1.950964	1.119150
16	1	0	-0.040148	2.707020	-0.882999
17	1	0	-1.027890	1.731612	1.852929
18	1	0	0.511479	-0.662174	2.559308
19	6	0	1.278665	0.577758	-0.924331
20	5	0	0.415239	-0.398870	1.409836
21	7	0	-1.890995	-0.765133	-0.618417
22	1	0	-0.967343	1.111753	-1.470022
23	1	0	-1.392842	-1.218105	-1.371662
24	1	0	-2.858491	-1.064166	-0.599012

oTS7-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.032680	0.703863	-1.308115
2	5	0	-0.075334	1.641718	-0.072898
3	5	0	1.022673	-0.667171	-1.155582
4	5	0	1.090126	0.894077	1.247947
5	5	0	1.467101	0.898402	-0.450630
6	5	0	0.244047	-1.549065	0.174676
7	5	0	-1.759312	-0.755244	0.069566
8	5	0	0.433263	-0.731858	1.613447
9	1	0	-0.099024	1.095638	-2.314287
10	1	0	-0.571335	2.691179	0.106547
11	1	0	1.518907	-1.104704	-2.131026
12	1	0	-0.911486	-1.251803	-1.980352
13	1	0	1.615881	1.610870	2.026759
14	1	0	2.231226	1.690718	-0.886524
15	1	0	0.218413	-2.728918	0.085601
16	1	0	-2.304895	-1.774091	0.342420
17	1	0	0.418084	-1.131201	2.727730
18	1	0	2.836987	-0.971816	0.628649
19	6	0	-0.675511	-0.701629	-1.073617
20	5	0	1.746486	-0.546246	0.460434
21	1	0	-0.085820	0.533836	1.640439
22	7	0	-2.286869	0.518838	0.510131
23	1	0	-3.002491	0.537312	1.222703
24	1	0	-2.452473	1.234655	-0.183978

oE-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.012219	0.413557	-1.270586
2	5	0	0.342801	1.604766	-0.329091
3	5	0	0.892072	-1.047992	-0.939586

4	5	0	1.524380	1.052501	0.885216
5	5	0	1.668096	0.556315	-0.774262
6	5	0	0.137275	-1.463958	0.603444
7	5	0	-2.113904	-0.545863	0.112403
8	5	0	0.524626	-0.296607	1.707690
9	1	0	-0.195079	0.638508	-2.314146
10	1	0	0.065506	2.745478	-0.472441
11	1	0	1.195934	-1.787285	-1.805219
12	1	0	-1.065768	-1.540936	-1.499897
13	1	0	2.196491	1.807204	1.494035
14	1	0	2.494638	0.895311	-1.545329
15	1	0	-0.003329	-2.616177	0.843180
16	1	0	-2.737117	-1.488501	0.482968
17	1	0	0.321498	-0.048049	2.843449
18	1	0	2.768575	-1.152853	0.872911
19	6	0	-0.796257	-0.818635	-0.723863
20	5	0	1.767034	-0.628426	0.520118
21	1	0	0.208224	1.268809	1.030996
22	7	0	-2.631618	0.728342	0.325166
23	1	0	-3.484972	0.877287	0.838566
24	1	0	-2.204315	1.579594	-0.008205

oTS8-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.570071	-0.988155	-0.881878
2	5	0	-1.895074	-0.425619	-0.226434
3	5	0	0.996941	-1.319533	-0.299585
4	5	0	-0.447312	0.131925	1.612999
5	5	0	-0.335872	-1.340286	0.827327
6	5	0	1.879495	0.226844	-0.254309
7	5	0	0.792223	1.426774	-0.877763
8	5	0	1.048564	1.292704	0.861902
9	1	0	-0.739904	-1.858326	-1.508959
10	1	0	-2.766479	-1.200271	0.008241
11	1	0	1.534540	-2.298361	-0.675334
12	1	0	0.838939	-0.227362	-2.421030
13	1	0	-1.056683	0.669722	2.459919
14	1	0	-0.622074	-2.406648	1.250648

15	1	0	3.019886	0.206972	-0.557116
16	1	0	1.010588	2.384445	-1.536470
17	1	0	1.503259	2.145808	1.539429
18	1	0	1.771070	-0.700618	2.172436
19	6	0	0.542421	-0.025088	-1.399416
20	5	0	1.153426	-0.412454	1.200673
21	1	0	0.047985	1.765238	0.170885
22	7	0	-2.212757	0.965095	-0.139074
23	1	0	-3.131378	1.247831	0.162817
24	1	0	-1.716503	1.693580	-0.628234

oP3-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.376550	1.289739	-0.695109
2	5	0	1.741969	0.504870	-0.518381
3	5	0	-0.804200	1.341023	0.521265
4	5	0	1.158333	-0.782821	0.849277
5	5	0	0.834849	0.972364	0.957746
6	5	0	-1.835221	-0.064370	0.335100
7	5	0	-1.363399	-0.901918	-1.108402
8	5	0	-0.921235	-1.522214	0.476726
9	1	0	0.484463	2.301602	-1.065387
10	1	0	2.792083	1.036032	-0.664971
11	1	0	-1.306235	2.364498	0.822382
12	1	0	-1.585073	1.257458	-1.715058
13	1	0	1.833298	-1.307462	1.668946
14	1	0	1.315126	1.790625	1.663048
15	1	0	-2.966683	0.128718	0.614862
16	1	0	-2.069546	-1.409600	-1.910600
17	1	0	-1.218938	-2.575032	0.923070
18	1	0	-0.590339	-0.266364	2.607939
19	6	0	-0.989960	0.624095	-1.068699
20	5	0	-0.431983	-0.160867	1.439761
21	1	0	-0.473294	-1.763023	-0.748538
22	7	0	1.693750	-1.014264	-0.626605
23	1	0	2.605679	-1.454511	-0.640711
24	1	0	1.108099	-1.416420	-1.351361

oTS9-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.072314	1.345196	-0.430324
2	5	0	1.981357	0.187367	-0.657074
3	5	0	-0.445544	1.443442	0.267053
4	5	0	0.771495	-1.162730	0.783373
5	5	0	1.036475	0.757061	1.066797
6	5	0	-1.852689	0.276566	0.361040
7	5	0	-1.633025	-0.635726	-1.130903
8	5	0	-1.168671	-1.350574	0.500483
9	1	0	1.455687	2.345722	-0.596778
10	1	0	3.151159	0.313484	-0.819293
11	1	0	-0.751625	2.532647	0.619751
12	1	0	-1.610823	1.557621	-1.696855
13	1	0	1.318210	-1.907270	1.526586
14	1	0	1.495287	1.355941	1.978324
15	1	0	-2.814920	0.725543	0.878619
16	1	0	-2.398899	-1.097732	-1.906525
17	1	0	-1.745760	-2.268338	0.973326
18	1	0	-0.634541	-0.165200	2.563105
19	6	0	-1.192760	0.802657	-1.043902
20	5	0	-0.420197	-0.072932	1.402762
21	1	0	-0.874398	-1.640308	-0.723022
22	7	0	1.413340	-1.221712	-0.677308
23	1	0	2.128009	-1.939999	-0.727629
24	1	0	0.765908	-1.359606	-1.450753

oF-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.483999	1.178624	-0.301493
2	5	0	2.094763	-0.106676	-0.708448
3	5	0	-0.174572	1.483969	0.021680
4	5	0	0.549473	-1.279616	0.760406

5	5	0	1.112027	0.683328	1.127594
6	5	0	-1.764707	0.547759	0.402024
7	5	0	-1.824033	-0.461950	-1.066106
8	5	0	-1.379006	-1.179058	0.571353
9	1	0	2.065382	2.091327	-0.361570
10	1	0	3.247902	-0.297624	-0.918883
11	1	0	-0.333640	2.622260	0.323597
12	1	0	-1.564782	1.636832	-1.751199
13	1	0	1.054432	-2.104523	1.446711
14	1	0	1.550274	1.200649	2.099155
15	1	0	-2.616389	1.156703	0.949586
16	1	0	-2.713695	-0.855230	-1.740645
17	1	0	-2.083455	-1.952353	1.123604
18	1	0	-0.639793	-0.065968	2.573269
19	6	0	-1.156355	0.874974	-1.096450
20	5	0	-0.401580	-0.025541	1.413195
21	1	0	-1.184346	-1.574956	-0.624648
22	7	0	1.160377	-1.307449	-0.714860
23	1	0	1.619274	-2.192862	-0.904834
24	1	0	0.448505	-1.144768	-1.430952

oTS10-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.452869	1.231385	-0.103349
2	5	0	1.852695	0.144797	-1.031807
3	5	0	-0.291264	1.463246	0.126459
4	5	0	0.607210	-1.262214	0.818677
5	5	0	1.026810	0.700487	1.265115
6	5	0	-1.821296	0.396877	0.360630
7	5	0	-1.692297	-0.491859	-1.192534
8	5	0	-1.264409	-1.292989	0.427453
9	1	0	1.931462	2.201604	-0.189981
10	1	0	2.597921	0.172763	-1.959749
11	1	0	-0.486652	2.580285	0.479735
12	1	0	-1.669618	1.679275	-1.672738
13	1	0	1.070044	-2.080253	1.546835
14	1	0	1.338653	1.211514	2.289339
15	1	0	-2.756283	0.876891	0.902054
16	1	0	-2.498940	-0.944988	-1.931274

17	1	0	-1.932994	-2.178570	0.839861
18	1	0	-0.797155	-0.224202	2.550643
19	6	0	-1.196997	0.905651	-1.078068
20	5	0	-0.481770	-0.100759	1.414589
21	1	0	-0.923867	-1.528182	-0.780452
22	7	0	1.394870	-1.260312	-0.588988
23	1	0	2.243968	-1.814384	-0.459897
24	1	0	0.905742	-1.739714	-1.345868

oG-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.831574	-0.638507	0.239941
2	5	0	-0.838792	-0.905068	-0.971731
3	5	0	-0.317244	-0.969644	1.029979
4	5	0	-0.361166	1.537936	-0.327300
5	5	0	-1.533886	0.589583	1.001251
6	5	0	1.363566	-0.391058	0.998925
7	5	0	1.892633	-0.457903	-0.669065
8	5	0	1.533512	1.124267	0.078054
9	1	0	-2.645412	-1.310166	0.488732
10	1	0	-1.076342	-1.750793	-1.779701
11	1	0	-0.441484	-1.814227	1.852978
12	1	0	0.940923	-2.426509	-0.247463
13	1	0	-0.643650	2.676275	-0.512644
14	1	0	-2.143022	1.044702	1.911175
15	1	0	2.055453	-0.804038	1.862185
16	1	0	2.914289	-0.776613	-1.169771
17	1	0	2.352825	1.960977	0.236786
18	1	0	0.351568	1.659714	2.097494
19	6	0	0.734128	-1.363495	-0.244758
20	5	0	0.196299	0.941005	1.169646
21	1	0	1.571348	0.768527	-1.147836
22	7	0	-0.674148	0.565117	-1.551731
23	1	0	-1.587207	0.822890	-1.922006
24	1	0	-0.020178	0.659866	-2.327709

oTS11-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.731902	-0.254096	0.586503
2	5	0	-0.797562	-1.328864	-0.232422
3	5	0	-0.307236	-0.393297	1.438522
4	5	0	-0.942485	0.924876	-1.003901
5	5	0	-1.223525	1.141349	0.781165
6	5	0	1.333286	0.309934	0.955180
7	5	0	1.935349	-0.710082	-0.349165
8	5	0	1.681521	0.987634	-0.609305
9	1	0	-2.671004	-0.539377	1.045045
10	1	0	-1.161275	-2.460066	-0.311184
11	1	0	-0.416064	-0.742197	2.565377
12	1	0	1.062979	-2.086275	1.128421
13	1	0	-1.619833	1.652278	-1.655756
14	1	0	-1.811278	1.965529	1.392908
15	1	0	1.967691	0.498014	1.935358
16	1	0	2.946373	-1.291935	-0.542972
17	1	0	2.560262	1.685134	-0.984365
18	1	0	0.429285	2.744117	0.364318
19	6	0	0.757752	-1.242198	0.520154
20	5	0	0.278745	1.601021	0.081045
21	1	0	1.604449	-0.031759	-1.437427
22	7	0	-0.756531	-0.521625	-1.588730
23	1	0	-1.587036	-0.765898	-2.122891
24	1	0	0.045602	-0.661283	-2.201259

oH-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.669839	-0.070888	-0.563817
2	5	0	0.938183	-1.152153	0.573169
3	5	0	0.509696	-0.883893	-1.249532
4	5	0	1.165358	1.088173	0.523123
5	5	0	0.577436	0.954389	-1.170576
6	5	0	-1.143673	0.042154	-1.000593

7	5	0	-1.850167	-0.821429	0.455921
8	5	0	-1.869158	0.918770	0.496221
9	1	0	2.643883	-0.132133	-1.023002
10	1	0	1.518564	-2.143199	0.877985
11	1	0	0.730702	-1.559719	-2.193131
12	1	0	-0.809596	-2.410849	-0.555880
13	1	0	1.877893	1.984148	0.840037
14	1	0	0.945520	1.604325	-2.087297
15	1	0	-1.788692	-0.083454	-1.985710
16	1	0	-2.828314	-1.466520	0.620807
17	1	0	-2.948171	1.378705	0.671620
18	1	0	-0.793386	2.716961	-0.650681
19	6	0	-0.565504	-1.428983	-0.164826
20	5	0	-0.564354	1.667258	-0.139264
21	1	0	-1.665447	0.026662	1.440078
22	7	0	0.855401	-0.002473	1.642687
23	1	0	1.661884	-0.069241	2.258053
24	1	0	0.024739	0.104509	2.217825

oTS12-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.667550	-0.009413	0.457701
2	5	0	-1.067039	0.249248	-1.141273
3	5	0	-1.049278	-1.360495	-0.082435
4	5	0	-0.599211	1.182678	0.820423
5	5	0	-0.464800	-0.619357	1.414171
6	5	0	0.648697	-1.433450	0.340541
7	5	0	1.611769	-0.461251	-0.894175
8	5	0	2.076158	0.868803	0.260677
9	1	0	-2.689456	-0.026481	0.803986
10	1	0	-1.820739	0.230564	-2.062169
11	1	0	-1.698420	-2.326974	-0.278726
12	1	0	0.136926	-1.666086	-1.989718
13	1	0	-0.849568	2.019077	1.625723
14	1	0	-0.755377	-1.015470	2.488141
15	1	0	1.217885	-2.449818	0.535461
16	1	0	2.542800	-0.954492	-1.443337
17	1	0	3.074044	1.504009	0.312055

18	1	0	1.552790	0.069121	2.366825
19	6	0	0.146675	-0.923098	-1.201790
20	5	0	1.045532	0.237814	1.300526
21	1	0	1.850502	0.818442	-1.021032
22	7	0	-0.506284	1.668286	-0.711346
23	1	0	-1.242926	2.355370	-0.854867
24	1	0	0.341637	2.039862	-1.130666

oI-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.372261	1.420072	0.671508
2	5	0	0.213073	1.211280	-0.928515
3	5	0	-1.545497	0.770370	-0.258799
4	5	0	0.916662	0.466107	1.025732
5	5	0	-1.107610	0.114768	1.284499
6	5	0	-1.466125	-0.915879	-0.032541
7	5	0	0.049277	-1.526677	-0.870542
8	5	0	1.430648	-1.436913	0.243869
9	1	0	-0.510879	2.381090	1.145219
10	1	0	0.144309	2.111989	-1.706923
11	1	0	-2.500426	1.379538	-0.588378
12	1	0	-1.116471	-0.220319	-2.323867
13	1	0	1.545582	0.664153	2.011720
14	1	0	-1.673635	0.128863	2.319393
15	1	0	-2.364098	-1.670855	-0.171318
16	1	0	-0.048139	-2.526314	-1.503264
17	1	0	2.443662	-1.864900	0.671244
18	1	0	-0.012055	-2.030755	1.900067
19	6	0	-0.650743	-0.162627	-1.349198
20	5	0	-0.002155	-1.294871	0.967055
21	1	0	1.497486	-1.387010	-0.998955
22	7	0	1.686325	0.909429	-0.391638
23	1	0	2.126598	1.795949	-0.158544
24	1	0	2.360445	0.386975	-0.942574

oTS13-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.370004	-1.437310	0.630777
2	5	0	-0.253251	-1.184552	-0.938041
3	5	0	1.537005	-0.778493	-0.290442
4	5	0	-0.829014	-0.449813	1.089642
5	5	0	1.121874	-0.131683	1.266482
6	5	0	1.471231	0.911071	-0.050458
7	5	0	-0.051480	1.535246	-0.838778
8	5	0	-1.436069	1.343417	0.269408
9	1	0	0.507773	-2.407454	1.084956
10	1	0	-0.215999	-2.074789	-1.731287
11	1	0	2.487732	-1.383722	-0.639070
12	1	0	1.081827	0.241714	-2.341171
13	1	0	-1.480686	-0.680754	2.050911
14	1	0	1.714233	-0.180559	2.285567
15	1	0	2.379086	1.651781	-0.196821
16	1	0	0.038652	2.558993	-1.431595
17	1	0	-2.459085	1.732067	0.708559
18	1	0	0.031402	2.034370	1.900630
19	6	0	0.633323	0.176088	-1.359032
20	5	0	0.024298	1.271328	0.990292
21	1	0	-1.478895	1.402561	-0.975515
22	7	0	-1.713076	-0.838482	-0.395503
23	1	0	-2.172779	-1.691383	-0.087406
24	1	0	-2.384666	-0.348733	-0.980235

oP4-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.283874	-0.553638	-1.405750
2	5	0	0.579014	0.842547	-1.086382
3	5	0	-1.404806	-0.969273	-0.197518
4	5	0	-1.293637	0.659184	-0.857046
5	5	0	0.104821	0.736465	1.464841
6	1	0	-0.512639	-0.856548	-2.418113
7	1	0	0.780970	1.574205	-2.005593

8	1	0	-2.287678	-1.720531	-0.415550
9	1	0	0.178141	-2.832489	-0.537865
10	1	0	-0.588625	2.575045	0.247344
11	1	0	-2.049560	1.177428	-1.600503
12	1	0	-0.429876	-1.641100	2.197757
13	1	0	2.225996	-0.994017	1.540498
14	1	0	0.525588	1.230160	2.454808
15	1	0	-2.457755	0.718285	1.477579
16	1	0	1.502707	-1.663015	-0.067529
17	7	0	1.902993	0.442569	-0.311308
18	1	0	2.296825	1.266296	0.138191
19	1	0	2.628534	0.074742	-0.929238
20	5	0	0.216658	-1.660894	-0.343454
21	5	0	1.425897	-0.644644	0.734683
22	5	0	-0.347469	-0.910988	1.269250
23	5	0	-1.491858	0.396627	0.879661
24	6	0	-0.395571	1.511711	0.201950

mTS1-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.327391	1.477835	-0.355833
2	5	0	1.106242	0.623979	0.704209
3	5	0	-1.241188	1.109416	-0.694403
4	5	0	-0.171085	-0.526085	1.268499
5	5	0	-0.600494	1.208630	0.964451
6	5	0	-1.420156	-0.614239	-1.038501
7	5	0	-1.260778	-1.563175	0.381991
8	1	0	0.664021	2.447552	-0.689479
9	1	0	1.897136	1.074621	1.464021
10	1	0	-1.891048	1.929666	-1.241219
11	1	0	0.693498	0.129299	-2.362128
12	1	0	0.104211	-1.068032	2.287173
13	1	0	-0.735784	2.021565	1.810823
14	1	0	-1.993221	-1.073436	-1.965832
15	1	0	0.687005	-2.021786	-0.661250
16	1	0	-1.656465	-2.627780	0.696080
17	1	0	-2.897384	0.169370	1.161401
18	5	0	-1.850718	0.010981	0.632359

19	1	0	2.795072	-0.833989	-0.990390
20	7	0	2.814339	-0.427401	-0.058608
21	1	0	3.051034	-1.158766	0.606846
22	1	0	3.555377	0.267007	-0.028070
23	6	0	0.047898	-1.200289	-0.365574
24	5	0	0.193065	0.164742	-1.288459

mA-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.593744	1.327139	-0.464863
2	5	0	1.492213	0.450434	0.558983
3	5	0	-1.073314	1.308577	-0.445780
4	5	0	0.012346	-0.657104	1.127286
5	5	0	-0.110783	1.134349	1.026964
6	5	0	-1.693764	-0.288243	-0.842697
7	5	0	-1.436722	-1.387630	0.464270
8	1	0	0.953671	2.283989	-0.821137
9	1	0	2.233572	0.984720	1.335136
10	1	0	-1.628945	2.302047	-0.762196
11	1	0	0.162678	0.150159	-2.576444
12	1	0	0.394289	-1.360473	2.009152
13	1	0	0.039207	1.909180	1.904227
14	1	0	-2.570864	-0.536627	-1.596359
15	1	0	0.021726	-2.138540	-1.048298
16	1	0	-1.964708	-2.388490	0.796565
17	1	0	-2.467879	0.548899	1.681011
18	5	0	-1.616861	0.225280	0.924479
19	1	0	3.306833	-0.188682	-0.462606
20	7	0	2.459728	-0.652071	-0.135443
21	1	0	2.011897	-1.121492	-0.922976
22	1	0	2.739156	-1.359056	0.544343
23	6	0	-0.277490	-1.213362	-0.563771
24	5	0	-0.042364	0.173577	-1.405608

mTS2-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.524964	-1.222260	-0.754863
2	5	0	-1.714916	-0.531248	0.124123
3	5	0	1.064573	-1.311550	-0.358831
4	5	0	-0.276461	0.264329	1.549010
5	5	0	-0.216469	-1.297998	0.899031
6	5	0	1.766516	0.293385	-0.477151
7	5	0	1.027883	1.347734	0.728792
8	1	0	-0.834572	-2.142495	-1.232387
9	1	0	-2.637502	-1.251610	0.342993
10	1	0	1.673027	-2.294957	-0.596933
11	1	0	0.424926	-0.126127	-2.706876
12	1	0	-0.908673	0.857956	2.347649
13	1	0	-0.452769	-2.283412	1.508361
14	1	0	2.845511	0.529601	-0.894104
15	1	0	0.664474	2.246049	-1.344683
16	1	0	1.519074	2.276561	1.271201
17	1	0	2.022738	-0.576819	2.034083
18	5	0	1.314540	-0.296144	1.124867
19	1	0	-3.035463	0.929030	-0.589471
20	7	0	-2.103783	0.908865	-0.182207
21	1	0	-0.756791	1.198604	-0.758130
22	1	0	-2.098168	1.593826	0.566403
23	6	0	0.472129	1.361941	-0.744606
24	5	0	0.357868	-0.099777	-1.525009

mB-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.311564	1.360281	-0.711527
2	5	0	1.673900	0.512761	-0.556479
3	5	0	-0.843425	1.381099	0.502375
4	5	0	1.130716	-0.739868	0.859669
5	5	0	0.807535	1.057897	0.907592
6	5	0	-1.794324	-0.072915	0.287985
7	5	0	-0.715454	-1.502115	0.543163
8	1	0	0.508897	2.352261	-1.100969

9	1	0	2.735374	1.018992	-0.713589
10	1	0	-1.345117	2.385219	0.870251
11	1	0	-1.766575	1.134373	-2.009033
12	1	0	1.837973	-1.198026	1.692092
13	1	0	1.343541	1.878532	1.568259
14	1	0	-2.949542	-0.145578	0.521525
15	1	0	-2.008936	-1.626751	-1.402058
16	1	0	-0.984006	-2.544252	1.038021
17	1	0	-0.531956	-0.162652	2.646800
18	5	0	-0.434231	-0.097995	1.468744
19	1	0	2.611710	-1.396529	-0.608632
20	7	0	1.674082	-1.011789	-0.617430
21	1	0	-0.448652	-0.846316	-1.655414
22	1	0	1.098340	-1.545377	-1.253455
23	6	0	-1.213087	-1.090013	-0.899488
24	5	0	-1.106816	0.692539	-1.134189

mTS3-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.375325	1.314148	-0.762516
2	5	0	1.713812	0.436912	-0.544653
3	5	0	-0.811114	1.429793	0.393449
4	5	0	1.092681	-0.734305	0.895117
5	5	0	0.831828	1.086435	0.863934
6	5	0	-1.809046	0.001265	0.341902
7	5	0	-0.754105	-1.421758	0.628721
8	1	0	0.590879	2.283671	-1.196106
9	1	0	2.803757	0.885683	-0.677571
10	1	0	-1.286765	2.464763	0.708970
11	1	0	-1.674536	1.097431	-2.056078
12	1	0	1.796033	-1.193787	1.729484
13	1	0	1.388048	1.914479	1.498011
14	1	0	-2.969717	-0.057197	0.534213
15	1	0	-2.227235	-1.357835	-1.100084
16	1	0	-1.014738	-2.478323	1.096350
17	1	0	-0.515542	-0.005421	2.673887
18	5	0	-0.431849	-0.009352	1.492913
19	1	0	0.982907	-1.520782	-1.238728

20	7	0	1.607104	-1.073693	-0.583443
21	1	0	-0.804585	-1.666478	-1.683127
22	1	0	2.499874	-1.551803	-0.566310
23	6	0	-1.194913	-1.018359	-0.896319
24	5	0	-1.012323	0.596353	-1.208546

mC-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.453042	1.333200	-0.662966
2	5	0	1.766357	0.436559	-0.494254
3	5	0	-0.757768	1.410390	0.477590
4	5	0	1.047531	-0.859780	0.838807
5	5	0	0.863340	0.968509	0.954941
6	5	0	-1.815672	0.022421	0.313905
7	5	0	-0.931968	-1.427387	0.574741
8	1	0	0.688930	2.334980	-1.003014
9	1	0	2.864692	0.875418	-0.589544
10	1	0	-1.187627	2.447852	0.844920
11	1	0	-1.587173	1.331199	-1.995056
12	1	0	1.696130	-1.430801	1.648344
13	1	0	1.428526	1.724583	1.666287
14	1	0	-2.974487	0.067238	0.538929
15	1	0	-2.156312	-1.292530	-1.554718
16	1	0	-1.258283	-2.518321	0.881836
17	1	0	-0.558992	-0.197803	2.638201
18	5	0	-0.451451	-0.088386	1.463412
19	1	0	1.074070	-1.412915	-1.414743
20	7	0	1.626762	-1.071151	-0.636669
21	1	0	-0.502363	-1.577486	-1.040166
22	1	0	2.510294	-1.566572	-0.615489
23	6	0	-1.325783	-0.844887	-1.022320
24	5	0	-0.958030	0.694342	-1.216620

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mTS4-N

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-1.414519	-0.489556	-1.103253
2	5	0	1.843398	0.297827	-0.423117
3	5	0	-1.866267	0.191296	0.221991
4	5	0	-0.652476	0.807597	-1.311132
5	5	0	0.928614	0.782426	1.087041
6	1	0	-2.100464	-0.930058	-1.813540
7	1	0	2.983546	0.614870	-0.496614
8	1	0	-2.983343	0.321677	0.585683
9	1	0	-1.900831	-2.103711	0.897437
10	1	0	1.006195	2.339348	-0.743592
11	1	0	-0.988332	1.506027	-2.213732
12	1	0	-0.824808	-0.242017	2.549433
13	1	0	1.393155	-1.789983	1.576231
14	1	0	1.556300	1.400510	1.875407
15	1	0	-0.987390	2.491562	0.936799
16	1	0	-0.662981	-2.089851	-0.544557
17	7	0	1.484312	-1.152602	-0.653878
18	1	0	2.269027	-1.790912	-0.709020
19	1	0	0.831153	-1.323300	-1.415711
20	5	0	-1.085522	-1.421257	0.361304
21	5	0	0.853057	-1.074251	0.802419
22	5	0	-0.522919	-0.113741	1.413096
23	5	0	-0.584065	1.437475	0.586424
24	6	0	0.656101	1.344088	-0.496282

mD-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.397286	-0.402154	-1.122266
2	5	0	1.824055	0.281547	-0.423923
3	5	0	-1.895390	0.177350	0.225828
4	5	0	-0.572216	0.840840	-1.359701
5	5	0	0.949910	0.750072	1.109226
6	1	0	-2.076581	-0.801897	-1.865753
7	1	0	2.964604	0.584450	-0.535270
8	1	0	-3.003876	0.335206	0.601324
9	1	0	-2.029370	-1.848483	0.868950

10	1	0	1.034459	2.357689	-0.672048
11	1	0	-0.819064	1.552901	-2.281448
12	1	0	-0.851005	-0.291087	2.538245
13	1	0	1.368998	-1.829614	1.562134
14	1	0	1.592991	1.348071	1.901207
15	1	0	-1.011465	2.455261	1.002644
16	1	0	-0.685090	-2.402620	-0.300937
17	7	0	1.437513	-1.164368	-0.662588
18	1	0	2.212187	-1.811437	-0.749490
19	1	0	0.738697	-1.334610	-1.385745
20	5	0	-1.083658	-1.427877	0.254775
21	5	0	0.842178	-1.093185	0.798495
22	5	0	-0.520144	-0.138352	1.412808
23	5	0	-0.557721	1.419822	0.658655
24	6	0	0.658427	1.366432	-0.448820

mTS5-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.336861	-0.434741	-1.167615
2	5	0	1.856182	0.304191	-0.450704
3	5	0	-1.848733	0.254795	0.155111
4	5	0	-0.585741	0.877874	-1.291993
5	5	0	0.899595	0.721754	1.163361
6	1	0	-2.027531	-0.780687	-1.926035
7	1	0	2.999411	0.598184	-0.556859
8	1	0	-2.976468	0.393735	0.478620
9	1	0	-2.058026	-1.994187	0.704300
10	1	0	1.100265	2.358960	-0.564648
11	1	0	-0.841095	1.645136	-2.164047
12	1	0	-0.908075	-0.307631	2.531842
13	1	0	1.227328	-1.966320	1.522037
14	1	0	1.574748	1.220865	1.995111
15	1	0	-0.953469	2.477126	1.016306
16	1	0	-0.430903	-2.292006	-0.154939
17	7	0	1.449068	-1.136989	-0.639763
18	1	0	2.210974	-1.799561	-0.734917
19	1	0	0.763408	-1.258225	-1.395610
20	5	0	-1.141795	-1.400576	0.218397

21	5	0	0.726821	-1.202650	0.768756
22	5	0	-0.564997	-0.155731	1.409387
23	5	0	-0.563586	1.424133	0.646829
24	6	0	0.718066	1.358837	-0.393809

mE-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.156525	0.574492	-1.227939
2	5	0	-1.872271	-0.402571	-0.532451
3	5	0	1.829720	-0.219766	0.076793
4	5	0	0.640194	-0.881984	-1.222876
5	5	0	-0.744161	-0.705124	1.237011
6	1	0	1.823269	0.855781	-2.035260
7	1	0	-2.998735	-0.742338	-0.678357
8	1	0	2.990252	-0.367002	0.252881
9	1	0	1.914687	2.290735	0.363477
10	1	0	-1.087507	-2.398085	-0.410272
11	1	0	0.931776	-1.666022	-2.065037
12	1	0	1.042190	0.367297	2.520056
13	1	0	-1.338081	1.817376	1.637175
14	1	0	-1.466685	-1.053953	2.103287
15	1	0	1.014160	-2.498129	0.954919
16	1	0	0.090858	2.164658	0.438617
17	7	0	-1.530771	1.058090	-0.570666
18	1	0	-2.311895	1.696595	-0.682915
19	1	0	-0.804111	1.205983	-1.301230
20	5	0	1.157906	1.415625	0.089094
21	5	0	-0.730716	1.236163	0.799391
22	5	0	0.718074	0.137506	1.404508
23	5	0	0.675115	-1.431586	0.576137
24	6	0	-0.732208	-1.377966	-0.312181

mTS6-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.977977	0.539964	-1.346144
2	5	0	-1.736349	-0.545884	-0.668990
3	5	0	1.822445	-0.135838	-0.109244
4	5	0	0.517870	-0.935159	-1.190308
5	5	0	-0.558156	-0.648997	1.411280
6	1	0	1.525010	0.787633	-2.248189
7	1	0	-2.683051	-0.948070	-1.264185
8	1	0	2.997524	-0.270492	-0.059635
9	1	0	1.783729	2.400121	0.018222
10	1	0	-0.995793	-2.485604	-0.109129
11	1	0	0.738402	-1.765938	-2.006777
12	1	0	1.300755	0.615005	2.376486
13	1	0	-1.233538	1.844570	1.695581
14	1	0	-1.203936	-0.943246	2.354157
15	1	0	1.247965	-2.367352	1.045759
16	1	0	0.001136	2.227897	0.355793
17	7	0	-1.660923	0.954519	-0.410677
18	1	0	-2.587698	1.351794	-0.263455
19	1	0	-1.261386	1.391831	-1.249643
20	5	0	1.048926	1.471688	-0.103114
21	5	0	-0.685150	1.260377	0.816169
22	5	0	0.856656	0.265825	1.334366
23	5	0	0.804414	-1.352084	0.635286
24	6	0	-0.703965	-1.443202	-0.053434

mTS7-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.874122	-0.586196	-1.244941
2	5	0	-0.349333	0.880250	-1.269635
3	5	0	-1.332830	-1.096373	0.293209
4	5	0	-1.857708	0.445876	-0.320633
5	5	0	0.552823	0.836482	0.982448
6	1	0	-1.305234	-1.040226	-2.127030
7	1	0	-0.054900	1.520253	-2.215810
8	1	0	-2.079051	-1.993260	0.459970
9	1	0	0.224440	-2.728571	-0.651208
10	1	0	-0.828516	2.548844	0.274227

11	1	0	-2.944615	0.773533	-0.634668
12	1	0	0.410393	-1.464474	2.201721
13	1	0	2.515164	-1.393922	0.808470
14	1	0	1.236944	1.542046	1.633492
15	1	0	-1.731377	0.641036	2.251672
16	1	0	1.423714	-1.302263	-0.879009
17	7	0	2.318203	0.592669	-0.441224
18	1	0	2.990673	1.096530	0.120618
19	1	0	2.721436	0.441043	-1.357811
20	5	0	0.239355	-1.559489	-0.442455
21	5	0	1.779338	-0.662775	0.222822
22	5	0	0.189186	-0.830891	1.229100
23	5	0	-1.149411	0.342981	1.269662
24	6	0	-0.653144	1.491271	0.141831

mF-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.233590	0.690915	-0.959485
2	5	0	0.810876	-0.754201	-1.350413
3	5	0	1.206845	1.004421	0.698003
4	5	0	1.826778	-0.489608	0.117081
5	5	0	-1.005463	-0.991507	0.638393
6	1	0	1.922092	1.244541	-1.584165
7	1	0	0.946325	-1.245093	-2.421399
8	1	0	1.927694	1.801449	1.186073
9	1	0	-0.034124	2.776095	-0.578089
10	1	0	0.640679	-2.566717	0.064264
11	1	0	2.944478	-0.858937	0.171525
12	1	0	-0.861101	1.410916	2.121050
13	1	0	-2.668744	1.580202	-0.000804
14	1	0	-1.525619	-1.702163	1.439535
15	1	0	0.806199	-0.971580	2.407065
16	1	0	-1.160799	1.372840	-1.265276
17	7	0	-2.003756	-0.602995	-0.515653
18	1	0	-2.962858	-0.848228	-0.295743
19	1	0	-1.786796	-0.963961	-1.439344
20	5	0	-0.085649	1.600610	-0.424303
21	5	0	-1.718107	0.902880	-0.210775

22	5	0	-0.523546	0.845231	1.136564
23	5	0	0.593920	-0.510010	1.341580
24	6	0	0.484843	-1.498828	-0.028144

mTS8-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.807324	0.595723	-1.290830
2	5	0	0.310727	-0.876363	-1.223099
3	5	0	1.454097	1.120423	0.181998
4	5	0	1.903969	-0.433635	-0.508855
5	5	0	-0.278694	-0.787034	1.129679
6	1	0	1.116053	1.041108	-2.226591
7	1	0	-0.143066	-1.516612	-2.108751
8	1	0	2.185826	2.045609	0.212922
9	1	0	-0.398038	2.603872	-0.586674
10	1	0	0.972310	-2.540824	0.240206
11	1	0	2.926013	-0.762556	-0.993901
12	1	0	-0.113978	1.513996	2.234392
13	1	0	-2.571607	1.371145	0.948022
14	1	0	-0.996647	-1.489218	1.751735
15	1	0	2.149405	-0.619442	2.069432
16	1	0	-1.537607	1.155193	-0.865335
17	7	0	-2.799355	-0.523835	-0.283278
18	1	0	-3.487104	-0.956785	0.312565
19	1	0	-2.530032	-1.100774	-1.063637
20	5	0	-0.267042	1.442057	-0.367530
21	5	0	-2.142312	0.654166	0.116460
22	5	0	0.080870	0.844944	1.276814
23	5	0	1.437109	-0.317768	1.177583
24	6	0	0.781065	-1.481025	0.148048

C2B7H9

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.419801	0.595490	1.259617
2	5	0	-1.072727	-0.017196	-0.939677
3	5	0	-1.072727	-0.017196	0.939677
4	5	0	-0.270009	1.377885	0.000000
5	5	0	0.419801	-0.983239	-1.069209
6	5	0	1.363394	0.620829	0.000000
7	5	0	0.419801	-0.983239	1.069209
8	1	0	0.683468	1.075898	2.188266
9	1	0	-1.953305	0.154982	-1.705643
10	1	0	0.683468	1.075898	-2.188266
11	1	0	-0.557411	2.519331	0.000000
12	1	0	0.960439	-1.675941	-1.857072
13	1	0	2.493767	0.952029	0.000000
14	1	0	0.960439	-1.675941	1.857072
15	1	0	-1.377233	-2.469498	-0.000000
16	6	0	0.419801	0.595490	-1.259617
17	5	0	-0.783120	-1.449368	-0.000000
18	1	0	-1.953305	0.154982	1.705643

pTS1-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.600915	1.264522	0.644860
2	5	0	-1.635325	0.556354	-0.399963
3	5	0	1.023720	1.270154	0.526911
4	5	0	-0.013317	-0.418855	-1.453860
5	5	0	-0.018995	1.224849	-0.947242
6	5	0	1.667301	-0.369854	0.712753
7	5	0	0.254776	-1.458477	0.736797
8	1	0	-0.921841	2.209235	1.066014
9	1	0	-2.438204	1.268271	-0.917735
10	1	0	1.622022	2.210582	0.917342
11	1	0	-0.020655	0.116824	2.724114
12	1	0	-0.379249	-0.897308	-2.472146
13	1	0	-0.174184	2.161898	-1.648870
14	1	0	2.693765	-0.660881	1.218108
15	1	0	0.146684	-2.571842	1.126952
16	1	0	1.634150	-2.039094	-1.023429
17	1	0	2.452138	0.573793	-1.606237

18	5	0	1.532767	0.324085	-0.909888
19	7	0	-2.214533	-0.782711	0.072158
20	6	0	1.091385	-1.209862	-0.592823
21	5	0	0.068573	0.061092	1.542822
22	1	0	-1.069487	-0.932562	0.921936
23	1	0	-3.169977	-0.670718	0.408851
24	1	0	-2.213756	-1.563922	-0.573880

pP1-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.528364	1.373845	-0.583569
2	5	0	1.783350	0.451021	-0.427238
3	5	0	-0.774008	1.431456	0.425438
4	5	0	0.816688	-0.977402	0.839471
5	5	0	0.765982	0.920025	1.051470
6	5	0	-1.826102	0.049291	0.100488
7	5	0	-1.203014	-1.059039	-1.066592
8	1	0	0.809825	2.381988	-0.863682
9	1	0	2.884222	0.891235	-0.480828
10	1	0	-1.253339	2.481516	0.673994
11	1	0	-1.316458	1.293856	-2.206759
12	1	0	1.297651	-1.609273	1.720672
13	1	0	1.312975	1.625469	1.825897
14	1	0	-2.985600	0.061234	0.320746
15	1	0	-1.873903	-1.737263	-1.765767
16	1	0	-1.296474	-2.165944	0.912714
17	1	0	-0.954007	-0.131728	2.563233
18	5	0	-0.652128	-0.022046	1.426307
19	7	0	1.651212	-1.061628	-0.506276
20	6	0	-0.831524	-1.317665	0.426413
21	5	0	-0.848949	0.702690	-1.294902
22	1	0	-0.341197	-0.459283	-1.807710
23	1	0	2.539074	-1.539672	-0.399675
24	1	0	1.128608	-1.477793	-1.278173

pTS2-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.548383	1.205599	-0.716563
2	5	0	1.853746	0.491146	-0.134172
3	5	0	-1.006614	1.370548	-0.185321
4	5	0	0.343538	-0.496453	1.403197
5	5	0	0.258706	1.198859	0.995809
6	5	0	-1.810663	-0.224644	-0.393880
7	5	0	-0.715394	-1.437900	-0.906346
8	1	0	0.825074	2.166999	-1.135863
9	1	0	2.752439	1.217479	0.148657
10	1	0	-1.573230	2.375877	-0.429677
11	1	0	-0.654167	0.435130	-2.707940
12	1	0	0.909613	-1.001721	2.304396
13	1	0	0.601657	2.125633	1.642637
14	1	0	-2.961380	-0.413538	-0.577510
15	1	0	-1.025675	-2.437557	-1.456190
16	1	0	-1.392391	-2.038941	1.166472
17	1	0	-1.965838	0.492918	2.115288
18	5	0	-1.271522	0.328853	1.173416
19	7	0	2.207768	-0.894653	-0.139360
20	6	0	-0.885775	-1.218970	0.673423
21	5	0	-0.452977	0.212074	-1.563442
22	1	0	0.276052	-0.952403	-1.530706
23	1	0	3.138069	-1.152812	0.151075
24	1	0	1.645654	-1.686686	-0.402585

pA-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.943109	-0.001224	0.000280
2	5	0	0.021902	-1.295337	0.169224
3	5	0	0.023770	1.294162	-0.168952
4	5	0	-1.485782	-0.796266	1.036595
5	5	0	0.022776	0.168492	1.294892
6	5	0	-1.484349	0.797151	-1.036801
7	5	0	-1.485678	-1.036216	-0.796834

8	1	0	2.025004	-0.001891	0.000379
9	1	0	0.508838	-2.361526	0.308565
10	1	0	0.512206	2.359690	-0.308173
11	1	0	0.510671	-0.309300	-2.360382
12	1	0	-1.978489	-1.449778	1.887007
13	1	0	0.510382	0.307440	2.360832
14	1	0	-1.975887	1.451362	-1.887352
15	1	0	-1.978289	-1.886351	-1.450776
16	1	0	-3.479105	0.001869	-0.000388
17	1	0	-1.976093	1.888006	1.450368
18	5	0	-1.484461	1.037181	0.796583
19	7	0	4.418093	0.000204	-0.000053
20	6	0	-2.402078	0.001102	-0.000225
21	5	0	0.022910	-0.169686	-1.294603
22	1	0	4.795999	0.921116	-0.203150
23	1	0	4.798249	-0.283596	0.898316
24	1	0	4.798241	-0.635139	-0.695722

pTS3-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.903069	0.993081	-0.327584
2	5	0	-2.268502	0.412848	0.274914
3	5	0	0.691229	1.377328	-0.572289
4	5	0	0.537587	-1.406998	-0.541464
5	5	0	-0.144510	-0.010636	-1.379047
6	5	0	1.727775	0.614188	0.684026
7	5	0	0.765390	-0.688943	1.396846
8	1	0	-1.308022	1.948758	-0.678586
9	1	0	-2.941861	1.159379	0.910974
10	1	0	0.895194	2.462600	-0.988178
11	1	0	-0.256864	1.692171	1.976670
12	1	0	0.380186	-2.549995	-0.807548
13	1	0	-0.471538	-0.005536	-2.520395
14	1	0	2.647590	1.140243	1.203131
15	1	0	0.871252	-1.209793	2.451493
16	1	0	2.707909	-1.559195	0.445137
17	1	0	2.448866	-0.045125	-1.903532
18	5	0	1.630377	-0.035534	-1.050770

19	7	0	-2.737498	-0.868713	0.031427
20	6	0	1.829571	-0.969173	0.238921
21	5	0	0.033357	0.997094	1.066637
22	1	0	-0.376778	-0.645580	0.941716
23	1	0	-3.607594	-1.198309	0.418545
24	1	0	-2.248380	-1.548807	-0.531694

pB-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.876092	0.985107	0.358404
2	5	0	2.202249	0.395939	-0.337315
3	5	0	-0.709288	1.408578	0.537640
4	5	0	-0.558601	-1.419104	0.472088
5	5	0	0.107520	0.050890	1.418894
6	5	0	-1.698845	0.601650	-0.729731
7	5	0	-0.643444	-0.721140	-1.319342
8	1	0	1.342141	1.917721	0.700230
9	1	0	2.805778	1.105720	-1.074571
10	1	0	-0.934691	2.487518	0.958987
11	1	0	0.229052	1.798097	-1.907025
12	1	0	-0.439989	-2.546484	0.808129
13	1	0	0.400210	0.043773	2.567561
14	1	0	-2.563238	1.124794	-1.342730
15	1	0	-0.597496	-1.316033	-2.338471
16	1	0	-2.755753	-1.519162	-0.488405
17	1	0	-2.411111	-0.135131	1.903959
18	5	0	-1.606805	-0.075921	1.039863
19	7	0	2.749398	-0.835594	-0.003836
20	6	0	-1.866719	-0.940645	-0.304583
21	5	0	-0.024366	1.022231	-1.052831
22	1	0	0.325672	-1.055484	-0.470211
23	1	0	3.608057	-1.159314	-0.420645
24	1	0	2.347246	-1.479250	0.660785

pB'-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.989454	0.682432	0.071415
2	5	0	-2.017641	-0.482306	-0.302285
3	5	0	0.432452	1.373201	0.537010
4	5	0	0.894501	-1.405454	0.487030
5	5	0	-0.191365	-0.116564	1.293965
6	5	0	1.736049	0.833067	-0.577204
7	5	0	1.095104	-0.684088	-1.282751
8	1	0	-1.666968	1.499524	0.316757
9	1	0	-1.705663	-1.495359	-0.831062
10	1	0	0.357433	2.467048	0.974432
11	1	0	-0.179362	1.600985	-2.060782
12	1	0	0.968989	-2.534434	0.825034
13	1	0	-0.673585	-0.198129	2.370752
14	1	0	2.547929	1.540386	-1.064205
15	1	0	1.317256	-1.262671	-2.288026
16	1	0	3.183610	-1.024765	-0.150834
17	1	0	2.201255	0.228126	2.143944
18	5	0	1.554317	0.118985	1.160949
19	7	0	-3.372613	-0.276798	-0.048131
20	6	0	2.176476	-0.647334	-0.107254
21	5	0	0.067616	0.873225	-1.160874
22	1	0	0.102476	-1.216255	-0.573321
23	1	0	-4.064919	-0.966325	-0.293154
24	1	0	-3.757460	0.538545	0.403216

pTS4-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.350991	-1.308867	0.049300
2	5	0	-1.665016	-0.026233	0.585060
3	5	0	0.907597	-1.063329	-1.028881
4	5	0	-0.329204	1.437832	-0.068538
5	5	0	-0.611817	-0.162484	-1.035475
6	5	0	2.054450	-0.146810	-0.096021
7	5	0	1.253107	0.271457	1.431989
8	1	0	-0.932873	-2.222334	0.043503

9	1	0	-1.570705	-0.372516	1.720970
10	1	0	1.149766	-1.815556	-1.905002
11	1	0	1.486039	-2.329464	1.230015
12	1	0	-0.729320	2.498867	-0.414204
13	1	0	-1.393630	-0.248796	-1.914378
14	1	0	3.234155	-0.167249	-0.164322
15	1	0	1.296814	0.455167	2.597207
16	1	0	1.837802	2.249729	0.356251
17	1	0	1.175794	1.329926	-2.150951
18	5	0	0.898560	0.720243	-1.179954
19	7	0	-3.008409	0.077265	0.110378
20	6	0	1.298956	1.314058	0.312066
21	5	0	1.061473	-1.338453	0.739635
22	1	0	-0.985849	1.151071	0.969724
23	1	0	-3.772284	0.065282	0.765418
24	1	0	-3.270388	0.372756	-0.814147

pC-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.192809	-1.421298	-0.053843
2	5	0	1.861478	-0.100295	-0.593932
3	5	0	-1.253250	-0.808585	1.092561
4	5	0	0.728975	1.219329	0.136528
5	5	0	0.501511	-0.399417	0.946818
6	5	0	-2.095843	0.335837	0.043911
7	5	0	-1.109231	0.236611	-1.428914
8	1	0	0.222955	-2.417266	-0.149300
9	1	0	1.632606	-0.675485	-1.607353
10	1	0	-1.622459	-1.395319	2.047649
11	1	0	-2.293172	-2.063017	-1.059738
12	1	0	1.267008	2.140015	0.662644
13	1	0	1.190795	-0.771860	1.833534
14	1	0	-3.196875	0.759262	0.094840
15	1	0	-1.074738	0.236370	-2.608889
16	1	0	-1.118113	2.415545	-0.685103
17	1	0	-0.902507	1.616466	2.032973
18	5	0	-0.766802	0.878431	1.123609
19	7	0	3.168047	-0.151845	-0.069382

20	6	0	-0.842452	1.396707	-0.446937
21	5	0	-1.613254	-1.204263	-0.614232
22	1	0	1.363812	1.095429	-0.953716
23	1	0	3.864591	-0.759147	-0.468126
24	1	0	3.433409	0.241223	0.819192

pTS5-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.382714	-1.399546	0.018345
2	5	0	2.246370	-0.278629	-0.696027
3	5	0	-1.525166	-0.703072	1.060414
4	5	0	0.695995	1.042018	0.185258
5	5	0	0.254427	-0.451704	1.087513
6	5	0	-2.120886	0.490778	-0.124672
7	5	0	-0.979353	0.184512	-1.449884
8	1	0	-0.033177	-2.423183	-0.057935
9	1	0	2.028697	-1.205142	-1.396014
10	1	0	-2.087264	-1.248178	1.943959
11	1	0	-2.441832	-1.939655	-1.152798
12	1	0	1.405765	1.912493	0.580028
13	1	0	0.913369	-0.857272	1.986072
14	1	0	-3.159921	1.043592	-0.222887
15	1	0	-0.802271	0.158214	-2.617664
16	1	0	-0.888003	2.414669	-0.822126
17	1	0	-0.989014	1.727788	1.960698
18	5	0	-0.875404	0.921515	1.105376
19	7	0	3.394273	-0.087421	0.041065
20	6	0	-0.717311	1.396714	-0.500196
21	5	0	-1.750092	-1.120815	-0.653390
22	1	0	1.521064	0.704356	-0.933339
23	1	0	4.115642	-0.787675	0.111873
24	1	0	3.527729	0.705918	0.650849

pD-N

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-1.196175	0.683276	-0.000000
2	5	0	0.352837	1.380808	0.000000
3	5	0	-0.451017	-0.970555	1.061046
4	5	0	-0.451017	0.686190	1.384284
5	5	0	1.063086	-0.032685	-0.943456
6	5	0	-0.451017	-0.970555	-1.061046
7	1	0	-2.210311	1.061343	-0.000000
8	1	0	0.625198	2.527908	0.000000
9	1	0	-0.818823	1.229583	-2.364187
10	1	0	-1.044440	-1.766145	1.697110
11	1	0	-0.818823	1.229583	2.364187
12	1	0	2.026698	-0.077510	-1.621948
13	1	0	-1.044440	-1.766145	-1.697110
14	1	0	1.171911	-2.263896	-0.000000
15	1	0	2.026698	-0.077510	1.621948
16	5	0	1.063086	-0.032685	0.943456
17	6	0	0.648113	-1.321735	-0.000000
18	5	0	-0.451017	0.686190	-1.384284

pTS6-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.211995	0.872067	-1.067130
2	5	0	-0.257816	1.545600	0.206077
3	5	0	-1.357530	0.304438	-0.431070
4	5	0	0.473904	-1.275301	0.535557
5	5	0	1.535705	-0.207528	-0.397411
6	5	0	1.148693	0.409361	1.063278
7	1	0	0.417437	1.382059	-1.999323
8	1	0	-1.749859	-1.826800	0.296539
9	1	0	-0.017075	-1.391774	-2.152361
10	1	0	-2.392835	0.627314	-0.892022
11	1	0	0.876222	-2.250861	1.064650
12	1	0	2.533083	-0.379890	-1.006447
13	1	0	1.798798	0.909887	1.913535
14	1	0	-1.226191	0.266719	2.280392
15	5	0	-0.631893	0.221673	1.262232

16	1	0	-0.340577	2.696404	0.448456
17	6	0	-1.001321	-1.061924	0.168054
18	5	0	0.056328	-0.777026	-1.150456

pP2-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.419801	0.595490	1.259617
2	5	0	-1.072727	-0.017196	-0.939677
3	5	0	-1.072727	-0.017196	0.939677
4	5	0	-0.270009	1.377885	0.000000
5	5	0	0.419801	-0.983239	-1.069209
6	5	0	1.363394	0.620829	0.000000
7	5	0	0.419801	-0.983239	1.069209
8	1	0	0.683468	1.075898	2.188266
9	1	0	-1.953305	0.154982	-1.705643
10	1	0	0.683468	1.075898	-2.188266
11	1	0	-0.557411	2.519331	0.000000
12	1	0	0.960439	-1.675941	-1.857072
13	1	0	2.493767	0.952029	0.000000
14	1	0	0.960439	-1.675941	1.857072
15	1	0	-1.377233	-2.469498	-0.000000
16	6	0	0.419801	0.595490	-1.259617
17	5	0	-0.783120	-1.449368	-0.000000
18	1	0	-1.953305	0.154982	1.705643