SUPPORTING INFORMATION

Computational Examination of the Mechanism of Alkene Epoxidation Catalyzed by Gallium(III) Complexes with N-Donor Ligands

Michael L. McKee* and Christian R. Goldsmith*

Department of Chemistry and Biochemistry, Auburn University, Auburn, AL 36849

*To whom correspondence should be addressed: mckeeml@auburn.edu and crgoldsmith@auburn.edu

Table S1. Charge, Point Group, Absolute Energies (Hartrees), Zero-Point Energy and Thermal Corrections (kcal mol^{-1}), Entropies (cal mol^{-1} K^{-1}) and Free Energies of Solvation in Acetonitrile (kcal mol^{-1})[a]

	Charge	PG	B3LYP/ 6-31+G(2d,p)	ZPE	TC	ΔS	ΔG(solv) an
Cl	−1	K	−460.27366	0.00	1.48	36.59	−65.16
HCl	0	C_{iv}	−460.80442	4.19	2.07	44.61	−3.59
AC	0	C_s	−229.11617	38.94	3.45	68.73	−6.14
AI	−1	C_s	−228.55255	30.30	3.38	69.37	−59.16
PA	0	C_s	−304.24845	40.96	4.10	75.01	−6.84
PI	−1	C_s	−303.66661	32.59	3.92	73.02	−62.87
C_2H_4	0	D_{2h}	−78.59988	32.15	2.50	52.33	−1.19
EO	0	C_{2v}	−153.80448	36.18	2.57	57.93	−3.54
C_6H_{10}	0	C_2	−234.67154	92.21	4.04	72.42	−4.14
OC_6H_{10}	0	C_1	−309.87911	95.65	4.33	76.73	−5.90
Ga	3	D_{2d}	−3065.66264	220.86	13.30	145.24	−326.55
phen	0	C_{2v}	−571.65069	107.26	6.34	92.84	−14.62
$Ga(AI)_3$	0	C_3	−2608.85531	98.26	10.64	134.66	−12.19
Hphen	1	C_s	−572.04713	116.37	6.35	93.98	−55.53
GaCl	2	C_2	−3526.35368	221.90	14.47	155.40	−157.68
$GaCl_2$	1	C_2	−3986.89578	222.10	15.74	163.88	−65.96
$GaCl_2$−AC	1	C_1	−4216.02573	261.84	19.76	200.44	−64.59
GaClAI−PA	1	C_1	−4059.44705	295.43	22.84	224.06	−63.68
$GaCl_2$AC	1	C_1	−4215.99036	261.03	19.55	196.85	−59.76
GaClAI	1	C_1	−3755.19163	254.00	17.96	182.77	−63.38
GaClAI−HCl	1	C_1	−4216.00818	259.65	19.68	202.31	−66.58
GaClAI−AC	1	C_1	−3984.31930	293.60	22.07	221.00	−62.46
GaClAI−PA	1	C_1	−4059.44952	295.54	22.73	224.06	−63.24
GaClAIPA−Cl	1	C_1	−4059.41155	295.53	22.20	216.49	−74.80
GaAIAC−Cl	1	C_1	−3984.29230	292.45	21.42	209.70	−72.04
GaAI	2	C_1	−3294.67209	254.06	15.90	165.39	−149.80
GaPI	2	C_1	−3369.80728	256.38	16.99	174.17	−149.80
$GaAI_2$	1	C_2	−3523.48697	285.90	20.18	198.88	−60.62
$GaAI_2$−HCl	1	C_1	−3984.30215	291.30	21.88	217.83	−65.60
$GaPI_2$	1	C_2	−3673.73339	289.68	21.59	210.40	−66.76
GaAIPIa	1	C_1	−3598.59390	287.81	20.90	207.17	−58.01
GaAIPIb	1	C_1	−3598.61654	295.53	22.20	216.49	−61.95
GaAIEO	2	C_1	−3448.47591	291.51	19.38	192.30	−149.52
TS1	1	C_1	−4215.98849	260.96	19.28	197.37	−59.23
TS2	1	C_1	−4215.97414	259.65	19.00	191.87	−71.89
TS3	1	C_1	−4059.39629	295.58	21.66	208.55	−63.88
TS4	1	C_1	−3598.59267	289.98	21.29	209.47	−58.45
TS5	1	C_1	−3523.48500	286.05	20.14	197.60	−60.45
TS6	1	C_1	−3984.29174	289.98	21.29	209.47	−70.34
TS7	1	C_1	−3677.16797	320.60	22.96	218.55	−59.55
TS8	2	C_1	−3448.37602	288.92	19.38	191.60	−147.90
TS88	2	C_1	−3448.37377	289.06	19.32	191.70	−147.07
TS9	2	C_1	−3604.45769	348.22	21.48	208.79	−146.40
$GaAI(OC_6H_{10})$	2	C_1	−3604.55831	350.49	21.46	209.23	−148.18

a) Geometries, zero-point energies, thermal corrections, and entropies at B3LYP/6-31G(d) and 298 K. Relative energies at B3LYP/6-31+G(2d,p) and solvation effects at SMD/B3LYP/6-31+G(2d,p).

Table S2. Cartesian Coordinates of Species in Table S1 optimized at the B3LYP/6-31G(d) Level

HCl Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	-1.217860
2	17	0	0.000000	0.000000	0.071639

AC Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.864675	0.373328	0.000000
2	6	0	0.000000	0.156210	0.000000
3	8	0	-1.247307	-0.382262	0.000000
4	6	0	1.060871	-0.916340	0.000000
5	1	0	2.047293	-0.452137	0.000000
6	1	0	0.947974	-1.554725	0.882318
7	1	0	0.947974	-1.554725	-0.882318
8	8	0	0.191833	1.350891	0.000000

AI Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.220219	0.000000
2	8	0	-1.160431	0.705181	0.000000
3	6	0	0.044313	-1.354764	0.000000
4	1	0	1.071452	-1.741812	0.000000
5	1	0	-0.485963	-1.746478	0.880584
6	1	0	-0.485963	-1.746478	-0.880584
7	8	0	1.114755	0.800074	0.000000

PA Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.476705	-1.810000	0.000000
2	1	0	-1.286000	-1.237636	0.000000
3	6	0	0.000000	0.447805	0.000000
4	8	0	-1.202854	0.622124	0.000000
5	6	0	1.068145	1.506478	0.000000
6	1	0	0.938796	2.137622	0.884359
7	1	0	2.068792	1.070968	0.000000
8	1	0	0.938796	2.137622	-0.884359
9	8	0	0.545903	-0.791409	0.000000

PI Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.769418	-1.830484	0.000000
2	6	0	0.000000	0.396641	0.000000
3	8	0	-1.106802	0.932457	0.000000
4	6	0	1.283504	1.239114	0.000000
5	1	0	1.295830	1.894302	0.881606

6	1	0	2.185460	0.619146	0.000000
7	1	0	1.295830	1.894302	-0.881606
8	8	0	0.316452	-0.879757	0.000000

C2H4 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.665525
2	1	0	0.000000	0.923969	1.238848
3	1	0	0.000000	-0.923969	1.238848
4	6	0	0.000000	0.000000	-0.665525
5	1	0	0.000000	0.923969	-1.238848
6	1	0	0.000000	-0.923969	-1.238848

EO Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.854903
2	6	0	0.000000	0.734769	-0.371703
3	6	0	0.000000	-0.734769	-0.371703
4	1	0	0.921024	-1.274082	-0.594699
5	1	0	-0.921024	-1.274082	-0.594699
6	1	0	0.921024	1.274082	-0.594699
7	1	0	-0.921024	1.274082	-0.594699

C6H10 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.005131	0.668537	1.306147
2	6	0	0.005131	-0.668537	1.306147
3	1	0	0.019001	-1.204547	2.254789
4	1	0	-0.019001	1.204547	2.254789
5	6	0	0.005131	1.502890	0.047799
6	6	0	-0.005131	-1.502890	0.047799
7	6	0	-0.371791	-0.671462	-1.192266
8	6	0	0.371791	0.671462	-1.192266
9	1	0	-0.983469	1.969860	-0.090259
10	1	0	0.708471	2.339393	0.163622
11	1	0	-0.708471	-2.339393	0.163622
12	1	0	0.983469	-1.969860	-0.090259
13	1	0	-0.150487	-1.236418	-2.106119
14	1	0	-1.454297	-0.481702	-1.192112
15	1	0	0.150487	1.236418	-2.106119
16	1	0	1.454297	0.481702	-1.192112

OC6H10 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.096930	-0.631536	-0.413515
2	6	0	0.989203	0.836185	-0.296322
3	8	0	1.514868	0.039390	0.783986
4	1	0	1.751490	1.446017	-0.785742
5	1	0	1.921680	-1.044427	-0.999923
6	6	0	-0.128261	-1.513016	-0.292511
7	6	0	-0.344016	1.519744	-0.033595

8	6	0	-1.551410	0.573195	-0.172077
9	6	0	-1.279677	-0.807329	0.440997
10	1	0	-0.447007	-1.793921	-1.307219
11	1	0	0.145047	-2.444916	0.220132
12	1	0	-0.454196	2.368058	-0.720764
13	1	0	-0.306575	1.941646	0.979515
14	1	0	-2.433844	1.032659	0.289365
15	1	0	-1.789458	0.443979	-1.237885
16	1	0	-2.181196	-1.429596	0.391479
17	1	0	-1.021495	-0.698074	1.501284

Ga Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	0.000000	0.000000	0.000000
2	7	0	0.000000	1.345285	1.413551
3	6	0	0.000000	0.713926	2.634116
4	6	0	0.000000	2.689606	1.358454
5	6	0	0.000000	1.424955	3.851900
6	6	0	0.000000	3.463042	2.524310
7	1	0	0.000000	3.148684	0.375234
8	6	0	0.000000	2.840811	3.765478
9	1	0	0.000000	4.544867	2.442529
10	1	0	0.000000	3.435909	4.675137
11	7	0	0.000000	-1.345285	1.413551
12	6	0	0.000000	-0.713926	2.634116
13	6	0	0.000000	-2.689606	1.358454
14	6	0	0.000000	-1.424955	3.851900
15	6	0	0.000000	-3.463042	2.524310
16	1	0	0.000000	-3.148684	0.375234
17	6	0	0.000000	-2.840811	3.765478
18	1	0	0.000000	-4.544867	2.442529
19	1	0	0.000000	-3.435909	4.675137
20	7	0	-1.345285	0.000000	-1.413551
21	6	0	-2.689606	0.000000	-1.358454
22	6	0	-0.713926	0.000000	-2.634116
23	6	0	-3.463042	0.000000	-2.524310
24	1	0	-3.148684	0.000000	-0.375234
25	6	0	-1.424955	0.000000	-3.851900
26	6	0	-2.840811	0.000000	-3.765478
27	1	0	-4.544867	0.000000	-2.442529
28	1	0	-3.435909	0.000000	-4.675137
29	7	0	1.345285	0.000000	-1.413551
30	6	0	0.713926	0.000000	-2.634116
31	6	0	2.689606	0.000000	-1.358454
32	6	0	1.424955	0.000000	-3.851900
33	6	0	3.463042	0.000000	-2.524310
34	1	0	3.148684	0.000000	-0.375234
35	6	0	2.840811	0.000000	-3.765478
36	1	0	4.544867	0.000000	-2.442529
37	1	0	3.435909	0.000000	-4.675137
38	6	0	-0.684070	0.000000	-5.082860
39	6	0	0.684070	0.000000	-5.082860
40	6	0	0.000000	-0.684070	5.082860
41	6	0	0.000000	0.684070	5.082860
42	1	0	-1.231804	0.000000	-6.020453
43	1	0	1.231804	0.000000	-6.020453
44	1	0	0.000000	-1.231804	6.020453
45	1	0	0.000000	1.231804	6.020453

phen Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	7	0	0.000000	1.381148	-1.563335
2	6	0	0.000000	0.729479	-0.378079
3	6	0	0.000000	2.704080	-1.548816
4	6	0	0.000000	1.417201	0.870581
5	6	0	0.000000	3.482574	-0.373097
6	1	0	0.000000	3.193771	-2.522387
7	6	0	0.000000	2.829070	0.841370
8	1	0	0.000000	4.566872	-0.432838
9	1	0	0.000000	3.383192	1.777367
10	7	0	0.000000	-1.381148	-1.563335
11	6	0	0.000000	-0.729479	-0.378079
12	6	0	0.000000	-2.704080	-1.548816
13	6	0	0.000000	-1.417201	0.870581
14	6	0	0.000000	-3.482574	-0.373097
15	1	0	0.000000	-3.193771	-2.522387
16	6	0	0.000000	-2.829070	0.841370
17	1	0	0.000000	-4.566872	-0.432838
18	1	0	0.000000	-3.383192	1.777367
19	6	0	0.000000	-0.680140	2.102014
20	6	0	0.000000	0.680140	2.102014
21	1	0	0.000000	-1.234823	3.037367
22	1	0	0.000000	1.234823	3.037367

Ga(AI)3 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	0.000000	0.000000	0.008472
2	8	0	0.499505	1.696315	-0.962123
3	6	0	0.000000	2.367100	0.003503
4	8	0	-0.494751	1.699827	0.974024
5	6	0	-0.036374	3.865113	-0.017622
6	8	0	-1.224718	-1.278381	0.974024
7	8	0	-1.718805	-0.415574	-0.962123
8	8	0	1.219300	-1.280742	-0.962123
9	8	0	1.719469	-0.421446	0.974024
10	6	0	-2.049968	-1.183550	0.003503
11	6	0	2.049968	-1.183550	0.003503
12	6	0	3.365473	-1.901056	-0.017622
13	6	0	-3.329099	-1.964057	-0.017622
14	1	0	3.285716	-2.822800	-0.596869
15	1	0	4.107432	-1.254784	-0.501312
16	1	0	3.701586	-2.107455	1.000141
17	1	0	-4.087475	-1.434113	-0.596869
18	1	0	-3.140391	-2.929749	-0.501312
19	1	0	-3.675903	-2.151940	1.000141
20	1	0	-0.025683	4.259395	1.000141
21	1	0	0.801759	4.256913	-0.596869
22	1	0	-0.967041	4.184533	-0.501312

Hphen Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.823371	-1.827179	0.000000
2	6	0	0.000000	-0.743411	0.000000
3	6	0	0.382944	-3.092085	0.000000
4	6	0	-1.401266	-0.935493	0.000000
5	6	0	-0.989368	-3.338033	0.000000
6	1	0	1.133117	-3.874008	0.000000
7	6	0	-1.874101	-2.266000	0.000000

8	1	0	-1.345178	-4.361526	0.000000
9	1	0	-2.945016	-2.448726	0.000000
10	7	0	1.938266	0.634259	0.000000
11	6	0	0.588869	0.563549	0.000000
12	6	0	2.481444	1.842070	0.000000
13	6	0	-0.277933	1.683391	0.000000
14	6	0	1.718346	3.033316	0.000000
15	1	0	3.567583	1.886877	0.000000
16	6	0	0.340089	2.956350	0.000000
17	1	0	2.224663	3.992841	0.000000
18	1	0	-0.270307	3.854921	0.000000
19	6	0	-1.700479	1.479119	0.000000
20	6	0	-2.243592	0.226376	0.000000
21	1	0	-2.347703	2.351394	0.000000
22	1	0	-3.320151	0.088869	0.000000
23	1	0	1.821813	-1.595098	0.000000

GaCl Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	0.000000	0.000000	0.856561
2	7	0	-1.279491	1.011904	-0.345183
3	6	0	-0.879420	2.289458	-0.612205
4	6	0	-2.422296	0.570068	-0.881768
5	6	0	-1.632864	3.176418	-1.411626
6	6	0	-3.223440	1.376652	-1.699670
7	1	0	-2.711526	-0.446407	-0.646585
8	6	0	-2.835598	2.679152	-1.963808
9	1	0	-4.143361	0.973477	-2.107938
10	1	0	-3.450026	3.323476	-2.586340
11	7	0	1.016481	1.821749	0.732727
12	6	0	0.343615	2.730778	-0.016738
13	6	0	2.111015	2.204391	1.393466
14	6	0	0.779268	4.062509	-0.186796
15	6	0	2.619545	3.509158	1.286665
16	1	0	2.589927	1.461301	2.023383
17	6	0	1.964420	4.434525	0.491672
18	1	0	3.515783	3.777877	1.834822
19	1	0	2.344164	5.447938	0.396931
20	7	0	-1.016481	-1.821749	0.732727
21	6	0	-2.111015	-2.204391	1.393466
22	6	0	-0.343615	-2.730778	-0.016738
23	6	0	-2.619545	-3.509158	1.286665
24	1	0	-2.589927	-1.461301	2.023383
25	6	0	-0.779268	-4.062509	-0.186796
26	6	0	-1.964420	-4.434525	0.491672
27	1	0	-3.515783	-3.777877	1.834822
28	1	0	-2.344164	-5.447938	0.396931
29	7	0	1.279491	-1.011904	-0.345183
30	6	0	0.879420	-2.289458	-0.612205
31	6	0	2.422296	-0.570068	-0.881768
32	6	0	1.632864	-3.176418	-1.411626
33	6	0	3.223440	-1.376652	-1.699670
34	1	0	2.711526	0.446407	-0.646585
35	6	0	2.835598	-2.679152	-1.963808
36	1	0	4.143361	-0.973477	-2.107938
37	1	0	3.450026	-3.323476	-2.586340
38	6	0	0.000000	-4.945206	-1.009261
39	6	0	1.152811	-4.517088	-1.602827
40	6	0	0.000000	4.945206	-1.009261
41	6	0	-1.152811	4.517088	-1.602827
42	1	0	-0.341568	-5.966449	-1.147298
43	1	0	1.735943	-5.192919	-2.220637
44	1	0	0.341568	5.966449	-1.147298

45	1	0	-1.735943	5.192919	-2.220637
46	17	0	0.000000	0.000000	3.028415

GaCl2 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	0.000000	0.000000	1.037107
2	7	0	-1.155441	0.865396	-0.575497
3	6	0	-0.802734	2.146403	-0.844248
4	6	0	-2.195052	0.343003	-1.214599
5	6	0	-1.484125	2.952235	-1.785204
6	6	0	-2.928682	1.059120	-2.174934
7	1	0	-2.461417	-0.676546	-0.959546
8	6	0	-2.575796	2.363850	-2.461476
9	1	0	-3.769175	0.585768	-2.670326
10	1	0	-3.131483	2.943688	-3.193040
11	7	0	0.919619	1.872313	0.777707
12	6	0	0.304655	2.689873	-0.111685
13	6	0	1.925032	2.341090	1.512733
14	6	0	0.705538	4.027886	-0.320715
15	6	0	2.389729	3.660653	1.374179
16	1	0	2.359808	1.640633	2.218394
17	6	0	1.785966	4.501904	0.458881
18	1	0	3.211937	4.002445	1.992957
19	1	0	2.126899	5.526265	0.336552
20	7	0	-0.919619	-1.872313	0.777707
21	6	0	-1.925032	-2.341090	1.512733
22	6	0	-0.304655	-2.689873	-0.111685
23	6	0	-2.389729	-3.660653	1.374179
24	1	0	-2.359808	-1.640633	2.218394
25	6	0	-0.705538	-4.027886	-0.320715
26	6	0	-1.785966	-4.501904	0.458881
27	1	0	-3.211937	-4.002445	1.992957
28	1	0	-2.126899	-5.526265	0.336552
29	7	0	1.155441	-0.865396	-0.575497
30	6	0	0.802734	-2.146403	-0.844248
31	6	0	2.195052	-0.343003	-1.214599
32	6	0	1.484125	-2.952235	-1.785204
33	6	0	2.928682	-1.059120	-2.174934
34	1	0	2.461417	0.676546	-0.959546
35	6	0	2.575796	-2.363850	-2.461476
36	1	0	3.769175	-0.585768	-2.670326
37	1	0	3.131483	-2.943688	-3.193040
38	6	0	0.000000	-4.821630	-1.287220
39	6	0	1.048351	-4.304908	-1.990787
40	6	0	0.000000	4.821630	-1.287220
41	6	0	-1.048351	4.304908	-1.990787
42	1	0	-0.314242	-5.849259	-1.443878
43	1	0	1.578837	-4.915805	-2.715144
44	1	0	0.314242	5.849259	-1.443878
45	1	0	-1.578837	4.915805	-2.715144
46	17	0	-1.544812	0.831716	2.471403
47	17	0	1.544812	-0.831716	2.471403

GaCl2-AC Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	-0.122954	-0.347282	-1.013077
2	6	0	1.363242	4.481069	0.028611
3	8	0	1.853296	3.439598	0.440759
4	6	0	1.828615	5.860694	0.420030

5	1	0	0.988532	6.446536	0.806272
6	1	0	2.615336	5.789016	1.171325
7	1	0	2.206549	6.386396	-0.463377
8	8	0	0.343355	4.523732	-0.836088
9	7	0	0.342990	-2.015012	0.260040
10	6	0	1.654164	-2.055846	0.603410
11	6	0	-0.449564	-3.007792	0.645581
12	6	0	2.216061	-3.099818	1.374352
13	6	0	0.012296	-4.083462	1.421552
14	1	0	-1.485854	-2.954378	0.331569
15	6	0	1.343658	-4.130589	1.788622
16	1	0	-0.676052	-4.868860	1.713367
17	1	0	1.728750	-4.954591	2.382744
18	7	0	1.898522	-0.024831	-0.618720
19	6	0	2.489867	-0.992926	0.126669
20	6	0	2.641338	0.950706	-1.131985
21	6	0	3.870924	-0.993765	0.415710
22	6	0	4.026006	1.027426	-0.899218
23	1	0	2.117051	1.678488	-1.737676
24	6	0	4.639611	0.064785	-0.123732
25	1	0	4.590863	1.845203	-1.331491
26	1	0	5.707667	0.105191	0.071201
27	7	0	-2.177864	-0.780368	-0.939881
28	6	0	-2.865802	-1.428655	-1.876246
29	6	0	-2.834793	-0.226380	0.108347
30	6	0	-4.261361	-1.579343	-1.796361
31	1	0	-2.280564	-1.831752	-2.696225
32	6	0	-4.233087	-0.334366	0.275972
33	6	0	-4.944027	-1.039723	-0.722501
34	1	0	-4.783894	-2.114384	-2.581475
35	1	0	-6.022316	-1.144989	-0.640271
36	7	0	-0.715826	0.599129	0.817271
37	6	0	-2.047941	0.503120	1.058970
38	6	0	0.038552	1.301669	1.655455
39	6	0	-2.673857	1.100445	2.175403
40	6	0	-0.492870	1.921090	2.800879
41	1	0	1.087364	1.403404	1.411640
42	6	0	-1.844263	1.821459	3.064602
43	1	0	0.166227	2.484351	3.451851
44	1	0	-2.279341	2.298085	3.938657
45	6	0	-4.842817	0.275273	1.423722
46	6	0	-4.093797	0.960074	2.335981
47	6	0	4.412888	-2.057388	1.213221
48	6	0	3.619126	-3.066559	1.675035
49	1	0	-5.917712	0.186188	1.549919
50	1	0	-4.565582	1.422057	3.198173
51	1	0	5.475648	-2.048107	1.436407
52	1	0	4.041336	-3.870455	2.270601
53	17	0	0.314379	-1.662084	-2.805690
54	17	0	-0.516660	1.645467	-2.113480
55	1	0	0.095356	3.604562	-1.092755

GaClAI-PA Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	0.314457	-0.317595	0.769646
2	6	0	-0.121774	-2.613320	2.501899
3	8	0	0.555857	-1.506590	2.236903
4	6	0	0.236878	-3.221339	3.844823
5	1	0	-0.318995	-4.147109	3.998010
6	1	0	1.312272	-3.423819	3.899478
7	1	0	0.001897	-2.512014	4.645682
8	8	0	-0.957131	-3.111642	1.758664
9	7	0	0.599173	0.996086	-0.893395

10	6	0	1.879888	1.424919	-1.026493
11	6	0	-0.323206	1.480808	-1.717808
12	6	0	2.289863	2.338763	-2.022160
13	6	0	-0.010563	2.387635	-2.746164
14	1	0	-1.345030	1.165663	-1.554426
15	6	0	1.293310	2.812744	-2.905461
16	1	0	-0.803522	2.749366	-3.390990
17	1	0	1.559861	3.515911	-3.689698
18	7	0	2.377430	0.066850	0.856234
19	6	0	2.834796	0.934119	-0.076586
20	6	0	3.202427	-0.372561	1.802943
21	6	0	4.177018	1.370166	-0.124600
22	6	0	4.554488	0.011875	1.839934
23	1	0	2.755596	-1.039915	2.530739
24	6	0	5.043922	0.874475	0.876519
25	1	0	5.195527	-0.368983	2.627241
26	1	0	6.085541	1.183573	0.885678
27	7	0	-1.633854	-0.711181	0.197102
28	6	0	-2.726338	-0.125768	0.675851
29	6	0	-1.756480	-1.739058	-0.680900
30	6	0	-4.014162	-0.529484	0.280837
31	1	0	-2.586468	0.698656	1.360351
32	6	0	-3.005427	-2.202513	-1.138763
33	6	0	-4.156795	-1.561003	-0.623677
34	1	0	-4.874399	-0.015957	0.694167
35	1	0	-5.141745	-1.889954	-0.943452
36	7	0	0.616413	-1.894985	-0.628262
37	6	0	-0.550031	-2.368029	-1.129036
38	6	0	1.752643	-2.483751	-0.982240
39	6	0	-0.613861	-3.449370	-2.036624
40	6	0	1.792737	-3.561793	-1.880150
41	1	0	2.662994	-2.093722	-0.541262
42	6	0	0.610869	-4.043191	-2.411474
43	1	0	2.745431	-4.009796	-2.139944
44	1	0	0.612547	-4.879543	-3.104951
45	6	0	-3.043653	-3.293412	-2.071907
46	6	0	-1.896813	-3.891071	-2.504834
47	6	0	4.571153	2.285784	-1.157761
48	6	0	3.666109	2.746883	-2.069125
49	1	0	-4.010970	-3.642055	-2.421423
50	1	0	-1.937234	-4.721291	-3.203597
51	1	0	5.605835	2.613391	-1.195612
52	1	0	3.972494	3.445744	-2.841894
53	17	0	-0.083727	1.544582	2.096343
54	1	0	-2.040176	2.698093	2.199951
55	8	0	-3.018006	2.825005	2.174463
56	8	0	-3.147208	4.036758	1.403863
57	6	0	-3.118512	3.815935	0.060926
58	8	0	-2.876172	2.754419	-0.466726
59	6	0	-3.451918	5.109501	-0.644821
60	1	0	-4.516188	5.100628	-0.905999
61	1	0	-3.259245	5.979456	-0.014253
62	1	0	-2.873108	5.172550	-1.568621

GaCl2AC Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	-0.420763	-1.014392	-0.266260
2	6	0	0.563169	-0.091581	2.556597
3	8	0	-0.052943	0.032639	1.483378
4	6	0	0.581728	1.007733	3.575745
5	1	0	-0.165022	1.761857	3.328711
6	1	0	0.405077	0.597596	4.573490
7	1	0	1.575401	1.470142	3.581542

8	8	0	1.254973	-1.148710	2.897631
9	7	0	-1.144578	0.740779	-1.092439
10	6	0	-2.414172	1.033478	-0.722281
11	6	0	-0.553440	1.472083	-2.029106
12	6	0	-3.123149	2.141926	-1.237106
13	6	0	-1.183915	2.585462	-2.607153
14	1	0	0.443225	1.170255	-2.321658
15	6	0	-2.458904	2.933280	-2.200300
16	1	0	-0.664931	3.156281	-3.369027
17	1	0	-2.963514	3.794568	-2.629309
18	7	0	-2.354003	-0.956862	0.576090
19	6	0	-3.060387	0.129419	0.184162
20	6	0	-2.926750	-1.855390	1.368352
21	6	0	-4.391555	0.366421	0.590704
22	6	0	-4.244657	-1.700055	1.833037
23	1	0	-2.318356	-2.712210	1.636613
24	6	0	-4.975891	-0.591671	1.450227
25	1	0	-4.673900	-2.457700	2.479187
26	1	0	-5.998141	-0.454624	1.791765
27	7	0	1.727011	-0.909247	-0.940899
28	6	0	1.953823	-2.042069	-1.619141
29	6	0	2.818970	-0.173756	-0.530309
30	6	0	3.225890	-2.551242	-1.904750
31	1	0	1.077373	-2.584119	-1.948983
32	6	0	4.139654	-0.681332	-0.704431
33	6	0	4.322668	-1.893359	-1.403319
34	1	0	3.313862	-3.472408	-2.469547
35	1	0	5.328185	-2.279539	-1.546055
36	7	0	1.473034	1.753602	0.018546
37	6	0	2.685517	1.160746	0.033634
38	6	0	1.347790	2.973894	0.514581
39	6	0	3.841700	1.831927	0.533330
40	6	0	2.414718	3.704092	1.073879
41	1	0	0.352222	3.412549	0.465047
42	6	0	3.666508	3.125682	1.075480
43	1	0	2.249836	4.700464	1.471353
44	1	0	4.528531	3.656201	1.471101
45	6	0	5.274374	0.026588	-0.186377
46	6	0	5.133207	1.225380	0.436742
47	6	0	-5.072453	1.529829	0.094996
48	6	0	-4.465779	2.378031	-0.784698
49	1	0	6.254967	-0.423704	-0.310085
50	1	0	5.994932	1.755211	0.832444
51	1	0	-6.092832	1.711548	0.419199
52	1	0	-4.998355	3.241674	-1.171819
53	17	0	-1.233108	-2.068444	-2.116784
54	17	0	0.185082	-3.017076	0.846404
55	1	0	1.093066	-1.886478	2.234409

GaClAI Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	0.049203	0.600335	-0.668611
2	6	0	-1.675668	2.895091	-0.189084
3	8	0	-0.462874	2.420290	-0.423065
4	6	0	-1.735305	4.411029	-0.206539
5	1	0	-1.031384	4.830256	0.520948
6	1	0	-1.437594	4.781168	-1.193485
7	1	0	-2.746024	4.749702	0.024263
8	8	0	-2.664244	2.203202	0.021026
9	7	0	1.046130	-1.311301	-0.528433
10	6	0	2.335152	-1.209304	-0.120639
11	6	0	0.585316	-2.506794	-0.877984
12	6	0	3.209389	-2.316916	-0.035560

13	6	0	1.372144	-3.669286	-0.819783
14	1	0	-0.441564	-2.549390	-1.222416
15	6	0	2.684363	-3.577301	-0.397205
16	1	0	0.944463	-4.620588	-1.116469
17	1	0	3.317695	-4.458687	-0.349418
18	7	0	1.931288	1.121328	0.107314
19	6	0	2.814826	0.101256	0.210592
20	6	0	2.336600	2.365754	0.348575
21	6	0	4.157223	0.288385	0.606507
22	6	0	3.655750	2.649250	0.743874
23	1	0	1.579506	3.130184	0.217792
24	6	0	4.563315	1.615105	0.878599
25	1	0	3.946507	3.676832	0.931961
26	1	0	5.587901	1.811210	1.182428
27	7	0	-1.761031	-0.316791	-1.146525
28	6	0	-2.264260	-0.443148	-2.370521
29	6	0	-2.500953	-0.691273	-0.076363
30	6	0	-3.539858	-0.991277	-2.589722
31	1	0	-1.625253	-0.110948	-3.182038
32	6	0	-3.784838	-1.260292	-0.199865
33	6	0	-4.297149	-1.404060	-1.509899
34	1	0	-3.915323	-1.077098	-3.603289
35	1	0	-5.286275	-1.829507	-1.655516
36	7	0	-0.711099	0.111940	1.269517
37	6	0	-1.933269	-0.469336	1.221239
38	6	0	-0.173911	0.377203	2.454226
39	6	0	-2.659705	-0.831471	2.377237
40	6	0	-0.815485	0.052175	3.659995
41	1	0	0.794284	0.865503	2.452724
42	6	0	-2.056599	-0.555685	3.623789
43	1	0	-0.336957	0.288069	4.604037
44	1	0	-2.577101	-0.813153	4.542008
45	6	0	-4.496576	-1.634446	0.990544
46	6	0	-3.956412	-1.430655	2.226072
47	6	0	5.020524	-0.855608	0.695136
48	6	0	4.564635	-2.104754	0.389939
49	1	0	-5.483677	-2.075397	0.887942
50	1	0	-4.506963	-1.708027	3.120047
51	1	0	6.050898	-0.706420	1.004014
52	1	0	5.227563	-2.962539	0.453567
53	17	0	0.790498	0.771908	-2.811055

GaClAI-HCl Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	0.365661	0.295384	-0.845076
2	6	0	-1.750131	2.314405	-0.990399
3	8	0	-0.482680	2.014447	-1.060879
4	6	0	-2.074303	3.765910	-1.270159
5	1	0	-1.406572	4.427653	-0.710265
6	1	0	-1.912207	3.966910	-2.335319
7	1	0	-3.112837	3.986462	-1.019358
8	8	0	-2.632313	1.482690	-0.735655
9	7	0	1.647014	-1.306138	-0.210285
10	6	0	2.846951	-0.876794	0.253049
11	6	0	1.435426	-2.614117	-0.306542
12	6	0	3.879871	-1.755109	0.652731
13	6	0	2.395002	-3.566632	0.074435
14	1	0	0.475449	-2.922730	-0.703810
15	6	0	3.617582	-3.139703	0.556149
16	1	0	2.169219	-4.622655	-0.023866
17	1	0	4.380717	-3.854424	0.851071
18	7	0	2.033246	1.330217	-0.093669
19	6	0	3.059105	0.540671	0.304404

20	6	0	2.198937	2.650675	-0.121871
21	6	0	4.299860	1.057628	0.737538
22	6	0	3.400475	3.255212	0.286362
23	1	0	1.347327	3.217089	-0.479235
24	6	0	4.447076	2.463634	0.721180
25	1	0	3.493163	4.334936	0.249141
26	1	0	5.384855	2.909111	1.041440
27	7	0	-1.201687	-1.022847	-1.214295
28	6	0	-1.540822	-1.512526	-2.403508
29	6	0	-1.975759	-1.289142	-0.134898
30	6	0	-2.670656	-2.332004	-2.567311
31	1	0	-0.886824	-1.250043	-3.228379
32	6	0	-3.123394	-2.105594	-0.202659
33	6	0	-3.458295	-2.632048	-1.471689
34	1	0	-2.914598	-2.711057	-3.553439
35	1	0	-4.339252	-3.259243	-1.576428
36	7	0	-0.508323	0.126179	1.091474
37	6	0	-1.599748	-0.677391	1.105218
38	6	0	-0.159151	0.750782	2.210710
39	6	0	-2.379527	-0.898029	2.261916
40	6	0	-0.867542	0.591693	3.411955
41	1	0	0.705333	1.403040	2.156465
42	6	0	-1.976884	-0.232877	3.440543
43	1	0	-0.546570	1.125601	4.299432
44	1	0	-2.549690	-0.363700	4.354123
45	6	0	-3.889086	-2.329098	0.991727
46	6	0	-3.532229	-1.749877	2.173497
47	6	0	5.327825	0.143430	1.149023
48	6	0	5.124750	-1.205077	1.111157
49	1	0	-4.773460	-2.956102	0.931791
50	1	0	-4.128911	-1.908722	3.066379
51	1	0	6.277970	0.547409	1.485569
52	1	0	5.911046	-1.888301	1.418024
53	17	0	1.265774	0.181069	-2.922242
54	17	0	-5.141650	1.894488	0.888886
55	1	0	-4.103562	1.800281	0.065406

GaClAl-AC Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	0.319775	-0.566464	0.494043
2	6	0	-4.755897	-1.758026	-0.536548
3	8	0	-4.238805	-0.656957	-0.625302
4	6	0	-6.210494	-2.051885	-0.808854
5	1	0	-6.728316	-1.135095	-1.091794
6	1	0	-6.297832	-2.792756	-1.610315
7	1	0	-6.676943	-2.485405	0.081826
8	8	0	-4.083788	-2.860254	-0.180009
9	7	0	1.566216	1.175096	0.406001
10	6	0	2.714682	0.962690	-0.279493
11	6	0	1.374540	2.354795	0.984529
12	6	0	3.712873	1.950868	-0.432603
13	6	0	2.305049	3.401403	0.886083
14	1	0	0.456870	2.479025	1.548174
15	6	0	3.472607	3.203191	0.173487
16	1	0	2.102970	4.347758	1.375397
17	1	0	4.211945	3.994285	0.084712
18	7	0	1.928996	-1.255469	-0.648115
19	6	0	2.912774	-0.343407	-0.836864
20	6	0	2.097100	-2.499570	-1.086386
21	6	0	4.104983	-0.642297	-1.528531
22	6	0	3.256287	-2.890498	-1.777841
23	1	0	1.281243	-3.186909	-0.891992
24	6	0	4.256059	-1.964565	-2.005016

25	1	0	3.352483	-3.915452	-2.118225
26	1	0	5.161760	-2.243198	-2.536627
27	7	0	-1.239077	0.533885	1.332263
28	6	0	-1.546382	0.574711	2.628072
29	6	0	-2.017793	1.189416	0.442145
30	6	0	-2.641167	1.317177	3.099865
31	1	0	-0.889121	0.007668	3.276623
32	6	0	-3.127270	1.972947	0.823620
33	6	0	-3.423985	2.023533	2.203309
34	1	0	-2.860071	1.327495	4.161858
35	1	0	-4.272010	2.608264	2.549054
36	7	0	-0.620232	0.247958	-1.234273
37	6	0	-1.677705	1.042946	-0.941736
38	6	0	-0.318018	0.038787	-2.512471
39	6	0	-2.454431	1.692651	-1.926066
40	6	0	-1.030880	0.636415	-3.562910
41	1	0	0.511749	-0.628895	-2.712461
42	6	0	-2.094287	1.471348	-3.271912
43	1	0	-0.743099	0.432980	-4.588412
44	1	0	-2.662413	1.946079	-4.066963
45	6	0	-3.881534	2.646934	-0.194885
46	6	0	-3.557266	2.513641	-1.512138
47	6	0	5.094987	0.385988	-1.688139
48	6	0	4.906354	1.630469	-1.164171
49	1	0	-4.729037	3.256442	0.104243
50	1	0	-4.143126	3.015858	-2.276175
51	1	0	6.007465	0.148138	-2.226766
52	1	0	5.665648	2.398089	-1.280137
53	17	0	-0.882406	-2.523784	0.292450
54	1	0	-3.143926	-2.614063	-0.023178
55	8	0	0.921369	-0.923767	2.265731
56	6	0	2.161085	-1.130526	2.679585
57	8	0	3.157405	-1.015170	1.976747
58	6	0	2.240690	-1.535919	4.139517
59	1	0	3.282441	-1.655164	4.439626
60	1	0	1.758356	-0.783194	4.772857
61	1	0	1.702308	-2.477666	4.291327

GaClAI-PA Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	0.076521	-0.473590	0.806257
2	6	0	-0.760581	4.807388	0.371375
3	8	0	-1.286271	3.881126	-0.203802
4	6	0	-1.411207	6.124824	0.721235
5	1	0	-1.380452	6.775596	-0.160012
6	1	0	-2.457545	5.949212	0.979376
7	1	0	-0.895757	6.628902	1.540897
8	8	0	1.281383	3.682117	0.363268
9	7	0	-0.531295	-1.859388	-0.688745
10	6	0	-1.779739	-1.606467	-1.149291
11	6	0	0.117306	-2.925358	-1.141729
12	6	0	-2.418836	-2.412011	-2.118103
13	6	0	-0.431920	-3.784016	-2.106903
14	1	0	1.103493	-3.108761	-0.730024
15	6	0	-1.697523	-3.526205	-2.599718
16	1	0	0.135951	-4.642301	-2.448477
17	1	0	-2.147833	-4.177050	-3.344028
18	7	0	-1.809380	0.247800	0.345292
19	6	0	-2.467897	-0.481343	-0.589404
20	6	0	-2.427667	1.259743	0.942979
21	6	0	-3.783631	-0.184349	-0.995928
22	6	0	-3.744028	1.621685	0.608381
23	1	0	-1.852222	1.796643	1.686843

24	6	0	-4.419268	0.908340	-0.360982
25	1	0	-4.209285	2.458901	1.115314
26	1	0	-5.436441	1.171340	-0.637789
27	7	0	2.036440	-1.212805	0.809356
28	6	0	2.535794	-2.066921	1.699143
29	6	0	2.851869	-0.668451	-0.124136
30	6	0	3.889058	-2.447175	1.676508
31	1	0	1.826915	-2.439396	2.429352
32	6	0	4.220865	-0.998936	-0.231830
33	6	0	4.728512	-1.922183	0.711128
34	1	0	4.258859	-3.145668	2.418900
35	1	0	5.776945	-2.205101	0.674126
36	7	0	0.957470	0.600520	-0.811383
37	6	0	2.266576	0.293759	-1.009519
38	6	0	0.402250	1.534549	-1.576792
39	6	0	3.059003	0.895416	-2.010175
40	6	0	1.106098	2.174360	-2.613181
41	1	0	-0.618608	1.813692	-1.353350
42	6	0	2.428841	1.855137	-2.836090
43	1	0	0.601980	2.929894	-3.204773
44	1	0	2.996939	2.344357	-3.622330
45	6	0	5.001850	-0.380562	-1.264993
46	6	0	4.441633	0.523613	-2.120404
47	6	0	-4.404809	-1.006567	-1.996332
48	6	0	-3.750031	-2.074049	-2.536523
49	1	0	6.052783	-0.640627	-1.349595
50	1	0	5.042321	0.991313	-2.894895
51	1	0	-5.417042	-0.767215	-2.308506
52	1	0	-4.232729	-2.695656	-3.284715
53	17	0	0.647445	1.227800	2.288678
54	1	0	1.092310	3.029889	1.082069
55	8	0	-0.309523	-1.726884	2.187836
56	6	0	-1.458818	-2.337373	2.431063
57	8	0	-2.450893	-2.262257	1.717452
58	6	0	-1.437386	-3.157218	3.707602
59	1	0	-2.393973	-3.662794	3.844904
60	1	0	-0.630930	-3.898147	3.673602
61	1	0	-1.238074	-2.503531	4.563576
62	8	0	0.531946	4.832712	0.800511

GaClAIPA-Cl Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	-0.139507	0.416340	0.014927
2	6	0	1.514353	2.244185	-2.064806
3	8	0	0.640652	1.600012	-1.473235
4	6	0	1.200527	3.444011	-2.913568
5	1	0	2.094843	3.826654	-3.406136
6	1	0	0.448130	3.182254	-3.664058
7	1	0	0.784172	4.219041	-2.261423
8	8	0	3.176957	0.892480	-1.219536
9	7	0	-1.412825	-0.820842	1.140621
10	6	0	-2.703782	-0.814091	0.731045
11	6	0	-1.086518	-1.512635	2.226590
12	6	0	-3.723383	-1.536336	1.390077
13	6	0	-2.025888	-2.277246	2.936892
14	1	0	-0.055437	-1.454621	2.547711
15	6	0	-3.342851	-2.293298	2.520809
16	1	0	-1.709546	-2.830200	3.814105
17	1	0	-4.090765	-2.868136	3.059729
18	7	0	-2.003668	0.679513	-0.986756
19	6	0	-3.023551	0.003454	-0.402794
20	6	0	-2.273670	1.500340	-1.997627
21	6	0	-4.361698	0.091518	-0.851147

22	6	0	-3.572442	1.660662	-2.508257
23	1	0	-1.428411	2.038279	-2.405974
24	6	0	-4.615501	0.951320	-1.943031
25	1	0	-3.741416	2.340604	-3.335940
26	1	0	-5.628717	1.054981	-2.321249
27	7	0	1.525989	-0.302490	0.956538
28	6	0	2.138961	0.221332	2.023208
29	6	0	2.093836	-1.368573	0.322028
30	6	0	3.313613	-0.367807	2.556011
31	1	0	1.630090	1.020292	2.534935
32	6	0	3.259029	-2.004954	0.782210
33	6	0	3.863049	-1.472044	1.955821
34	1	0	3.765910	0.089436	3.427580
35	1	0	4.763591	-1.932898	2.351344
36	7	0	0.336024	-1.159574	-1.259109
37	6	0	1.449598	-1.830849	-0.862758
38	6	0	-0.276038	-1.537300	-2.377778
39	6	0	1.979984	-2.930701	-1.581518
40	6	0	0.175597	-2.612590	-3.156005
41	1	0	-1.149625	-0.969013	-2.672668
42	6	0	1.300265	-3.312198	-2.757890
43	1	0	-0.357832	-2.881093	-4.060957
44	1	0	1.670930	-4.148248	-3.344506
45	6	0	3.771930	-3.124412	0.049933
46	6	0	3.160342	-3.572351	-1.087704
47	6	0	-5.376669	-0.666984	-0.176105
48	6	0	-5.069206	-1.450116	0.897451
49	1	0	4.673194	-3.609624	0.413164
50	1	0	3.565869	-4.415455	-1.638527
51	1	0	-6.400066	-0.596950	-0.532251
52	1	0	-5.845017	-2.013157	1.407695
53	17	0	3.397322	2.552011	1.144100
54	1	0	3.380322	1.441312	-0.354077
55	8	0	-0.507849	1.344401	3.011041
56	6	0	-0.588884	2.245260	2.179740
57	8	0	-0.487398	2.054123	0.875457
58	6	0	-0.770587	3.698389	2.555871
59	1	0	-1.508130	4.180793	1.908196
60	1	0	-1.065207	3.784376	3.602529
61	1	0	0.186062	4.212745	2.406179
62	8	0	2.803407	1.984704	-2.072113

GaAlAC-Cl Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	0.053282	0.344941	-0.040063
2	6	0	-1.245308	2.510511	1.833996
3	8	0	-0.718633	1.431679	1.435560
4	6	0	-0.850908	3.056219	3.181948
5	1	0	-0.075079	3.815686	3.023835
6	1	0	-1.701033	3.547760	3.658779
7	1	0	-0.456456	2.264316	3.821530
8	8	0	-2.102473	3.217643	1.211823
9	7	0	1.153672	-1.045466	-1.215445
10	6	0	2.478702	-1.053315	-0.929169
11	6	0	0.707447	-1.835016	-2.186477
12	6	0	3.413878	-1.858535	-1.617967
13	6	0	1.556147	-2.678289	-2.922649
14	1	0	-0.353805	-1.789686	-2.399792
15	6	0	2.908702	-2.692170	-2.640655
16	1	0	1.142202	-3.300774	-3.708080
17	1	0	3.588086	-3.329241	-3.199987
18	7	0	1.978443	0.562875	0.743568
19	6	0	2.924212	-0.176266	0.113590

20	6	0	2.350326	1.437201	1.673340
21	6	0	4.297565	-0.098209	0.433699
22	6	0	3.693334	1.583025	2.059832
23	1	0	1.563204	2.028409	2.116818
24	6	0	4.665746	0.816246	1.447076
25	1	0	3.950898	2.304236	2.827293
26	1	0	5.710634	0.914558	1.728125
27	7	0	-1.701957	-0.323552	-0.839039
28	6	0	-2.315107	0.193626	-1.904259
29	6	0	-2.304733	-1.317678	-0.132056
30	6	0	-3.557854	-0.320695	-2.349942
31	1	0	-1.769842	0.949840	-2.447834
32	6	0	-3.543851	-1.872716	-0.494117
33	6	0	-4.166930	-1.338689	-1.657257
34	1	0	-4.021612	0.127861	-3.220160
35	1	0	-5.125005	-1.735445	-1.980813
36	7	0	-0.404114	-1.225449	1.291059
37	6	0	-1.597075	-1.811375	1.006008
38	6	0	0.280990	-1.652971	2.345553
39	6	0	-2.149165	-2.857318	1.784524
40	6	0	-0.180470	-2.687790	3.175307
41	1	0	1.219370	-1.151031	2.552376
42	6	0	-1.393613	-3.290042	2.896824
43	1	0	0.415119	-2.997631	4.026787
44	1	0	-1.774336	-4.089099	3.526981
45	6	0	-4.085743	-2.928814	0.309016
46	6	0	-3.417976	-3.403421	1.404432
47	6	0	5.226255	-0.929618	-0.279065
48	6	0	4.801942	-1.777766	-1.259827
49	1	0	-5.047698	-3.349673	0.031181
50	1	0	-3.842130	-4.202613	2.004694
51	1	0	6.279996	-0.866826	-0.024240
52	1	0	5.512897	-2.399925	-1.795148
53	17	0	-3.333892	2.729493	-1.285817
54	1	0	-2.471146	2.922300	0.243807
55	8	0	0.234822	1.651051	-1.389465
56	6	0	0.583490	2.912027	-1.150302
57	8	0	0.980340	3.308517	-0.059695
58	6	0	0.406387	3.819101	-2.344819
59	1	0	0.897457	4.776915	-2.168092
60	1	0	0.798036	3.349620	-3.252156
61	1	0	-0.668438	3.982327	-2.491355

GaAI Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	0.000372	0.066891	-0.659551
2	8	0	0.403230	-0.769123	-2.453661
3	6	0	-0.000458	0.299376	-3.036087
4	8	0	-0.402068	1.234841	-2.253651
5	6	0	-0.005158	0.453546	-4.520934
6	1	0	0.639749	1.293519	-4.801019
7	1	0	0.341561	-0.456711	-5.009937
8	1	0	-1.015801	0.705642	-4.858521
9	7	0	-0.952127	1.205537	0.736378
10	6	0	-2.252415	0.846326	0.924270
11	6	0	-0.465818	2.237014	1.428640
12	6	0	-3.115692	1.520671	1.814686
13	6	0	-1.245895	2.960700	2.341705
14	1	0	0.569830	2.500435	1.250083
15	6	0	-2.569693	2.607472	2.536006
16	1	0	-0.805084	3.792946	2.878892
17	1	0	-3.193171	3.159306	3.233791
18	7	0	-1.852688	-0.864544	-0.671925

19	6	0	-2.739379	-0.261427	0.159968
20	6	0	-2.258074	-1.883333	-1.432620
21	6	0	-4.083216	-0.674892	0.281801
22	6	0	-3.576899	-2.363587	-1.379096
23	1	0	-1.517020	-2.315968	-2.096504
24	6	0	-4.487593	-1.765455	-0.524497
25	1	0	-3.867528	-3.195289	-2.011370
26	1	0	-5.512069	-2.123136	-0.471467
27	7	0	1.854131	0.979865	-0.487615
28	6	0	2.260016	2.128590	-1.032217
29	6	0	2.740605	0.223615	0.208149
30	6	0	3.579393	2.587538	-0.886032
31	1	0	1.518597	2.684651	-1.596327
32	6	0	4.085012	0.603460	0.408016
33	6	0	4.490066	1.831370	-0.167409
34	1	0	3.870570	3.527593	-1.341530
35	1	0	5.515004	2.170498	-0.045794
36	7	0	0.951692	-1.325787	0.485038
37	6	0	2.252584	-1.012520	0.739186
38	6	0	0.464197	-2.472736	0.961007
39	6	0	3.115390	-1.850275	1.478420
40	6	0	1.243743	-3.363348	1.712745
41	1	0	-0.571951	-2.694348	0.734975
42	6	0	2.568189	-3.057241	1.971761
43	1	0	0.801946	-4.284572	2.075626
44	1	0	3.191261	-3.736759	2.546379
45	6	0	4.944676	-0.265065	1.162920
46	6	0	4.477965	-1.440195	1.678403
47	6	0	-4.943271	0.026410	1.193799
48	6	0	-4.477577	1.077371	1.930710
49	1	0	5.978519	0.028993	1.315761
50	1	0	5.136707	-2.089919	2.246319
51	1	0	-5.976609	-0.293480	1.286245
52	1	0	-5.136611	1.601408	2.616036

GaPI Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	0.010384	0.555401	-0.237672
2	8	0	0.490831	1.537568	-1.839471
3	6	0	-0.412705	3.247695	-0.583933
4	8	0	-0.542945	2.402439	0.334542
5	6	0	-0.808270	4.680622	-0.461601
6	1	0	-0.252197	5.139055	0.363107
7	1	0	-0.609898	5.223831	-1.386354
8	1	0	-1.872955	4.739630	-0.212460
9	8	0	0.095762	2.918514	-1.745002
10	7	0	-0.894388	-0.304815	1.399340
11	6	0	-2.183506	-0.681188	1.171994
12	6	0	-0.376445	-0.512174	2.611059
13	6	0	-3.002209	-1.271886	2.158988
14	6	0	-1.109813	-1.099850	3.652252
15	1	0	0.649183	-0.198657	2.763315
16	6	0	-2.421975	-1.478911	3.431575
17	1	0	-0.641535	-1.244544	4.619398
18	1	0	-3.009509	-1.930631	4.225889
19	7	0	-1.858780	0.114101	-1.034375
20	6	0	-2.707676	-0.445100	-0.137888
21	6	0	-2.291791	0.385602	-2.266537
22	6	0	-4.042174	-0.782958	-0.447125
23	6	0	-3.605538	0.086622	-2.665679
24	1	0	-1.570994	0.843169	-2.936462
25	6	0	-4.478517	-0.497318	-1.763149
26	1	0	-3.921744	0.318544	-3.676770

27	1	0	-5.497354	-0.735543	-2.055756
28	7	0	1.853689	0.801140	0.698583
29	6	0	2.247024	1.778238	1.516654
30	6	0	2.760510	-0.125242	0.292976
31	6	0	3.566334	1.868435	1.987994
32	1	0	1.490114	2.497562	1.810294
33	6	0	4.108637	-0.116675	0.713913
34	6	0	4.496790	0.924130	1.589678
35	1	0	3.841972	2.678323	2.654330
36	1	0	5.523446	0.977232	1.940902
37	7	0	0.995044	-1.067263	-1.001550
38	6	0	2.296444	-1.135520	-0.609552
39	6	0	0.530736	-1.983057	-1.851861
40	6	0	3.183911	-2.133760	-1.067428
41	6	0	1.334607	-3.018426	-2.350084
42	1	0	-0.506111	-1.889301	-2.152395
43	6	0	2.660160	-3.095741	-1.961768
44	1	0	0.911422	-3.739048	-3.040849
45	1	0	3.303360	-3.884167	-2.342311
46	6	0	4.992769	-1.142434	0.235257
47	6	0	4.547664	-2.111843	-0.616378
48	6	0	-4.856847	-1.380864	0.573678
49	6	0	-4.355853	-1.617814	1.821817
50	1	0	6.027921	-1.131782	0.562393
51	1	0	5.224726	-2.881545	-0.973839
52	1	0	-5.883352	-1.642598	0.335846
53	1	0	-4.980138	-2.070748	2.585913

GaAI2 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	0.000000	0.000000	0.725122
2	6	0	2.285442	-0.749685	2.341849
3	8	0	1.381144	0.160340	2.027349
4	6	0	3.133354	-0.364345	3.540091
5	1	0	3.876285	-1.137606	3.739034
6	1	0	3.637890	0.591311	3.358770
7	1	0	2.495548	-0.229237	4.420296
8	8	0	2.450370	-1.804678	1.740708
9	7	0	-1.413364	0.350330	-0.828537
10	6	0	-1.538953	1.659492	-1.152925
11	6	0	-2.200391	-0.533534	-1.431499
12	6	0	-2.451746	2.130247	-2.122338
13	6	0	-3.137930	-0.165509	-2.409719
14	1	0	-2.089921	-1.568357	-1.128401
15	6	0	-3.261919	1.165886	-2.760337
16	1	0	-3.756970	-0.926124	-2.872456
17	1	0	-3.981961	1.478956	-3.511273
18	7	0	0.134687	2.074781	0.476665
19	6	0	-0.710598	2.589351	-0.443858
20	6	0	0.877353	2.893017	1.215095
21	6	0	-0.812800	3.971239	-0.701815
22	6	0	0.836917	4.287024	1.036504
23	1	0	1.511878	2.409553	1.948559
24	6	0	0.000000	4.826199	0.077479
25	1	0	1.457236	4.923092	1.658139
26	1	0	-0.047989	5.900631	-0.077127
27	7	0	-0.134687	-2.074781	0.476665
28	6	0	-0.877353	-2.893017	1.215095
29	6	0	0.710598	-2.589351	-0.443858
30	6	0	-0.836917	-4.287024	1.036504
31	1	0	-1.511878	-2.409553	1.948559
32	6	0	0.812800	-3.971239	-0.701815
33	6	0	0.000000	-4.826199	0.077479

34	1	0	-1.457236	-4.923092	1.658139
35	1	0	0.047989	-5.900631	-0.077127
36	7	0	1.413364	-0.350330	-0.828537
37	6	0	1.538953	-1.659492	-1.152925
38	6	0	2.200391	0.533534	-1.431499
39	6	0	2.451746	-2.130247	-2.122338
40	6	0	3.137930	0.165509	-2.409719
41	1	0	2.089921	1.568357	-1.128401
42	6	0	3.261919	-1.165886	-2.760337
43	1	0	3.756970	0.926124	-2.872456
44	1	0	3.981961	-1.478956	-3.511273
45	6	0	1.736519	-4.423724	-1.704586
46	6	0	2.520680	-3.540688	-2.386893
47	6	0	-1.736519	4.423724	-1.704586
48	6	0	-2.520680	3.540688	-2.386893
49	1	0	1.807808	-5.489121	-1.902654
50	1	0	3.223342	-3.893556	-3.135908
51	1	0	-1.807808	5.489121	-1.902654
52	1	0	-3.223342	3.893556	-3.135908
53	8	0	-2.450370	1.804678	1.740708
54	6	0	-2.285442	0.749685	2.341849
55	8	0	-1.381144	-0.160340	2.027349
56	6	0	-3.133354	0.364345	3.540091
57	1	0	-2.495548	0.229237	4.420296
58	1	0	-3.876285	1.137606	3.739034
59	1	0	-3.637890	-0.591311	3.358770

GaAI2-HCl Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	0.125176	0.432264	0.026361
2	6	0	-1.827365	1.965770	1.405023
3	8	0	-0.758630	1.225974	1.545967
4	6	0	-2.324141	2.632162	2.667645
5	1	0	-1.809848	3.595304	2.772436
6	1	0	-3.396559	2.827340	2.602552
7	1	0	-2.098861	2.028251	3.549594
8	8	0	-2.384230	2.134901	0.311874
9	7	0	1.449938	-0.721722	-1.223515
10	6	0	2.751968	-0.568057	-0.879530
11	6	0	1.155060	-1.476745	-2.274699
12	6	0	3.815974	-1.176040	-1.583919
13	6	0	2.139727	-2.130765	-3.034584
14	1	0	0.105993	-1.558806	-2.535855
15	6	0	3.470072	-1.983169	-2.690603
16	1	0	1.846652	-2.734675	-3.886250
17	1	0	4.251668	-2.471995	-3.265498
18	7	0	1.973820	0.821588	0.884008
19	6	0	3.034666	0.274404	0.246722
20	6	0	2.172974	1.657107	1.898766
21	6	0	4.369096	0.514304	0.639283
22	6	0	3.466966	1.951458	2.362526
23	1	0	1.282183	2.078509	2.345394
24	6	0	4.561805	1.382342	1.739161
25	1	0	3.591004	2.631767	3.197571
26	1	0	5.570180	1.600875	2.079842
27	7	0	-1.543195	-0.443244	-0.841454
28	6	0	-2.277691	0.124064	-1.794079
29	6	0	-1.957563	-1.600027	-0.275248
30	6	0	-3.465364	-0.468359	-2.256609
31	1	0	-1.896191	1.057350	-2.188137
32	6	0	-3.132394	-2.270011	-0.677745
33	6	0	-3.891963	-1.661598	-1.704222
34	1	0	-4.043799	0.029620	-3.026051

35	1	0	-4.811778	-2.130846	-2.041809
36	7	0	-0.059477	-1.406038	1.147544
37	6	0	-1.148957	-2.127257	0.785395
38	6	0	0.699166	-1.857741	2.139077
39	6	0	-1.519602	-3.339247	1.411552
40	6	0	0.421987	-3.056753	2.817202
41	1	0	1.549414	-1.245891	2.418783
42	6	0	-0.686085	-3.799257	2.455082
43	1	0	1.072622	-3.380302	3.622150
44	1	0	-0.928065	-4.725557	2.968683
45	6	0	-3.484544	-3.499898	-0.025006
46	6	0	-2.708536	-4.015085	0.972522
47	6	0	5.430489	-0.119391	-0.091738
48	6	0	5.164995	-0.933059	-1.154684
49	1	0	-4.388704	-4.013388	-0.338290
50	1	0	-2.986619	-4.944239	1.460986
51	1	0	6.455479	0.065627	0.215819
52	1	0	5.975852	-1.403940	-1.702462
53	17	0	-5.328432	2.361172	-0.267514
54	1	0	-4.040400	2.412157	0.058809
55	8	0	0.188028	1.745246	-1.349946
56	6	0	0.438089	3.016913	-1.060656
57	8	0	0.773433	3.409490	0.049322
58	6	0	0.253421	3.951812	-2.238376
59	1	0	0.673112	4.932383	-2.009881
60	1	0	0.717750	3.539843	-3.139407
61	1	0	-0.818095	4.064261	-2.441808

GaPI2 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	0.000000	0.000000	0.804512
2	8	0	-2.652653	-0.306292	1.761831
3	7	0	1.363739	-0.397057	-0.800336
4	6	0	1.459783	-1.716891	-1.093992
5	6	0	2.105581	0.465043	-1.487128
6	6	0	2.310728	-2.224109	-2.101747
7	6	0	2.969537	0.061116	-2.517654
8	1	0	2.018236	1.509762	-1.210233
9	6	0	3.073208	-1.282929	-2.826852
10	1	0	3.553542	0.803460	-3.050410
11	1	0	3.741932	-1.622864	-3.612839
12	7	0	-0.136165	-2.067280	0.624432
13	6	0	0.669890	-2.619706	-0.308601
14	6	0	-0.831641	-2.853141	1.440244
15	6	0	0.768284	-4.011276	-0.510669
16	6	0	-0.786845	-4.253811	1.324410
17	1	0	-1.431092	-2.348176	2.188585
18	6	0	0.000000	-4.832825	0.346059
19	1	0	-1.367798	-4.863783	2.007214
20	1	0	0.045139	-5.912926	0.236965
21	7	0	0.136165	2.067280	0.624432
22	6	0	0.831641	2.853141	1.440244
23	6	0	-0.669890	2.619706	-0.308601
24	6	0	0.786845	4.253811	1.324410
25	1	0	1.431092	2.348176	2.188585
26	6	0	-0.768284	4.011276	-0.510669
27	6	0	0.000000	4.832825	0.346059
28	1	0	1.367798	4.863783	2.007214
29	1	0	-0.045139	5.912926	0.236965
30	7	0	-1.363739	0.397057	-0.800336
31	6	0	-1.459783	1.716891	-1.093992
32	6	0	-2.105581	-0.465043	-1.487128
33	6	0	-2.310728	2.224109	-2.101747

34	6	0	-2.969537	-0.061116	-2.517654
35	1	0	-2.018236	-1.509762	-1.210233
36	6	0	-3.073208	1.282929	-2.826852
37	1	0	-3.553542	-0.803460	-3.050410
38	1	0	-3.741932	1.622864	-3.612839
39	6	0	-1.636569	4.501118	-1.544840
40	6	0	-2.369439	3.644000	-2.312564
41	6	0	1.636569	-4.501118	-1.544840
42	6	0	2.369439	-3.644000	-2.312564
43	1	0	-1.704513	5.573602	-1.701650
44	1	0	-3.025764	4.025624	-3.089040
45	1	0	1.704513	-5.573602	-1.701650
46	1	0	3.025764	-4.025624	-3.089040
47	8	0	-1.321226	0.070426	2.187042
48	8	0	1.321226	-0.070426	2.187042
49	8	0	2.652653	0.306292	1.761831
50	6	0	3.468572	-0.766982	1.577930
51	6	0	-3.468572	0.766982	1.577930
52	6	0	-4.902977	0.288943	1.506324
53	1	0	-5.349924	0.382155	2.502621
54	1	0	-5.464638	0.927575	0.821390
55	1	0	-4.974214	-0.757394	1.200345
56	6	0	4.902977	-0.288943	1.506324
57	1	0	5.349924	-0.382155	2.502621
58	1	0	5.464638	-0.927575	0.821390
59	1	0	4.974214	0.757394	1.200345
60	8	0	-3.104335	1.915968	1.491493
61	8	0	3.104335	-1.915968	1.491493

GaAlPIa Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	0.166666	0.878265	0.308903
2	6	0	0.401023	3.586240	-0.574427
3	8	0	-0.338159	2.609397	-0.805154
4	6	0	0.115200	4.975751	-1.055253
5	1	0	-0.021323	4.964289	-2.141121
6	1	0	-0.817449	5.328988	-0.602792
7	1	0	0.926832	5.655558	-0.792249
8	8	0	1.744011	2.117576	0.527033
9	7	0	-0.743963	-1.278728	0.707342
10	6	0	-1.975320	-1.593383	0.226450
11	6	0	-0.107805	-2.186830	1.440145
12	6	0	-2.563790	-2.870259	0.430321
13	6	0	-0.608904	-3.474561	1.687021
14	1	0	0.833961	-1.889610	1.870734
15	6	0	-1.834169	-3.826007	1.167793
16	1	0	-0.031284	-4.166255	2.290403
17	1	0	-2.258084	-4.812263	1.335669
18	7	0	-2.169730	0.642101	-0.621027
19	6	0	-2.736904	-0.576209	-0.457928
20	6	0	-2.906208	1.610872	-1.158860
21	6	0	-4.057383	-0.870565	-0.893665
22	6	0	-4.227789	1.422653	-1.600920
23	1	0	-2.418670	2.570985	-1.257333
24	6	0	-4.799932	0.174358	-1.483928
25	1	0	-4.772732	2.256075	-2.031481
26	1	0	-5.813836	-0.015165	-1.825858
27	7	0	2.009716	-0.173721	0.962408
28	6	0	2.611020	-0.149511	2.146108
29	6	0	2.656512	-0.712349	-0.093726
30	6	0	3.883740	-0.720922	2.341975
31	1	0	2.044216	0.289615	2.958209
32	6	0	3.922354	-1.332034	0.008333

33	6	0	4.532767	-1.325083	1.283824
34	1	0	4.336292	-0.684539	3.326893
35	1	0	5.508547	-1.784691	1.415210
36	7	0	0.836204	0.069584	-1.430233
37	6	0	2.009090	-0.615579	-1.369610
38	6	0	0.230765	0.202067	-2.608882
39	6	0	2.617483	-1.186581	-2.512258
40	6	0	0.750203	-0.347871	-3.789179
41	1	0	-0.689250	0.770206	-2.612368
42	6	0	1.942916	-1.043888	-3.743666
43	1	0	0.215331	-0.211389	-4.722391
44	1	0	2.373977	-1.471480	-4.644694
45	6	0	4.512976	-1.911902	-1.164200
46	6	0	3.882440	-1.850836	-2.371866
47	6	0	-4.598642	-2.184322	-0.708570
48	6	0	-3.876386	-3.147475	-0.075366
49	1	0	5.479922	-2.398049	-1.072892
50	1	0	4.336890	-2.289612	-3.255101
51	1	0	-5.602712	-2.388546	-1.069121
52	1	0	-4.290981	-4.139148	0.081440
53	8	0	-0.022618	0.128772	3.446752
54	6	0	-0.718091	1.059210	3.047823
55	8	0	-0.755797	1.490161	1.804914
56	6	0	-1.632042	1.841177	3.970634
57	1	0	-1.619778	1.406530	4.970763
58	1	0	-1.300344	2.884140	4.019730
59	1	0	-2.652944	1.846369	3.575379
60	8	0	1.496367	3.474115	0.120057

GaAIPIb Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	0.041618	0.463249	0.029677
2	6	0	0.516810	3.774644	-1.458712
3	8	0	-0.426882	3.638195	-2.205274
4	6	0	1.074680	5.103054	-0.999426
5	1	0	1.458055	5.642544	-1.871397
6	1	0	0.262453	5.697849	-0.572159
7	1	0	1.875357	4.986305	-0.267036
8	8	0	0.826605	1.471709	-1.393708
9	7	0	-0.949187	-1.028589	1.150474
10	6	0	-2.200065	-1.296060	0.696860
11	6	0	-0.514701	-1.653037	2.238412
12	6	0	-3.063075	-2.227974	1.314254
13	6	0	-1.294245	-2.607670	2.913519
14	1	0	0.469898	-1.381039	2.595758
15	6	0	-2.564594	-2.898494	2.454242
16	1	0	-0.895936	-3.093947	3.796901
17	1	0	-3.187929	-3.626654	2.965853
18	7	0	-1.769565	0.320589	-0.983157
19	6	0	-2.647048	-0.560500	-0.449475
20	6	0	-2.128218	1.070342	-2.021770
21	6	0	-3.944947	-0.759236	-0.963543
22	6	0	-3.407434	0.941225	-2.598866
23	1	0	-1.391391	1.790586	-2.372956
24	6	0	-4.309203	0.030819	-2.080672
25	1	0	-3.670960	1.568202	-3.443558
26	1	0	-5.299118	-0.079620	-2.515275
27	7	0	1.915266	0.154843	0.919324
28	6	0	2.418668	0.832580	1.948876
29	6	0	2.719344	-0.696544	0.231628
30	6	0	3.758190	0.689312	2.351695
31	1	0	1.723277	1.464037	2.487069
32	6	0	4.071842	-0.915123	0.576035

33	6	0	4.583864	-0.182820	1.671479
34	1	0	4.121523	1.263780	3.196502
35	1	0	5.621151	-0.314667	1.966895
36	7	0	0.849172	-1.131043	-1.179432
37	6	0	2.144299	-1.396472	-0.881220
38	6	0	0.295128	-1.747303	-2.215614
39	6	0	2.930728	-2.312670	-1.617946
40	6	0	0.989162	-2.682310	-3.001702
41	1	0	-0.735353	-1.496616	-2.437979
42	6	0	2.307555	-2.965661	-2.704559
43	1	0	0.488215	-3.158869	-3.837065
44	1	0	2.873066	-3.677515	-3.299377
45	6	0	4.847597	-1.849059	-0.189898
46	6	0	4.299316	-2.522928	-1.240776
47	6	0	-4.799341	-1.721649	-0.326029
48	6	0	-4.375358	-2.426173	0.764237
49	1	0	5.886128	-2.007959	0.085054
50	1	0	4.893935	-3.226840	-1.815420
51	1	0	-5.797799	-1.875876	-0.724582
52	1	0	-5.033189	-3.146511	1.241534
53	8	0	-0.293804	1.174344	3.181088
54	6	0	-0.823899	1.950617	2.383926
55	8	0	-0.685758	1.882752	1.079667
56	6	0	-1.698592	3.101599	2.841762
57	1	0	-1.762453	3.119958	3.930355
58	1	0	-1.288162	4.049031	2.476941
59	1	0	-2.701137	3.003428	2.411702
60	8	0	1.250042	2.769751	-0.922834

GaAlEO Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	-0.025745	0.604199	0.003316
2	7	0	-0.780706	-0.881211	1.232917
3	6	0	-2.036829	-1.254880	0.869863
4	6	0	-0.231912	-1.437236	2.311304
5	6	0	-2.790360	-2.211999	1.586116
6	6	0	-0.899426	-2.402307	3.080301
7	1	0	0.762449	-1.101912	2.582388
8	6	0	-2.177221	-2.791031	2.720779
9	1	0	-0.411316	-2.824682	3.951472
10	1	0	-2.716816	-3.531070	3.305003
11	7	0	-1.824966	0.281489	-0.941060
12	6	0	-2.600590	-0.623320	-0.286043
13	6	0	-2.324551	0.931937	-1.991642
14	6	0	-3.913778	-0.941133	-0.696085
15	6	0	-3.618582	0.675838	-2.471566
16	1	0	-1.677161	1.659336	-2.461033
17	6	0	-4.412565	-0.256946	-1.829722
18	1	0	-3.984851	1.222745	-3.333059
19	1	0	-5.418588	-0.464936	-2.183190
20	7	0	1.852965	0.630074	0.902491
21	6	0	2.234525	1.391200	1.930258
22	6	0	2.740366	-0.233312	0.346873
23	6	0	3.536119	1.318356	2.455825
24	1	0	1.473905	2.052233	2.330108
25	6	0	4.065923	-0.377648	0.810141
26	6	0	4.449896	0.438399	1.901464
27	1	0	3.809528	1.952008	3.292323
28	1	0	5.459479	0.367941	2.296748
29	7	0	0.989240	-0.800927	-1.163573
30	6	0	2.271357	-1.010731	-0.760701
31	6	0	0.525920	-1.498575	-2.199920
32	6	0	3.138980	-1.930782	-1.389661

33	6	0	1.311677	-2.437610	-2.886844
34	1	0	-0.494692	-1.298307	-2.504047
35	6	0	2.616435	-2.658071	-2.484147
36	1	0	0.887217	-2.977889	-3.725717
37	1	0	3.242880	-3.379136	-3.001670
38	6	0	4.927819	-1.323252	0.157031
39	6	0	4.481520	-2.069113	-0.896375
40	6	0	-4.658674	-1.917303	0.048609
41	6	0	-4.118037	-2.530390	1.141557
42	1	0	5.946313	-1.435055	0.516225
43	1	0	5.142010	-2.780121	-1.383261
44	1	0	-5.667198	-2.157823	-0.273602
45	1	0	-4.690221	-3.265536	1.699061
46	6	0	1.788955	2.380186	-2.162709
47	6	0	0.856839	3.327090	-1.538423
48	8	0	0.556231	1.899605	-1.538756
49	8	0	-0.554614	1.984495	1.173814
50	1	0	1.092171	3.728790	-0.558200
51	1	0	0.170821	3.911208	-2.141589
52	1	0	2.699278	2.106526	-1.636181
53	1	0	1.799581	2.252486	-3.241340
54	6	0	-1.395404	2.976899	0.866444
55	6	0	-1.836394	3.786421	2.063881
56	1	0	-0.966962	4.210607	2.577904
57	1	0	-2.501566	4.590096	1.747701
58	1	0	-2.350677	3.142078	2.784910
59	8	0	-1.758527	3.210918	-0.277412

TS1 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	0.347315	1.106096	-0.137080
2	6	0	-0.040558	-0.705424	2.847387
3	8	0	0.389539	-0.563426	1.702577
4	6	0	0.212849	-1.936903	3.673235
5	1	0	-0.727182	-2.485994	3.798414
6	1	0	0.945428	-2.575884	3.179809
7	1	0	0.560530	-1.657916	4.671977
8	8	0	-0.788651	0.190795	3.473476
9	7	0	1.014906	-0.439157	-1.304268
10	6	0	2.300209	-0.792166	-1.063980
11	6	0	0.362945	-0.991030	-2.321078
12	6	0	2.972055	-1.780284	-1.817273
13	6	0	0.952879	-1.973103	-3.130685
14	1	0	-0.651409	-0.651406	-2.485772
15	6	0	2.249665	-2.379964	-2.872166
16	1	0	0.386136	-2.398248	-3.951361
17	1	0	2.723653	-3.143174	-3.483111
18	7	0	2.311616	0.896743	0.600666
19	6	0	2.995699	-0.081703	-0.031854
20	6	0	2.916917	1.619656	1.533818
21	6	0	4.342874	-0.387335	0.255253
22	6	0	4.255419	1.383936	1.895665
23	1	0	2.318596	2.391745	2.005088
24	6	0	4.967999	0.382877	1.262441
25	1	0	4.714798	1.997246	2.662873
26	1	0	6.004614	0.188431	1.523097
27	7	0	-1.804826	1.111879	-0.777227
28	6	0	-2.065253	2.330929	-1.266861
29	6	0	-2.869490	0.292328	-0.481361
30	6	0	-3.353710	2.831463	-1.483719
31	1	0	-1.207481	2.948063	-1.498973
32	6	0	-4.208153	0.757748	-0.624154
33	6	0	-4.431456	2.054302	-1.131873

34	1	0	-3.472758	3.828850	-1.891683
35	1	0	-5.449962	2.415206	-1.245358
36	7	0	-1.421818	-1.577395	-0.064046
37	6	0	-2.676073	-1.086999	-0.072507
38	6	0	-1.229476	-2.837967	0.291699
39	6	0	-3.805066	-1.887815	0.269278
40	6	0	-2.270409	-3.708360	0.667620
41	1	0	-0.198357	-3.185914	0.282932
42	6	0	-3.562871	-3.225389	0.653682
43	1	0	-2.052818	-4.733833	0.948725
44	1	0	-4.401528	-3.861390	0.924049
45	6	0	-5.316294	-0.077994	-0.261196
46	6	0	-5.126882	-1.347111	0.185902
47	6	0	4.991604	-1.426970	-0.494546
48	6	0	4.335874	-2.091583	-1.489707
49	1	0	-6.316868	0.333135	-0.358232
50	1	0	-5.970278	-1.974103	0.460601
51	1	0	6.026245	-1.664212	-0.265305
52	1	0	4.843010	-2.861747	-2.063209
53	17	0	1.104125	2.589975	-1.664072
54	17	0	-0.333863	2.540870	1.521324
55	1	0	-0.849601	1.003526	2.909196

TS2 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	0.108487	0.314130	-0.351193
2	6	0	-1.532914	1.827737	1.908919
3	8	0	-0.603459	1.162958	1.365837
4	6	0	-1.933553	1.500595	3.324614
5	1	0	-1.538430	2.276921	3.990032
6	1	0	-3.022529	1.522854	3.419023
7	1	0	-1.535925	0.532204	3.631081
8	8	0	-2.158368	2.796674	1.361547
9	7	0	1.506520	-1.349905	-0.718504
10	6	0	2.769196	-1.056606	-0.335332
11	6	0	1.278729	-2.478167	-1.380105
12	6	0	3.867291	-1.914740	-0.578061
13	6	0	2.302689	-3.392871	-1.675692
14	1	0	0.255403	-2.665904	-1.691001
15	6	0	3.595400	-3.116635	-1.268389
16	1	0	2.071097	-4.300042	-2.222840
17	1	0	4.405296	-3.808122	-1.483334
18	7	0	1.890139	1.009732	0.466189
19	6	0	2.973573	0.207855	0.309193
20	6	0	2.050468	2.230482	0.974799
21	6	0	4.272126	0.591392	0.707517
22	6	0	3.307842	2.692284	1.400524
23	1	0	1.172138	2.865747	0.998529
24	6	0	4.414675	1.875737	1.280709
25	1	0	3.390947	3.695477	1.803153
26	1	0	5.395671	2.215467	1.601102
27	7	0	-1.892632	0.373387	-1.038540
28	6	0	-2.374594	1.267399	-1.899246
29	6	0	-2.723784	-0.552875	-0.506096
30	6	0	-3.731027	1.261397	-2.278143
31	1	0	-1.675521	2.006621	-2.272366
32	6	0	-4.093502	-0.636468	-0.830512
33	6	0	-4.588117	0.314744	-1.754386
34	1	0	-4.084266	2.012195	-2.975918
35	1	0	-5.637005	0.295144	-2.036997
36	7	0	-0.831196	-1.326205	0.701902
37	6	0	-2.151390	-1.465662	0.438488
38	6	0	-0.270251	-2.114202	1.612713

39	6	0	-2.964575	-2.440932	1.062192
40	6	0	-0.997208	-3.099814	2.299569
41	1	0	0.784581	-1.958502	1.812797
42	6	0	-2.340662	-3.272877	2.017737
43	1	0	-0.498178	-3.716900	3.038534
44	1	0	-2.921727	-4.035728	2.528457
45	6	0	-4.891841	-1.653217	-0.204778
46	6	0	-4.352795	-2.517419	0.704408
47	6	0	5.364274	-0.314593	0.484854
48	6	0	5.172362	-1.515601	-0.133382
49	1	0	-5.944586	-1.717344	-0.463838
50	1	0	-4.970477	-3.274859	1.177542
51	1	0	6.357579	-0.014708	0.805454
52	1	0	6.009850	-2.183437	-0.311704
53	17	0	0.760425	0.937253	-2.424254
54	17	0	-0.579935	3.845584	-0.677547
55	1	0	-1.595021	3.218867	0.480778

TS3 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	-0.144266	-0.909009	-0.121101
2	6	0	1.997778	-1.590655	2.217129
3	8	0	1.135139	-0.918505	1.657092
4	6	0	2.440209	-1.344958	3.633005
5	1	0	1.759887	-1.882111	4.304280
6	1	0	3.453203	-1.713172	3.804318
7	1	0	2.373808	-0.277507	3.851315
8	8	0	2.258111	-2.966531	0.359717
9	7	0	-1.086963	0.578063	-1.326921
10	6	0	-2.210379	1.067995	-0.764602
11	6	0	-0.771189	0.941463	-2.561222
12	6	0	-3.063017	1.987110	-1.412549
13	6	0	-1.550797	1.855992	-3.290081
14	1	0	0.116459	0.491341	-2.991090
15	6	0	-2.694110	2.382271	-2.717884
16	1	0	-1.255582	2.130799	-4.296705
17	1	0	-3.316013	3.086257	-3.263749
18	7	0	-1.667392	-0.300805	1.107188
19	6	0	-2.520855	0.593928	0.549271
20	6	0	-1.918279	-0.760375	2.330117
21	6	0	-3.678604	1.061103	1.207134
22	6	0	-3.041135	-0.342114	3.063382
23	1	0	-1.228342	-1.501004	2.710872
24	6	0	-3.925816	0.559810	2.504785
25	1	0	-3.206768	-0.750273	4.054068
26	1	0	-4.809310	0.883556	3.048067
27	7	0	1.694424	-0.289148	-0.962223
28	6	0	2.230083	-1.146067	-1.838995
29	6	0	2.381996	0.850369	-0.642487
30	6	0	3.476252	-0.943508	-2.446584
31	1	0	1.628424	-2.012353	-2.073938
32	6	0	3.656008	1.115626	-1.213832
33	6	0	4.195552	0.184834	-2.127665
34	1	0	3.851092	-1.682430	-3.145695
35	1	0	5.170321	0.374201	-2.568749
36	7	0	0.596935	1.581917	0.795504
37	6	0	1.822325	1.819180	0.277912
38	6	0	0.092367	2.452657	1.655215
39	6	0	2.573372	2.982631	0.607213
40	6	0	0.756636	3.628065	2.055365
41	1	0	-0.890528	2.222141	2.058258
42	6	0	1.999946	3.893214	1.523025
43	1	0	0.288311	4.302206	2.764911

44	1	0	2.547936	4.790636	1.796972
45	6	0	4.375323	2.305185	-0.862707
46	6	0	3.859153	3.203635	0.017734
47	6	0	-4.530484	2.001026	0.531618
48	6	0	-4.237173	2.445140	-0.724383
49	1	0	5.347840	2.468779	-1.317648
50	1	0	4.409665	4.101162	0.284545
51	1	0	-5.423153	2.348632	1.043169
52	1	0	-4.893461	3.150107	-1.225992
53	17	0	-0.534915	-3.289400	1.045114
54	1	0	1.348404	-3.378683	0.537442
55	8	0	-0.351323	-2.066822	-1.636373
56	6	0	-1.613576	-2.428158	-1.825325
57	8	0	-2.542723	-1.894236	-1.229969
58	6	0	-1.797209	-3.557262	-2.810042
59	1	0	-2.842473	-3.628677	-3.113673
60	1	0	-1.152534	-3.428730	-3.684406
61	1	0	-1.504486	-4.491068	-2.315914
62	8	0	2.651771	-2.629373	1.702586

TS4 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	-0.044492	0.713701	-0.321182
2	6	0	-0.340281	3.672336	0.492512
3	8	0	0.216370	2.765566	1.116467
4	6	0	-0.128862	5.139514	0.744460
5	1	0	-0.378315	5.361376	1.786928
6	1	0	0.926439	5.388616	0.593217
7	1	0	-0.745900	5.749439	0.082917
8	8	0	-1.485893	2.044748	-0.642911
9	7	0	0.720465	-1.358316	-0.679812
10	6	0	1.934021	-1.642661	-0.143590
11	6	0	0.125090	-2.288142	-1.418917
12	6	0	2.556907	-2.907809	-0.293946
13	6	0	0.661152	-3.570486	-1.615772
14	1	0	-0.806083	-2.014443	-1.887124
15	6	0	1.871896	-3.889392	-1.041115
16	1	0	0.121315	-4.286217	-2.225800
17	1	0	2.317550	-4.871492	-1.172748
18	7	0	2.021940	0.618036	0.650905
19	6	0	2.632211	-0.590008	0.543714
20	6	0	2.715307	1.628944	1.171961
21	6	0	3.940186	-0.833250	1.036693
22	6	0	4.024643	1.486882	1.662008
23	1	0	2.197353	2.574670	1.229288
24	6	0	4.632838	0.251373	1.615718
25	1	0	4.532398	2.350237	2.078093
26	1	0	5.637793	0.102278	2.001039
27	7	0	-1.944079	-0.232868	-1.004121
28	6	0	-2.493963	-0.207786	-2.212986
29	6	0	-2.672212	-0.681951	0.040256
30	6	0	-3.793481	-0.697394	-2.446669
31	1	0	-1.865916	0.170683	-3.011161
32	6	0	-3.976041	-1.211569	-0.097143
33	6	0	-4.528771	-1.213245	-1.398127
34	1	0	-4.200582	-0.666121	-3.451442
35	1	0	-5.529121	-1.606953	-1.556302
36	7	0	-0.858974	0.023363	1.431615
37	6	0	-2.078547	-0.572199	1.341714
38	6	0	-0.315311	0.183601	2.636180
39	6	0	-2.785192	-1.038624	2.475615
40	6	0	-0.934681	-0.262665	3.812151
41	1	0	0.635482	0.695832	2.670442

42	6	0	-2.168648	-0.877771	3.734735
43	1	0	-0.443312	-0.107370	4.766096
44	1	0	-2.677014	-1.225520	4.629802
45	6	0	-4.661943	-1.693845	1.067378
46	6	0	-4.086802	-1.618561	2.301175
47	6	0	4.521614	-2.137358	0.908966
48	6	0	3.853294	-3.137759	0.272750
49	1	0	-5.656638	-2.113496	0.948412
50	1	0	-4.613594	-1.979391	3.179535
51	1	0	5.515348	-2.303503	1.314456
52	1	0	4.301134	-4.120757	0.160115
53	8	0	0.176518	0.056290	-3.434580
54	6	0	0.892014	0.969652	-3.025770
55	8	0	0.974059	1.346350	-1.770213
56	6	0	1.777437	1.777632	-3.954184
57	1	0	1.405926	2.807319	-4.005527
58	1	0	2.799162	1.822451	-3.564480
59	1	0	1.774577	1.341783	-4.953993
60	8	0	-1.191985	3.440742	-0.481744

TS5 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	-0.333377	0.775527	-0.238235
2	6	0	0.110973	-1.775491	-2.490505
3	8	0	-0.283531	-1.315124	-1.417096
4	6	0	-0.107708	-3.207507	-2.894323
5	1	0	-0.762818	-3.704973	-2.178874
6	1	0	-0.537097	-3.253472	-3.899386
7	1	0	0.858300	-3.723240	-2.931452
8	8	0	0.781708	-1.080918	-3.393227
9	7	0	-0.844466	-0.438013	1.319953
10	6	0	-2.107580	-0.921864	1.231827
11	6	0	-0.125690	-0.683436	2.408155
12	6	0	-2.683843	-1.736223	2.231671
13	6	0	-0.619058	-1.472772	3.458539
14	1	0	0.865267	-0.250767	2.439121
15	6	0	-1.889371	-2.011728	3.366452
16	1	0	0.001051	-1.649215	4.330257
17	1	0	-2.288716	-2.631820	4.164316
18	7	0	-2.281837	0.275714	-0.806929
19	6	0	-2.878412	-0.546520	0.083092
20	6	0	-2.952846	0.692199	-1.871836
21	6	0	-4.202943	-1.008480	-0.065421
22	6	0	-4.274620	0.274256	-2.112176
23	1	0	-2.431636	1.366450	-2.539783
24	6	0	-4.899513	-0.572405	-1.216339
25	1	0	-4.793117	0.632333	-2.994508
26	1	0	-5.922549	-0.899178	-1.381147
27	7	0	1.772358	1.270956	0.467369
28	6	0	1.812217	2.590743	0.680778
29	6	0	2.964365	0.596031	0.380492
30	6	0	2.993595	3.330876	0.807101
31	1	0	0.851971	3.078682	0.761199
32	6	0	4.206861	1.288483	0.449666
33	6	0	4.197648	2.682777	0.661041
34	1	0	2.936064	4.398930	0.985137
35	1	0	5.139646	3.221506	0.715493
36	7	0	1.832055	-1.519355	0.329386
37	6	0	3.000672	-0.850812	0.275550
38	6	0	1.850750	-2.842184	0.265425
39	6	0	4.254075	-1.519105	0.158964
40	6	0	3.030470	-3.599449	0.135020
41	1	0	0.882637	-3.336217	0.318162

42	6	0	4.235347	-2.929151	0.079301
43	1	0	2.983588	-4.682799	0.088875
44	1	0	5.173361	-3.469856	-0.014080
45	6	0	5.446511	0.579532	0.311666
46	6	0	5.473788	-0.770551	0.157430
47	6	0	-4.755304	-1.862326	0.949113
48	6	0	-4.028532	-2.208779	2.051066
49	1	0	6.368078	1.153664	0.339805
50	1	0	6.415959	-1.301339	0.054778
51	1	0	-5.773870	-2.219624	0.829191
52	1	0	-4.462060	-2.842373	2.819105
53	17	0	0.331497	1.710211	-2.203625
54	1	0	0.830663	-0.134531	-3.097377
55	8	0	-0.987553	2.202731	0.849840
56	6	0	-1.838563	3.139684	0.435080
57	8	0	-2.289468	3.213591	-0.696126
58	6	0	-2.199563	4.130862	1.525710
59	1	0	-2.963303	4.820613	1.164831
60	1	0	-2.558222	3.604563	2.416296
61	1	0	-1.312334	4.700419	1.826160

TS6 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	0.040372	0.362458	-0.000092
2	6	0	-1.285783	2.410061	1.908983
3	8	0	-0.716240	1.328996	1.520181
4	6	0	-0.994387	2.857880	3.323779
5	1	0	-0.184593	3.597353	3.288739
6	1	0	-1.869427	3.349971	3.752316
7	1	0	-0.682716	2.016677	3.946628
8	8	0	-2.059484	3.145389	1.250020
9	7	0	1.146502	-0.978931	-1.250989
10	6	0	2.472064	-0.992529	-0.966600
11	6	0	0.707275	-1.721526	-2.261277
12	6	0	3.412838	-1.756052	-1.694685
13	6	0	1.561117	-2.520680	-3.039640
14	1	0	-0.353809	-1.672919	-2.474985
15	6	0	2.913710	-2.540177	-2.758401
16	1	0	1.151053	-3.104836	-3.855983
17	1	0	3.597389	-3.143469	-3.349079
18	7	0	1.963830	0.533815	0.784113
19	6	0	2.913508	-0.166871	0.119207
20	6	0	2.327537	1.360820	1.759233
21	6	0	4.285904	-0.097603	0.445074
22	6	0	3.668771	1.492379	2.156541
23	1	0	1.533582	1.920369	2.231737
24	6	0	4.646763	0.764731	1.505694
25	1	0	3.920960	2.173392	2.961575
26	1	0	5.690600	0.854387	1.793531
27	7	0	-1.723988	-0.303837	-0.824894
28	6	0	-2.342846	0.246425	-1.866951
29	6	0	-2.305925	-1.341189	-0.168719
30	6	0	-3.587474	-0.242845	-2.320874
31	1	0	-1.818330	1.051726	-2.360260
32	6	0	-3.546207	-1.887147	-0.547365
33	6	0	-4.187667	-1.296046	-1.667871
34	1	0	-4.063461	0.243892	-3.163790
35	1	0	-5.149833	-1.678216	-1.997237
36	7	0	-0.390474	-1.311349	1.238435
37	6	0	-1.580193	-1.890161	0.934887
38	6	0	0.307696	-1.789697	2.261474
39	6	0	-2.116132	-2.981634	1.657917
40	6	0	-0.136354	-2.873747	3.036757

41	1	0	1.243355	-1.291133	2.487598
42	6	0	-1.346710	-3.470589	2.737103
43	1	0	0.470224	-3.224709	3.864231
44	1	0	-1.714899	-4.306834	3.324953
45	6	0	-4.071858	-2.990879	0.203366
46	6	0	-3.386344	-3.517259	1.261786
47	6	0	5.219647	-0.885867	-0.308882
48	6	0	4.800413	-1.684894	-1.332173
49	1	0	-5.033571	-3.404110	-0.086212
50	1	0	-3.796169	-4.351937	1.822526
51	1	0	6.272992	-0.830265	-0.050691
52	1	0	5.515148	-2.274497	-1.898446
53	17	0	-3.296486	2.984440	-1.215365
54	1	0	-2.515656	2.969251	0.126705
55	8	0	0.194388	1.693553	-1.333551
56	6	0	0.615079	2.927536	-1.064881
57	8	0	1.055309	3.267155	0.027000
58	6	0	0.466066	3.879174	-2.228914
59	1	0	1.004273	4.806540	-2.028696
60	1	0	0.826101	3.420544	-3.154872
61	1	0	-0.600413	4.098833	-2.359498

TS7 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	-0.067101	-0.031456	0.718484
2	6	0	1.904241	2.976507	0.876682
3	8	0	0.831215	3.533129	0.648119
4	6	0	3.231684	3.723325	0.752788
5	1	0	3.495924	4.126952	1.737147
6	1	0	4.043326	3.062549	0.437675
7	1	0	3.121338	4.556233	0.054985
8	8	0	2.075091	1.730247	1.240611
9	7	0	-1.087989	-1.208144	-0.818764
10	6	0	-2.278263	-0.661977	-1.168876
11	6	0	-0.752057	-2.387456	-1.324446
12	6	0	-3.173492	-1.276789	-2.073312
13	6	0	-1.572290	-3.074206	-2.238236
14	1	0	0.186961	-2.812326	-0.994595
15	6	0	-2.780692	-2.522829	-2.613497
16	1	0	-1.252851	-4.035175	-2.625786
17	1	0	-3.435458	-3.035698	-3.312613
18	7	0	-1.715328	1.155134	0.265987
19	6	0	-2.615482	0.605220	-0.586361
20	6	0	-1.950016	2.355119	0.792250
21	6	0	-3.829400	1.242148	-0.925712
22	6	0	-3.132925	3.061080	0.506148
23	1	0	-1.160887	2.760227	1.413696
24	6	0	-4.074323	2.505510	-0.338414
25	1	0	-3.288168	4.037542	0.951324
26	1	0	-4.996432	3.032886	-0.567620
27	7	0	1.651050	-1.197597	0.642434
28	6	0	2.003415	-2.117872	1.534927
29	6	0	2.491564	-0.911985	-0.381324
30	6	0	3.221785	-2.811538	1.446035
31	1	0	1.286601	-2.335700	2.313028
32	6	0	3.724597	-1.575087	-0.565945
33	6	0	4.078257	-2.549242	0.394697
34	1	0	3.466717	-3.552757	2.198301
35	1	0	5.020600	-3.081484	0.298409
36	7	0	0.918261	0.752244	-1.022254
37	6	0	2.085411	0.117441	-1.291527
38	6	0	0.535146	1.743482	-1.817189
39	6	0	2.910920	0.450151	-2.387915

40	6	0	1.280586	2.137808	-2.942737
41	1	0	-0.375380	2.261412	-1.548834
42	6	0	2.465472	1.492366	-3.232435
43	1	0	0.922068	2.954537	-3.559216
44	1	0	3.065044	1.783509	-4.090430
45	6	0	4.540066	-1.225161	-1.694496
46	6	0	4.146463	-0.257832	-2.571906
47	6	0	-4.724897	0.589962	-1.838661
48	6	0	-4.409748	-0.618464	-2.388704
49	1	0	5.483411	-1.744834	-1.833891
50	1	0	4.771814	0.002985	-3.420654
51	1	0	-5.660985	1.081089	-2.087759
52	1	0	-5.093340	-1.102939	-3.079788
53	8	0	0.585708	1.163410	2.148929
54	6	0	-1.048479	1.159871	3.743582
55	6	0	0.192218	0.600299	3.905410
56	1	0	-1.887944	0.559119	3.419039
57	1	0	-1.204389	2.218920	3.921597
58	1	0	0.305176	-0.475858	3.863952
59	1	0	0.999817	1.151819	4.373108
60	8	0	-1.160627	-1.120317	1.902443
61	6	0	-1.369282	-2.416587	1.973554
62	8	0	-0.677422	-3.272427	1.423496
63	6	0	-2.559890	-2.789418	2.840404
64	1	0	-2.689419	-3.872227	2.859038
65	1	0	-2.412433	-2.420188	3.861330
66	1	0	-3.468158	-2.312318	2.456254

TS8 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	0.033145	0.749164	-0.000225
2	7	0	0.724323	-0.865579	-1.192643
3	6	0	1.973188	-1.275079	-0.848840
4	6	0	0.125306	-1.457930	-2.222563
5	6	0	2.658335	-2.315265	-1.516642
6	6	0	0.721479	-2.503659	-2.945369
7	1	0	-0.860615	-1.096518	-2.490474
8	6	0	1.986285	-2.936810	-2.593717
9	1	0	0.188952	-2.952166	-3.776631
10	1	0	2.471000	-3.740958	-3.140052
11	7	0	1.897963	0.398489	0.839224
12	6	0	2.607707	-0.590978	0.237702
13	6	0	2.461043	1.099491	1.825350
14	6	0	3.914518	-0.947257	0.637469
15	6	0	3.756019	0.815635	2.288055
16	1	0	1.859553	1.896350	2.245456
17	6	0	4.481395	-0.206104	1.701006
18	1	0	4.175929	1.406332	3.094662
19	1	0	5.485462	-0.440144	2.043795
20	7	0	-1.833583	0.699656	-0.885442
21	6	0	-2.250342	1.459014	-1.897895
22	6	0	-2.683301	-0.209550	-0.343006
23	6	0	-3.547529	1.343098	-2.425160
24	1	0	-1.528715	2.159796	-2.300267
25	6	0	-3.999248	-0.406633	-0.814894
26	6	0	-4.420330	0.411863	-1.890446
27	1	0	-3.848436	1.982370	-3.247745
28	1	0	-5.425622	0.303517	-2.287912
29	7	0	-0.929703	-0.701241	1.192270
30	6	0	-2.189931	-0.977348	0.761587
31	6	0	-0.438504	-1.399233	2.215944
32	6	0	-3.014347	-1.955731	1.361966
33	6	0	-1.176627	-2.400375	2.866872

34	1	0	0.566310	-1.149636	2.538242
35	6	0	-2.464592	-2.679159	2.445301
36	1	0	-0.732683	-2.937279	3.697834
37	1	0	-3.057035	-3.443549	2.940133
38	6	0	-4.818916	-1.404940	-0.186166
39	6	0	-4.343935	-2.151535	0.853787
40	6	0	4.586208	-2.012460	-0.052844
41	6	0	3.981687	-2.669806	-1.085011
42	1	0	-5.829181	-1.556291	-0.553995
43	1	0	-4.972147	-2.904137	1.320411
44	1	0	5.590255	-2.283492	0.258995
45	1	0	4.499477	-3.470587	-1.604142
46	6	0	-1.073277	2.164840	2.961873
47	6	0	-2.070646	2.414782	2.073175
48	8	0	-0.137352	2.441507	1.025961
49	8	0	0.734376	1.838375	-1.499779
50	1	0	-2.723071	1.623883	1.720430
51	1	0	-0.891906	1.166169	3.345309
52	6	0	1.225663	2.948353	-1.105686
53	6	0	1.975803	3.827347	-2.068466
54	1	0	2.673951	3.223792	-2.654519
55	1	0	1.257305	4.276844	-2.764072
56	1	0	2.501985	4.624167	-1.542325
57	8	0	1.100923	3.353225	0.090341
58	1	0	-2.306559	3.424186	1.757847
59	1	0	-0.496953	2.971698	3.399676

TS88 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	0.015243	0.755125	0.044694
2	7	0	0.711598	-0.823202	-1.212498
3	6	0	1.956439	-1.241871	-0.867555
4	6	0	0.128592	-1.373651	-2.273331
5	6	0	2.654406	-2.253355	-1.565438
6	6	0	0.738752	-2.388059	-3.029472
7	1	0	-0.854837	-1.003278	-2.540472
8	6	0	1.999397	-2.832351	-2.676543
9	1	0	0.219895	-2.804303	-3.885816
10	1	0	2.493896	-3.613223	-3.247327
11	7	0	1.855438	0.368810	0.882790
12	6	0	2.573524	-0.598141	0.253852
13	6	0	2.399412	1.026323	1.908834
14	6	0	3.872557	-0.971825	0.663099
15	6	0	3.684134	0.719941	2.384604
16	1	0	1.790404	1.808324	2.346314
17	6	0	4.419653	-0.276721	1.767421
18	1	0	4.088867	1.274428	3.223968
19	1	0	5.417066	-0.526414	2.118538
20	7	0	-1.852178	0.750334	-0.797567
21	6	0	-2.287500	1.582891	-1.743201
22	6	0	-2.686654	-0.207937	-0.318265
23	6	0	-3.589506	1.497427	-2.262058
24	1	0	-1.576708	2.319238	-2.098204
25	6	0	-4.007075	-0.377569	-0.789033
26	6	0	-4.447870	0.518951	-1.791523
27	1	0	-3.905648	2.195981	-3.028784
28	1	0	-5.457186	0.433206	-2.184291
29	7	0	-0.911154	-0.799808	1.154357
30	6	0	-2.172662	-1.056070	0.715477
31	6	0	-0.409913	-1.557143	2.128314
32	6	0	-2.985957	-2.078670	1.253006
33	6	0	-1.137267	-2.604627	2.716766
34	1	0	0.592293	-1.319163	2.466596

35	6	0	-2.423651	-2.868491	2.282718
36	1	0	-0.685175	-3.189466	3.510138
37	1	0	-3.007202	-3.668617	2.729204
38	6	0	-4.811374	-1.428694	-0.230952
39	6	0	-4.319065	-2.247598	0.744507
40	6	0	4.556954	-2.008121	-0.058177
41	6	0	3.971196	-2.623323	-1.126620
42	1	0	-5.824582	-1.559909	-0.598368
43	1	0	-4.936782	-3.037727	1.160376
44	1	0	5.555551	-2.291503	0.260116
45	1	0	4.499119	-3.402075	-1.668593
46	6	0	-1.660719	1.785512	2.629161
47	6	0	-1.493921	3.097823	2.308715
48	8	0	-0.077235	2.484585	1.019875
49	8	0	0.745861	1.834890	-1.467275
50	1	0	-2.172766	3.600594	1.628227
51	1	0	-0.802578	3.733086	2.849905
52	1	0	-2.462073	1.204272	2.189097
53	1	0	-1.048438	1.302315	3.383192
54	6	0	1.289805	2.919411	-1.082392
55	6	0	2.075674	3.763498	-2.047593
56	1	0	2.648107	4.529150	-1.523274
57	1	0	2.735374	3.127770	-2.643908
58	1	0	1.374493	4.254090	-2.733128
59	8	0	1.193410	3.336279	0.115586

TS9 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	-0.080330	0.250010	0.386123
2	7	0	-1.660948	-1.142599	0.737574
3	6	0	-2.851485	-0.721487	0.237142
4	6	0	-1.627714	-2.291691	1.407305
5	6	0	-4.051452	-1.456240	0.371243
6	6	0	-2.764867	-3.095001	1.589941
7	1	0	-0.670766	-2.592884	1.816982
8	6	0	-3.977539	-2.682211	1.070700
9	1	0	-2.681592	-4.023475	2.143798
10	1	0	-4.872777	-3.283493	1.201438
11	7	0	-1.683656	1.198896	-0.538776
12	6	0	-2.865988	0.539368	-0.442800
13	6	0	-1.647862	2.397629	-1.123182
14	6	0	-4.071437	1.049617	-0.973113
15	6	0	-2.797344	2.982731	-1.678696
16	1	0	-0.680454	2.885304	-1.144226
17	6	0	-4.005676	2.312026	-1.608425
18	1	0	-2.726496	3.956995	-2.149487
19	1	0	-4.906590	2.748463	-2.030702
20	7	0	1.306803	-1.060269	1.176692
21	6	0	1.766574	-1.071976	2.426897
22	6	0	1.762039	-1.983170	0.291868
23	6	0	2.711856	-2.017406	2.858727
24	1	0	1.363295	-0.319130	3.093600
25	6	0	2.700238	-2.979791	0.637928
26	6	0	3.175767	-2.972342	1.971040
27	1	0	3.063652	-1.991216	3.884094
28	1	0	3.902323	-3.715498	2.287530
29	7	0	0.393656	-0.885181	-1.319603
30	6	0	1.255261	-1.901213	-1.045795
31	6	0	-0.089001	-0.773709	-2.556531
32	6	0	1.677749	-2.837516	-2.015810
33	6	0	0.263066	-1.663451	-3.583754
34	1	0	-0.762856	0.054776	-2.743440
35	6	0	1.145756	-2.694902	-3.318007

36	1	0	-0.154165	-1.527265	-4.575286
37	1	0	1.438057	-3.390449	-4.099597
38	6	0	3.112300	-3.921671	-0.365437
39	6	0	2.617259	-3.856208	-1.636234
40	6	0	-5.274899	0.279404	-0.829715
41	6	0	-5.263757	-0.923910	-0.185858
42	1	0	3.830219	-4.689955	-0.094935
43	1	0	2.936479	-4.572965	-2.386682
44	1	0	-6.198891	0.675358	-1.239951
45	1	0	-6.179504	-1.497127	-0.077629
46	6	0	2.293582	1.999196	-1.615210
47	6	0	3.047245	1.260228	-0.753247
48	8	0	0.997019	1.884997	0.270785
49	8	0	-0.588998	0.863631	2.214109
50	1	0	3.004690	0.176270	-0.812222
51	1	0	1.677634	1.489499	-2.353673
52	6	0	-0.438130	2.118922	2.350559
53	6	0	-0.940303	2.822510	3.580320
54	1	0	-1.957204	2.490445	3.806113
55	1	0	-0.302628	2.544242	4.427650
56	1	0	-0.907981	3.905084	3.454753
57	8	0	0.143025	2.830064	1.467015
58	6	0	2.395952	3.494081	-1.713610
59	6	0	4.026080	1.868358	0.211665
60	6	0	4.378527	3.321995	-0.150008
61	6	0	3.123789	4.125273	-0.516057
62	1	0	2.931775	3.722610	-2.649096
63	1	0	1.397181	3.932208	-1.839925
64	1	0	4.931748	1.248767	0.245628
65	1	0	3.589754	1.823710	1.220399
66	1	0	4.905624	3.792691	0.686207
67	1	0	5.075039	3.322431	-0.998730
68	1	0	3.389580	5.160516	-0.753285
69	1	0	2.442213	4.153659	0.341305

GaAl(OC6H10) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	-0.095455	0.113639	0.423911
2	7	0	-1.316108	-1.574939	0.589677
3	6	0	-2.537590	-1.380503	0.026003
4	6	0	-1.072263	-2.731503	1.202668
5	6	0	-3.561991	-2.353919	0.053560
6	6	0	-2.023648	-3.760314	1.275610
7	1	0	-0.097284	-2.845910	1.661438
8	6	0	-3.268005	-3.575154	0.701570
9	1	0	-1.776411	-4.683190	1.788264
10	1	0	-4.023615	-4.354126	0.750294
11	7	0	-1.752120	0.778920	-0.604296
12	6	0	-2.774665	-0.115675	-0.603871
13	6	0	-1.944259	1.989536	-1.126333
14	6	0	-4.034307	0.164553	-1.177728
15	6	0	-3.160549	2.352368	-1.725096
16	1	0	-1.108488	2.673358	-1.072544
17	6	0	-4.203965	1.445254	-1.753665
18	1	0	-3.272227	3.345452	-2.145486
19	1	0	-5.155555	1.709049	-2.206607
20	7	0	1.557662	-0.880157	1.230103
21	6	0	1.907426	-0.924681	2.517111
22	6	0	2.306053	-1.544284	0.313629
23	6	0	3.034013	-1.645810	2.949380
24	1	0	1.256367	-0.385497	3.195841
25	6	0	3.450774	-2.296792	0.654879
26	6	0	3.804287	-2.330350	2.025206

27	1	0	3.286029	-1.659236	4.004037
28	1	0	4.677329	-2.894273	2.341849
29	7	0	0.788292	-0.684014	-1.306543
30	6	0	1.885526	-1.445699	-1.052109
31	6	0	0.381179	-0.557251	-2.568534
32	6	0	2.619454	-2.106899	-2.061892
33	6	0	1.043793	-1.177865	-3.639804
34	1	0	-0.486623	0.069008	-2.738666
35	6	0	2.160039	-1.955589	-3.390650
36	1	0	0.672788	-1.040617	-4.649425
37	1	0	2.688446	-2.445498	-4.203654
38	6	0	4.175474	-2.966734	-0.388877
39	6	0	3.774819	-2.876556	-1.691228
40	6	0	-5.056836	-0.842906	-1.139183
41	6	0	-4.828907	-2.053220	-0.551545
42	1	0	5.053566	-3.547669	-0.123655
43	1	0	4.331475	-3.385180	-2.472448
44	1	0	-6.021868	-0.621033	-1.584488
45	1	0	-5.609529	-2.807244	-0.524096
46	6	0	2.377240	2.083015	-0.267837
47	6	0	1.666843	2.749224	0.839379
48	8	0	0.935694	1.821194	-0.070757
49	8	0	-0.514379	0.685604	2.175132
50	1	0	1.765273	2.310812	1.829063
51	1	0	2.990231	1.216457	-0.027155
52	6	0	-1.194253	1.795111	2.475707
53	6	0	-1.568646	1.895556	3.937070
54	1	0	-2.197106	1.045635	4.223867
55	1	0	-0.671004	1.856006	4.563865
56	1	0	-2.102818	2.827362	4.123606
57	8	0	-1.474769	2.650528	1.648917
58	6	0	2.720369	2.827574	-1.532866
59	6	0	1.258722	4.204136	0.761857
60	6	0	1.885802	4.949593	-0.432302
61	6	0	1.890664	4.109572	-1.716466
62	1	0	3.786742	3.083952	-1.463631
63	1	0	2.620562	2.154549	-2.393996
64	1	0	1.554953	4.684007	1.701634
65	1	0	0.164332	4.239665	0.741748
66	1	0	1.348489	5.889345	-0.592841
67	1	0	2.920175	5.224133	-0.187226
68	1	0	2.309436	4.687615	-2.546170
69	1	0	0.863453	3.850242	-2.005452