Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Mechanistic Insights into the Different Chemoselectivities of Rh_2(II)-Catalyzed Ring Expansion of Cyclobutanol-Substituted Aryl Azide and C-H Bond Amination of Cyclopentanol-Substituted Aryl Azide: A DFT Study

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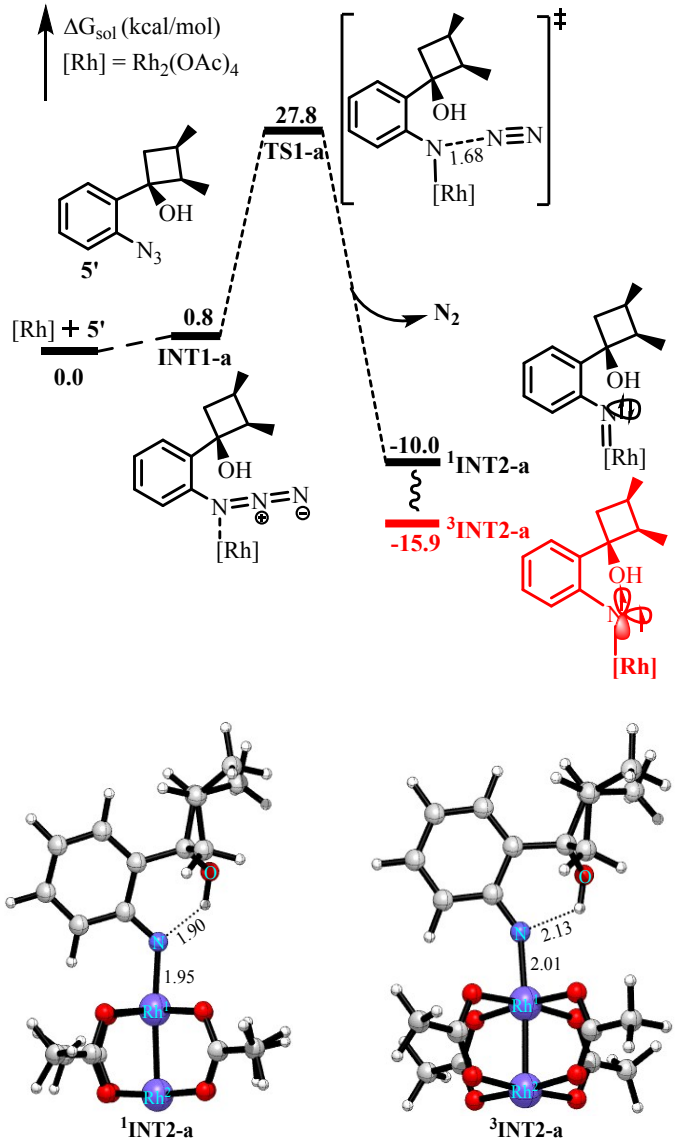

Figure S1. Energy profiles (in kcal/mol) for the formation of the key Rh_2(II)-*N*-arylnitrene intermediate with the substrate **5'**. Bond lengths are shown in Å.

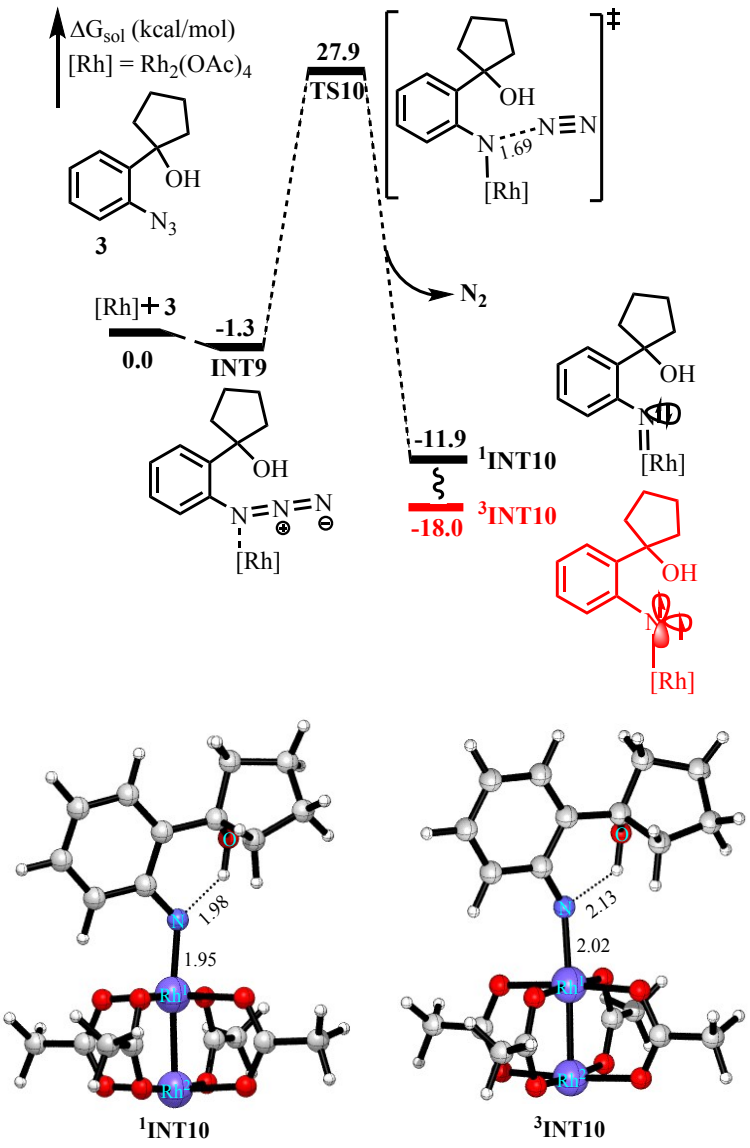

Figure S2. Energy profiles (in kcal/mol) for the formation of the key Rh_2(II)-*N*-arylnitrene intermediate with the substrate **3**. Bond lengths are shown in Å.

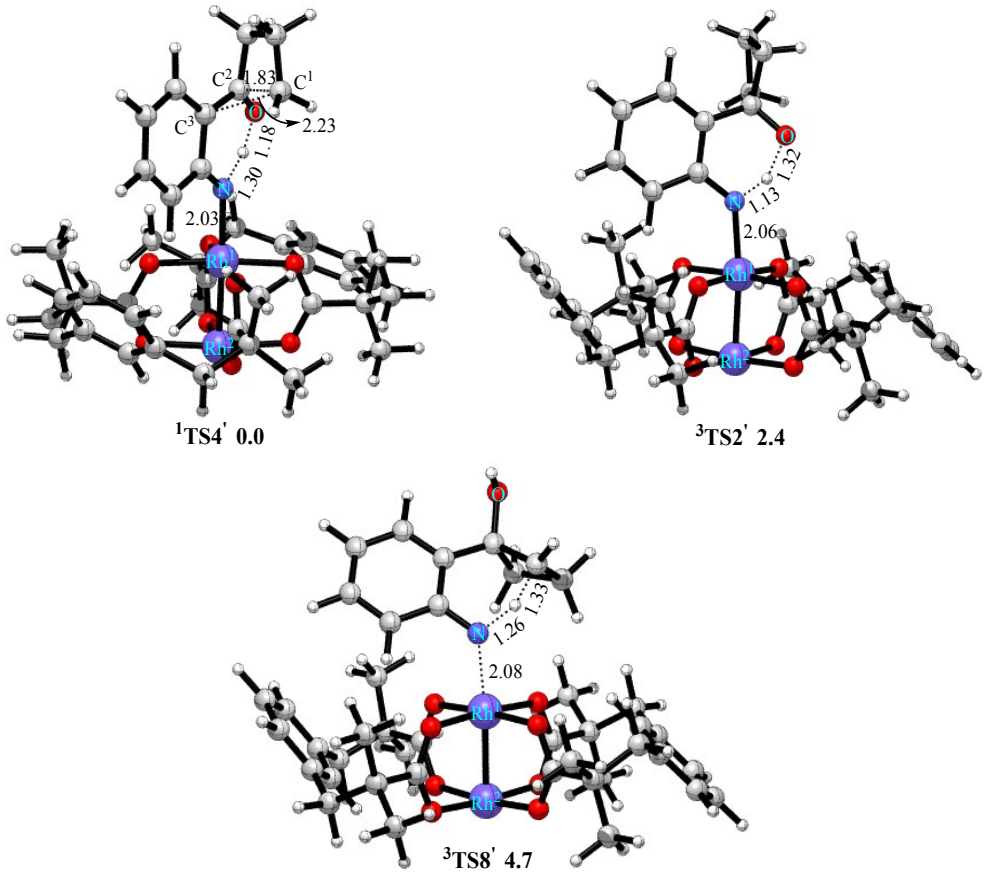

Figure S3. Optimized TS structures for the intramolecular proton transfer from O-H group of *o*-cyclobutanol moiety in singlet state (**^{1}TS4'**) and the HAA from both O-H (**^{3}TS2'**) and C-H bonds (**^{3}TS8'**) in triplet state using the full size catalyst model (Rh_2esp_2). The relative energies are shown in kcal/mol. Bond lengths are shown in Å.

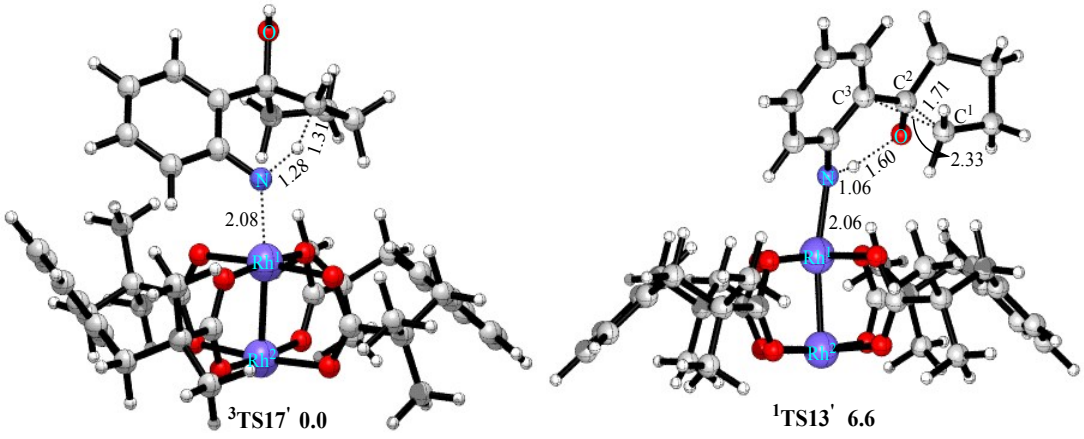

Figure S4. Optimized TS structures for the intramolecular HAA from the C-H bond of the *o*-cyclopentanol group (**^{3}TS17'**) and the competitive proton transfer from O-H group of the *o*-cyclopentanol moiety along with the ring-expansion (**^{1}TS13'**) using the full size catalyst model (Rh_2esp_2). The relative energies are shown in kcal/mol. Bond lengths are shown in Å.

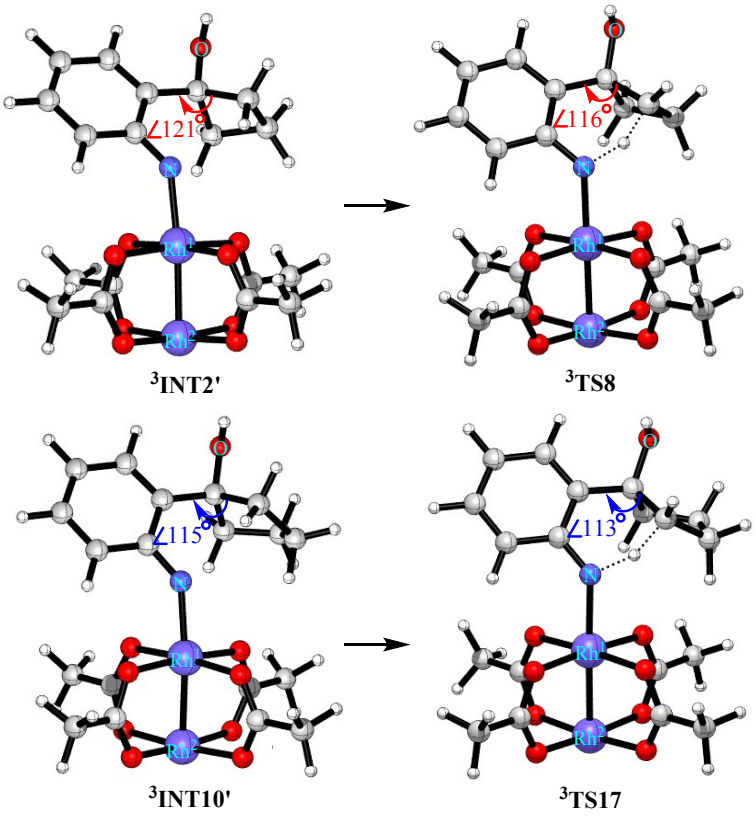

Figure S5. The mentioned bond angles in Scheme 2 are shown in 3D structures.

Cartesian Coordinates and Energies

$Rh_2(OAc)_4$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.861541	-1.856382	0.001281
2	8	0	-1.519357	-1.387531	1.127892
3	8	0	-1.383618	-1.523324	-1.124859
4	6	0	-2.955039	-2.882486	-0.008845
5	1	0	-2.757121	-3.633272	-0.777296
6	1	0	-3.055379	-3.347819	0.973210
7	1	0	-3.898670	-2.387895	-0.262636
8	6	0	-1.861445	1.855424	-0.007670
9	8	0	-1.387411	1.522723	1.120251
10	8	0	-1.514777	1.386907	-1.133002
11	6	0	-2.955470	2.881021	-0.000829
12	1	0	-2.756333	3.635568	0.763675
13	1	0	-3.057997	3.341679	-0.984846
14	1	0	-3.898256	2.387354	0.257807
15	6	0	1.865101	1.859701	0.003355
16	8	0	1.523149	1.390583	1.129639
17	8	0	1.396640	1.517288	-1.124191
18	6	0	2.918856	2.926778	-0.008182
19	1	0	3.308325	3.098777	0.996274
20	1	0	3.726909	2.633408	-0.684203
21	1	0	2.487025	3.852291	-0.401448
22	6	0	1.864284	-1.861517	0.011348
23	8	0	1.391411	-1.518747	1.135816
24	8	0	1.526748	-1.392669	-1.117517
25	6	0	2.928890	-2.917771	0.003801
26	1	0	3.850597	-2.495321	-0.407955
27	1	0	3.111291	-3.292403	1.012031
28	1	0	2.624731	-3.735838	-0.655345
29	45	0	0.002091	0.001798	1.193292
30	45	0	0.006593	-0.002842	-1.191227

Zero-point correction= 0.211186 (Hartree/Particle)
Thermal correction to Energy= 0.232435
Thermal correction to Enthalpy= 0.233380
Thermal correction to Gibbs Free Energy= 0.160357
Sum of electronic and zero-point Energies= -1132.367109
Sum of electronic and thermal Energies= -1132.345859
Sum of electronic and thermal Enthalpies= -1132.344915
Sum of electronic and thermal Free Energies= -1132.417937
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1134.95538518

1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.063375	0.043534	0.014828
2	6	0	-0.182967	0.681461	0.102431
3	6	0	-0.191454	2.072430	0.069655
4	6	0	0.982202	2.809595	-0.056716
5	6	0	2.202597	2.153728	-0.154054
6	6	0	2.245825	0.766375	-0.115264
7	1	0	-1.142605	2.593356	0.153240
8	1	0	0.940554	3.895364	-0.077190
9	1	0	3.126336	2.717448	-0.255698
10	1	0	3.199772	0.246042	-0.182281
11	7	0	1.043442	-1.382003	0.085503
12	7	0	2.109903	-1.981520	-0.046398
13	7	0	3.034981	-2.637616	-0.153679
14	6	0	-1.445808	-0.137856	0.237141
15	6	0	-2.819258	0.549378	0.161497
16	6	0	-1.881204	-1.005597	-0.970994
17	6	0	-3.340967	-0.670762	-0.620008
18	1	0	-2.796343	1.439529	-0.477082
19	1	0	-3.273493	0.797194	1.125911
20	1	0	-1.571301	-0.546136	-1.917901

21	1	0	-1.560478	-2.052916	-0.957403
22	1	0	-4.034651	-0.485784	-1.444983
23	1	0	-3.771791	-1.418503	0.051699
24	8	0	-1.437283	-0.899811	1.429622
25	1	0	-0.730077	-1.552842	1.335649

Zero-point correction= 0.199684 (Hartree/Particle)
Thermal correction to Energy= 0.211634
Thermal correction to Enthalpy= 0.212578
Thermal correction to Gibbs Free Energy= 0.161472
Sum of electronic and zero-point Energies= -626.466995
Sum of electronic and thermal Energies= -626.455044
Sum of electronic and thermal Enthalpies= -626.454100
Sum of electronic and thermal Free Energies= -626.505207
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -626.81436630

INT1

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1	6	0	-2.433364	1.460138	0.678812
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3	6	0	-4.293399	0.965244	-0.709424
4	6	0	-4.361467	2.287286	-1.124223
5	6	0	-3.461015	3.217630	-0.617647
6	6	0	-2.489549	2.794565	0.273332
7	1	0	-5.011688	0.257399	-1.118544
8	1	0	-5.122377	2.590634	-1.839241
9	1	0	-3.499893	4.258872	-0.926802
10	1	0	-1.743146	3.493961	0.645684
11	7	0	-1.319960	1.049913	1.496219
12	7	0	-0.928236	1.853526	2.356393
13	7	0	-0.482658	2.499437	3.177047
14	45	0	0.461610	0.216758	0.350626
15	45	0	2.327793	-0.637499	-0.914036
16	8	0	0.013385	-1.741645	0.844057
17	6	0	0.734804	-2.687512	0.384580
18	8	0	1.744942	-2.551073	-0.354129
19	8	0	2.763906	1.324084	-1.384795
20	6	0	2.027219	2.253582	-0.949428
21	8	0	1.007216	2.121917	-0.202675
22	8	0	3.454526	-0.469672	0.810790
23	6	0	2.918558	-0.012539	1.859507
24	8	0	1.708346	0.353180	1.989691
25	8	0	1.070618	-0.750608	-2.552728
26	6	0	-0.139491	-0.412212	-2.416896
27	8	0	-0.684214	0.035266	-1.360973
28	6	0	-3.367867	-0.963475	0.606552
29	6	0	-4.744690	-1.650101	0.789740
30	6	0	-3.077228	-1.997353	-0.515118
31	6	0	-4.179941	-2.893145	0.076475
32	1	0	-5.551973	-1.179245	0.220893
33	1	0	-5.049309	-1.745514	1.836214
34	1	0	-3.354350	-1.601125	-1.499996
35	1	0	-2.047193	-2.371408	-0.559259
36	1	0	-4.836622	-3.416326	-0.625034
37	1	0	-3.777281	-3.616449	0.792520
38	8	0	-2.644955	-1.263845	1.770338
39	6	0	2.372388	3.649137	-1.379203
40	1	0	3.453751	3.749201	-1.494376
41	1	0	1.910555	3.839732	-2.353962
42	1	0	1.987820	4.379470	-0.664775
43	6	0	3.791201	0.140519	3.070519
44	1	0	3.236890	-0.138245	3.969917
45	1	0	4.696178	-0.460823	2.969621
46	1	0	4.074506	1.193730	3.169678
47	6	0	-1.035528	-0.581628	-3.608946
48	1	0	-0.481959	-0.384491	-4.529696
49	1	0	-1.381828	-1.620874	-3.640347
50	1	0	-1.906393	0.073065	-3.527815
51	6	0	0.336428	-4.074125	0.794087
52	1	0	0.710596	-4.808415	0.078571
53	1	0	0.772189	-4.290050	1.775562
54	1	0	-0.751462	-4.139576	0.891848

55	1	0	-1.712907	-1.412030	1.544469

Zero-point correction= 0.413278 (Hartree/Particle)
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Thermal correction to Enthalpy= 0.448260
Thermal correction to Gibbs Free Energy= 0.348504
Sum of electronic and zero-point Energies= -1758.848964
Sum of electronic and thermal Energies= -1758.814926
Sum of electronic and thermal Enthalpies= -1758.813982
Sum of electronic and thermal Free Energies= -1758.913738
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1761.79755662

TS1

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1	6	0	-2.219779	1.431783	0.745293
2	6	0	-3.332449	0.669582	0.304572
3	6	0	-4.226493	1.318347	-0.557270
4	6	0	-4.095904	2.652159	-0.907857
5	6	0	-3.018033	3.398060	-0.428847
6	6	0	-2.073530	2.777485	0.359914
7	1	0	-5.070477	0.760273	-0.955171
8	1	0	-4.837974	3.114326	-1.554614
9	1	0	-2.909050	4.447151	-0.692085
10	1	0	-1.188795	3.309014	0.704674
11	7	0	-1.215659	0.766103	1.436700
12	7	0	-0.691699	1.714720	2.744347
13	7	0	0.061909	1.709753	3.569171
14	45	0	0.453167	0.255206	0.347154
15	45	0	2.258218	-0.713197	-0.969113
16	8	0	-0.121897	-1.693803	0.784565
17	6	0	0.538072	-2.672833	0.304575
18	8	0	1.564819	-2.592575	-0.419063
19	8	0	2.796715	1.232901	-1.429143
20	6	0	2.155002	2.198354	-0.936830
21	8	0	1.150441	2.123271	-0.155733
22	8	0	3.414300	-0.616966	0.751326
23	6	0	2.906491	-0.181364	1.818316
24	8	0	1.718022	0.256981	1.962442
25	8	0	0.971171	-0.750332	-2.586810
26	6	0	-0.198727	-0.301968	-2.439397
27	8	0	-0.690681	0.199468	-1.380075
28	6	0	-3.516310	-0.813023	0.575927
29	6	0	-4.941610	-1.416959	0.596969
30	6	0	-3.206430	-1.771094	-0.610200
31	6	0	-4.391710	-2.641334	-0.159583
32	1	0	-5.666412	-0.860923	-0.004809
33	1	0	-5.343631	-1.561908	1.604180
34	1	0	-3.403760	-1.285402	-1.574576
35	1	0	-2.195219	-2.195464	-0.616595
36	1	0	-5.022638	-3.081049	-0.937793
37	1	0	-4.075419	-3.427046	0.532483
38	8	0	-2.921240	-1.276818	1.758758
39	6	0	2.597788	3.587596	-1.293643
40	1	0	3.478577	3.556673	-1.936569
41	1	0	1.781396	4.107716	-1.803951
42	1	0	2.819242	4.146623	-0.379675
43	6	0	3.759388	-0.197900	3.052330
44	1	0	3.678613	-1.185036	3.520107
45	1	0	4.806163	-0.034800	2.787353
46	1	0	3.415212	0.551066	3.768548
47	6	0	-1.128694	-0.393518	-3.614247
48	1	0	-0.577306	-0.260786	-4.547659
49	1	0	-1.576484	-1.393985	-3.625310
50	1	0	-1.929756	0.343760	-3.522489
51	6	0	0.034103	-4.042716	0.655545
52	1	0	0.031493	-4.674815	-0.236271
53	1	0	0.715494	-4.499407	1.380703
54	1	0	-0.966700	-3.984518	1.091471
55	1	0	-1.957032	-1.276827	1.651129

Zero-point correction= 0.409243 (Hartree/Particle)
Thermal correction to Energy= 0.443777

Thermal correction to Enthalpy= 0.444722
Thermal correction to Gibbs Free Energy= 0.343366
Sum of electronic and zero-point Energies= -1758.805162
Sum of electronic and thermal Energies= -1758.770628
Sum of electronic and thermal Enthalpies= -1758.769684
Sum of electronic and thermal Free Energies= -1758.871040
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1761.74938414

N_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.552597
2	7	0	0.000000	0.000000	-0.552597

Zero-point correction= 0.005622 (Hartree/Particle)
Thermal correction to Energy= 0.007982
Thermal correction to Enthalpy= 0.008927
Thermal correction to Gibbs Free Energy= -0.012827
Sum of electronic and zero-point Energies= -109.453327
Sum of electronic and thermal Energies= -109.450967
Sum of electronic and thermal Enthalpies= -109.450023
Sum of electronic and thermal Free Energies= -109.471777
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -109.48464411

^{1}INT2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.468869	0.797645	-0.328377
2	6	0	3.869240	0.406609	-0.358783
3	6	0	4.822960	1.391514	-0.161471
4	6	0	4.456875	2.727924	0.006376
5	6	0	3.117286	3.129400	0.003420
6	6	0	2.132858	2.181387	-0.146320
7	1	0	5.878615	1.133096	-0.156001
8	1	0	5.237671	3.475514	0.133766
9	1	0	2.862537	4.178902	0.123868
10	1	0	1.081932	2.449724	-0.160786
11	7	0	1.568970	-0.166334	-0.464191
12	45	0	-0.346645	-0.035956	-0.135526
13	45	0	-2.762171	-0.074521	0.270914
14	8	0	-0.233131	-1.691508	1.109117
15	6	0	-1.281920	-2.104335	1.699525
16	8	0	-2.443402	-1.627062	1.595178
17	8	0	-2.917350	1.480774	-1.091145
18	6	0	-1.873417	1.980206	-1.580203
19	8	0	-0.672978	1.615821	-1.342864
20	8	0	-2.910439	-1.440049	-1.277791
21	6	0	-1.876473	-1.731976	-1.936393
22	8	0	-0.699097	-1.289137	-1.742383
23	8	0	-2.416925	1.288996	1.802024
24	6	0	-1.236086	1.600610	2.097625
25	8	0	-0.173816	1.210365	1.507543
26	6	0	4.221966	-1.059971	-0.505857
27	6	0	4.133543	-1.766471	0.885798
28	6	0	5.722737	-1.391873	-0.496944
29	6	0	5.657252	-1.615449	1.024298
30	1	0	5.838109	-2.339999	-1.031991
31	1	0	6.437218	-0.672957	-0.913077
32	1	0	6.215442	-2.462553	1.432742
33	1	0	5.931012	-0.718354	1.592737
34	6	0	-2.029424	3.103148	-2.564888
35	1	0	-1.253635	3.856849	-2.409228
36	1	0	-1.903048	2.703587	-3.576643
37	1	0	-3.022736	3.547254	-2.480251
38	6	0	-2.019394	-2.709451	-3.067651
39	1	0	-1.578901	-2.287854	-3.975531
40	1	0	-1.459341	-3.618811	-2.828399
41	1	0	-3.069711	-2.954678	-3.232717
42	6	0	-1.022169	2.516186	3.269453
43	1	0	-0.512110	1.964584	4.065625
44	1	0	-0.370608	3.345755	2.980738

45	1	0	-1.976646	2.892981	3.640071
46	6	0	-1.091074	-3.291414	2.599840
47	1	0	-0.807153	-4.157512	1.993722
48	1	0	-0.270148	-3.099176	3.296124
49	1	0	-2.010548	-3.510937	3.144722
50	8	0	3.554968	-1.662595	-1.568794
51	1	0	3.478595	-1.330692	1.648119
52	1	0	3.837674	-2.805899	0.703622
53	1	0	2.605302	-1.519988	-1.398125

Zero-point correction= 0.401812 (Hartree/Particle)
Thermal correction to Energy= 0.434378
Thermal correction to Enthalpy= 0.435322
Thermal correction to Gibbs Free Energy= 0.336645
Sum of electronic and zero-point Energies= -1649.394264
Sum of electronic and thermal Energies= -1649.361698
Sum of electronic and thermal Enthalpies= -1649.360754
Sum of electronic and thermal Free Energies= -1649.459431
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1652.30670833

^{3}INT2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.639561	0.874606	-0.244831
2	6	0	3.987438	0.363545	-0.319766
3	6	0	5.024268	1.263096	-0.164325
4	6	0	4.790552	2.626676	0.052282
5	6	0	3.484862	3.121797	0.118125
6	6	0	2.412843	2.268583	-0.027957
7	1	0	6.051092	0.907532	-0.208828
8	1	0	5.634076	3.303258	0.166297
9	1	0	3.312387	4.182583	0.283783
10	1	0	1.382727	2.609616	0.012848
11	7	0	1.629379	0.039366	-0.379879
12	45	0	-0.371496	-0.081030	-0.126970
13	45	0	-2.765533	0.009636	0.245754
14	8	0	-0.340223	-1.828758	0.972285
15	6	0	-1.433975	-2.269520	1.447723
16	8	0	-2.575337	-1.747002	1.313231
17	8	0	-2.815646	1.765749	-0.843653
18	6	0	-1.738500	2.196970	-1.337516
19	8	0	-0.584181	1.678546	-1.206569
20	8	0	-2.986264	-1.068261	-1.504294
21	6	0	-1.959191	-1.420871	-2.147379
22	8	0	-0.751541	-1.168424	-1.839337
23	8	0	-2.401985	1.079384	1.975374
24	6	0	-1.206320	1.337695	2.282294
25	8	0	-0.167660	1.013351	1.624606
26	6	0	4.151729	-1.128498	-0.529427
27	6	0	3.862617	-1.908439	0.784530
28	6	0	5.590805	-1.656911	-0.450312
29	6	0	5.378965	-1.932423	1.048142
30	1	0	5.623501	-2.589407	-1.023309
31	1	0	6.420646	-1.020429	-0.775502
32	1	0	5.811083	-2.847237	1.463237
33	1	0	5.693388	-1.084136	1.667731
34	6	0	-1.813497	3.429339	-2.191146
35	1	0	-2.705648	4.008551	-1.945842
36	1	0	-0.910678	4.032132	-2.070102
37	1	0	-1.872895	3.124212	-3.241333
38	6	0	-2.158321	-2.224391	-3.399014
39	1	0	-1.644690	-1.736338	-4.232204
40	1	0	-1.700539	-3.210005	-3.269602
41	1	0	-3.220760	-2.335711	-3.620435
42	6	0	-0.964392	2.085149	3.561636
43	1	0	-0.563417	1.390012	4.306489
44	1	0	-0.213930	2.863916	3.403645
45	1	0	-1.894742	2.515345	3.936042
46	6	0	-1.338605	-3.543892	2.234510
47	1	0	-0.565090	-3.443852	3.000993
48	1	0	-2.299050	-3.785986	2.691864
49	1	0	-1.032154	-4.355653	1.567475
50	8	0	3.493705	-1.563770	-1.688991

51	1	0	3.199584	-1.451002	1.527095
52	1	0	3.481282	-2.901256	0.518070
53	1	0	2.542506	-1.420522	-1.571153

Zero-point correction= 0.400401 (Hartree/Particle)
Thermal correction to Energy= 0.433314
Thermal correction to Enthalpy= 0.434258
Thermal correction to Gibbs Free Energy= 0.333812
Sum of electronic and zero-point Energies= -1649.400237
Sum of electronic and thermal Energies= -1649.367324
Sum of electronic and thermal Enthalpies= -1649.366380
Sum of electronic and thermal Free Energies= -1649.466826
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1652.31138770

MECP1
Singlet-A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.522066	0.841079	-0.275785
2	6	0	3.905667	0.408517	-0.342631
3	6	0	4.892392	1.362601	-0.176435
4	6	0	4.571648	2.708861	0.020557
5	6	0	3.242744	3.141564	0.078590
6	6	0	2.224063	2.224635	-0.052951
7	1	0	5.940073	1.071950	-0.209877
8	1	0	5.376005	3.433589	0.129860
9	1	0	3.020005	4.194646	0.231841
10	1	0	1.177559	2.511832	-0.019097
11	7	0	1.590222	-0.083704	-0.435594
12	45	0	-0.346538	-0.034376	-0.126783
13	45	0	-2.759645	-0.061925	0.252771
14	8	0	-0.250444	-1.762509	1.009563
15	6	0	-1.324020	-2.261590	1.474408
16	8	0	-2.490434	-1.803898	1.331443
17	8	0	-2.872309	1.682357	-0.865803
18	6	0	-1.819656	2.153639	-1.368291
19	8	0	-0.638710	1.692422	-1.230437
20	8	0	-2.930121	-1.177846	-1.483831
21	6	0	-1.885395	-1.491807	-2.115751
22	8	0	-0.691128	-1.170468	-1.816740
23	8	0	-2.409610	1.036635	1.976721
24	6	0	-1.230032	1.363915	2.269090
25	8	0	-0.178609	1.104157	1.596983
26	6	0	4.180248	-1.071827	-0.524557
27	6	0	3.959937	-1.831375	0.818599
28	6	0	5.654136	-1.498032	-0.442274
29	6	0	5.476436	-1.757581	1.063290
30	1	0	5.744528	-2.438545	-0.996081
31	1	0	6.440127	-0.817148	-0.786890
32	1	0	5.967671	-2.638179	1.486364
33	1	0	5.749377	-0.883096	1.666574
34	6	0	-1.947740	3.362772	-2.249463
35	1	0	-2.861743	3.911775	-2.015312
36	1	0	-1.070185	4.005292	-2.149009
37	1	0	-1.999620	3.029015	-3.291377
38	6	0	-2.032518	-2.339047	-3.346319
39	1	0	-1.526684	-1.855096	-4.186790
40	1	0	-1.535338	-3.299777	-3.178993
41	1	0	-3.085894	-2.503118	-3.577982
42	6	0	-1.011295	2.115598	3.551216
43	1	0	-0.593543	1.427841	4.293981
44	1	0	-0.282411	2.915479	3.399027
45	1	0	-1.953331	2.517317	3.928466
46	6	0	-1.159514	-3.532084	2.257609
47	1	0	-0.381459	-3.399116	3.014634
48	1	0	-2.102074	-3.821164	2.724915
49	1	0	-0.824423	-4.325768	1.582254
50	8	0	3.540950	-1.579625	-1.657348
51	1	0	3.274828	-1.398167	1.555270
52	1	0	3.632968	-2.848713	0.574374
53	1	0	2.588547	-1.440201	-1.514265

Zero-point correction= 0.398635 (Hartree/Particle)

Thermal correction to Energy= 0.430931
Thermal correction to Enthalpy= 0.431875
Thermal correction to Gibbs Free Energy= 0.334980
Sum of electronic and zero-point Energies= -1651.880036
Sum of electronic and thermal Energies= -1651.847739
Sum of electronic and thermal Enthalpies= -1651.846795
Sum of electronic and thermal Free Energies= -1651.943691
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1652.30561168

Triplet-B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.522066	0.841079	-0.275785
2	6	0	3.905667	0.408517	-0.342631
3	6	0	4.892392	1.362601	-0.176435
4	6	0	4.571648	2.708861	0.020557
5	6	0	3.242744	3.141564	0.078590
6	6	0	2.224063	2.224635	-0.052951
7	1	0	5.940073	1.071950	-0.209877
8	1	0	5.376005	3.433589	0.129860
9	1	0	3.020005	4.194646	0.231841
10	1	0	1.177559	2.511832	-0.019097
11	7	0	1.590222	-0.083704	-0.435594
12	45	0	-0.346538	-0.034376	-0.126783
13	45	0	-2.759645	-0.061925	0.252771
14	8	0	-0.250444	-1.762509	1.009563
15	6	0	-1.324020	-2.261590	1.474408
16	8	0	-2.490434	-1.803898	1.331443
17	8	0	-2.872309	1.682357	-0.865803
18	6	0	-1.819656	2.153639	-1.368291
19	8	0	-0.638710	1.692422	-1.230437
20	8	0	-2.930121	-1.177846	-1.483831
21	6	0	-1.885395	-1.491807	-2.115751
22	8	0	-0.691128	-1.170468	-1.816740
23	8	0	-2.409610	1.036635	1.976721
24	6	0	-1.230032	1.363915	2.269090
25	8	0	-0.178609	1.104157	1.596983
26	6	0	4.180248	-1.071827	-0.524557
27	6	0	3.959937	-1.831375	0.818599
28	6	0	5.654136	-1.498032	-0.442274
29	6	0	5.476436	-1.757581	1.063290
30	1	0	5.744528	-2.438545	-0.996081
31	1	0	6.440127	-0.817148	-0.786890
32	1	0	5.967671	-2.638179	1.486364
33	1	0	5.749377	-0.883096	1.666574
34	6	0	-1.947740	3.362772	-2.249463
35	1	0	-2.861743	3.911775	-2.015312
36	1	0	-1.070185	4.005292	-2.149009
37	1	0	-1.999620	3.029015	-3.291377
38	6	0	-2.032518	-2.339047	-3.346319
39	1	0	-1.526684	-1.855096	-4.186790
40	1	0	-1.535338	-3.299777	-3.178993
41	1	0	-3.085894	-2.503118	-3.577982
42	6	0	-1.011295	2.115598	3.551216
43	1	0	-0.593543	1.427841	4.293981
44	1	0	-0.282411	2.915479	3.399027
45	1	0	-1.953331	2.517317	3.928466
46	6	0	-1.159514	-3.532084	2.257609
47	1	0	-0.381459	-3.399116	3.014634
48	1	0	-2.102074	-3.821164	2.724915
49	1	0	-0.824423	-4.325768	1.582254
50	8	0	3.540950	-1.579625	-1.657348
51	1	0	3.274828	-1.398167	1.555270
52	1	0	3.632968	-2.848713	0.574374
53	1	0	2.588547	-1.440201	-1.514265

Zero-point correction= 0.397320 (Hartree/Particle)
Thermal correction to Energy= 0.429750
Thermal correction to Enthalpy= 0.430694
Thermal correction to Gibbs Free Energy= 0.332388
Sum of electronic and zero-point Energies= -1651.881966
Sum of electronic and thermal Energies= -1651.849536
Sum of electronic and thermal Enthalpies= -1651.848592

Sum of electronic and thermal Free Energies= -1651.946898
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1652.30510228

^{3}TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.608332	0.812564	-0.254479
2	6	0	3.983395	0.388187	-0.309473
3	6	0	4.981620	1.339749	-0.219098
4	6	0	4.674317	2.693254	-0.055226
5	6	0	3.341185	3.111072	0.028553
6	6	0	2.315761	2.196271	-0.065258
7	1	0	6.025206	1.037058	-0.279784
8	1	0	5.478158	3.422952	0.004841
9	1	0	3.111676	4.166271	0.155106
10	1	0	1.270680	2.488758	-0.033446
11	7	0	1.637195	-0.084044	-0.395779
12	45	0	-0.413052	-0.073306	-0.143673
13	45	0	-2.805567	-0.038499	0.263413
14	8	0	-0.352443	-1.898864	0.810354
15	6	0	-1.439620	-2.407143	1.229954
16	8	0	-2.590049	-1.895093	1.145907
17	8	0	-2.871028	1.812523	-0.654667
18	6	0	-1.806138	2.292239	-1.128697
19	8	0	-0.649477	1.764003	-1.083998
20	8	0	-3.042727	-0.941379	-1.579447
21	6	0	-2.017989	-1.247834	-2.250139
22	8	0	-0.808625	-1.034087	-1.924419
23	8	0	-2.416775	0.863273	2.083347
24	6	0	-1.220606	1.125467	2.385737
25	8	0	-0.189517	0.889609	1.681026
26	6	0	4.226326	-1.107056	-0.336658
27	6	0	4.702551	-1.640895	1.052828
28	6	0	5.618065	-1.528496	-0.910695
29	6	0	6.148848	-1.651798	0.528273
30	1	0	5.508998	-2.502237	-1.397367
31	1	0	6.096396	-0.830946	-1.606285
32	1	0	6.748837	-2.538646	0.751624
33	1	0	6.713836	-0.768492	0.846259
34	6	0	-1.889491	3.625879	-1.814811
35	1	0	-2.922567	3.974183	-1.854427
36	1	0	-1.274409	4.351800	-1.273856
37	1	0	-1.478838	3.541724	-2.825136
38	6	0	-2.225836	-1.942316	-3.564437
39	1	0	-1.703344	-1.395249	-4.354236
40	1	0	-1.782095	-2.941471	-3.514888
41	1	0	-3.289262	-2.020350	-3.795207
42	6	0	-0.968058	1.781108	3.713425
43	1	0	-0.339000	1.127485	4.325324
44	1	0	-0.415250	2.712770	3.561550
45	1	0	-1.908589	1.981576	4.228715
46	6	0	-1.317979	-3.753078	1.883362
47	1	0	-0.599365	-3.693798	2.705906
48	1	0	-2.286900	-4.092695	2.252369
49	1	0	-0.921291	-4.470524	1.158566
50	8	0	3.192437	-1.769080	-0.933277
51	1	0	4.476809	-1.032677	1.935002
52	1	0	4.298465	-2.649874	1.187144
53	1	0	2.106880	-1.098386	-0.633200

Zero-point correction= 0.394098 (Hartree/Particle)
Thermal correction to Energy= 0.426486
Thermal correction to Enthalpy= 0.427430
Thermal correction to Gibbs Free Energy= 0.328007
Sum of electronic and zero-point Energies= -1649.381343
Sum of electronic and thermal Energies= -1649.348955
Sum of electronic and thermal Enthalpies= -1649.348011
Sum of electronic and thermal Free Energies= -1649.447434
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1652.28442346

^{3}INT3

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	2.559451	0.952404	-0.703559
2	6	0	3.914697	0.477555	-0.600086
3	6	0	4.909656	1.386154	-0.286879
4	6	0	4.622829	2.736999	-0.061465
5	6	0	3.304409	3.194969	-0.117675
6	6	0	2.283016	2.319214	-0.419845
7	1	0	5.939829	1.048806	-0.200483
8	1	0	5.432006	3.424206	0.173718
9	1	0	3.083367	4.242115	0.073651
10	1	0	1.245080	2.639178	-0.483161
11	7	0	1.542988	0.146897	-1.034678
12	45	0	-0.417082	0.086779	-0.339017
13	45	0	-2.630077	-0.242200	0.610005
14	8	0	-0.052165	-1.920567	0.004602
15	6	0	-0.959074	-2.619446	0.560213
16	8	0	-2.098183	-2.223450	0.924774
17	8	0	-3.002433	1.754631	0.234540
18	6	0	-2.099683	2.460895	-0.289421
19	8	0	-0.932732	2.078024	-0.622235
20	8	0	-3.280513	-0.708954	-1.301365
21	6	0	-2.452506	-0.679557	-2.253597
22	8	0	-1.220966	-0.377335	-2.180201
23	8	0	-1.818242	0.254732	2.449679
24	6	0	-0.585921	0.506159	2.533831
25	8	0	0.255805	0.512761	1.580970
26	6	0	4.198504	-1.004114	-0.749429
27	6	0	3.562280	-1.784586	0.570270
28	6	0	5.556371	-1.531090	-0.228753
29	6	0	4.965149	-1.740698	1.169920
30	1	0	5.736972	-2.484682	-0.735374
31	1	0	6.444192	-0.900185	-0.332360
32	1	0	5.284117	-2.626600	1.725847
33	1	0	5.096522	-0.855168	1.801273
34	6	0	-2.427850	3.897606	-0.580641
35	1	0	-3.330293	4.199676	-0.046730
36	1	0	-1.585987	4.539091	-0.307978
37	1	0	-2.593182	4.011406	-1.657133
38	6	0	-2.964787	-1.066615	-3.611509
39	1	0	-2.299564	-0.700000	-4.395196
40	1	0	-3.011515	-2.159119	-3.671638
41	1	0	-3.978241	-0.682565	-3.749627
42	6	0	-0.037265	0.802632	3.901458
43	1	0	0.376158	-0.119530	4.324034
44	1	0	0.770708	1.534913	3.836092
45	1	0	-0.831711	1.158518	4.560132
46	6	0	-0.634696	-4.071102	0.773119
47	1	0	0.435055	-4.201703	0.952847
48	1	0	-1.219742	-4.471083	1.603552
49	1	0	-0.895919	-4.628632	-0.132676
50	8	0	3.662232	-1.575150	-1.816035
51	1	0	2.725607	-1.243096	1.021949
52	1	0	3.253770	-2.783705	0.250321
53	1	0	1.854109	-0.757976	-1.396302

Zero-point correction= 0.399774 (Hartree/Particle)
Thermal correction to Energy= 0.432681
Thermal correction to Enthalpy= 0.433625
Thermal correction to Gibbs Free Energy= 0.332773
Sum of electronic and zero-point Energies= -1649.387934
Sum of electronic and thermal Energies= -1649.355028
Sum of electronic and thermal Enthalpies= -1649.354084
Sum of electronic and thermal Free Energies= -1649.454936
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1652.29644945

^{3}TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.525627	0.987254	-0.788487
2	6	0	3.871487	0.493161	-0.662188
3	6	0	4.868011	1.376535	-0.283434
4	6	0	4.592046	2.724021	-0.028531

5	6	0	3.281937	3.200737	-0.113347
6	6	0	2.258809	2.347562	-0.471602
7	1	0	5.890047	1.020452	-0.174390
8	1	0	5.401517	3.393032	0.253461
9	1	0	3.067756	4.244466	0.103064
10	1	0	1.225841	2.680407	-0.545644
11	7	0	1.507722	0.198299	-1.156454
12	45	0	-0.422492	0.103795	-0.383972
13	45	0	-2.571458	-0.280649	0.684419
14	8	0	-0.045907	-1.920243	-0.165658
15	6	0	-0.920639	-2.650252	0.401536
16	8	0	-2.039029	-2.278092	0.846470
17	8	0	-2.958078	1.736972	0.437971
18	6	0	-2.090806	2.469085	-0.110230
19	8	0	-0.946362	2.105462	-0.530490
20	8	0	-3.340378	-0.647275	-1.200328
21	6	0	-2.577114	-0.558239	-2.202444
22	8	0	-1.341370	-0.265000	-2.192296
23	8	0	-1.644650	0.107180	2.497957
24	6	0	-0.411543	0.364378	2.515298
25	8	0	0.366074	0.431719	1.510063
26	6	0	4.147414	-0.976787	-0.869361
27	6	0	3.421917	-1.770907	0.625001
28	6	0	5.438014	-1.564401	-0.262911
29	6	0	4.844013	-1.736375	1.137979
30	1	0	5.594212	-2.530367	-0.753515
31	1	0	6.353639	-0.969688	-0.350452
32	6	0	-2.447855	3.912531	-0.323088
33	1	0	-3.182429	4.234658	0.417516
34	1	0	-1.554983	4.540220	-0.284318
35	1	0	-2.892748	4.019750	-1.318314
36	6	0	0.226231	0.628285	3.850554
37	1	0	1.079430	-0.042628	3.988315
38	1	0	0.612365	1.652132	3.870514
39	1	0	-0.495897	0.489305	4.656398
40	6	0	-0.551505	-4.097743	0.564288
41	1	0	-1.417540	-4.682389	0.878429
42	1	0	-0.146306	-4.485819	-0.374165
43	1	0	0.234786	-4.182400	1.322167
44	8	0	3.591044	-1.556248	-1.867334
45	1	0	2.633205	-1.141758	1.043575
46	1	0	3.060482	-2.736618	0.268349
47	1	0	1.826208	-0.701994	-1.527526
48	1	0	5.016605	-0.850377	1.758699
49	1	0	5.163575	-2.623832	1.693572
50	6	0	-3.197330	-0.802267	-3.548444
51	1	0	-2.429546	-0.956508	-4.308372
52	1	0	-3.867669	-1.663803	-3.494724
53	1	0	-3.801904	0.068805	-3.821937

Zero-point correction= 0.398951 (Hartree/Particle)
Thermal correction to Energy= 0.431434
Thermal correction to Enthalpy= 0.432378
Thermal correction to Gibbs Free Energy= 0.333172
Sum of electronic and zero-point Energies= -1649.387738
Sum of electronic and thermal Energies= -1649.355255
Sum of electronic and thermal Enthalpies= -1649.354311
Sum of electronic and thermal Free Energies= -1649.453516
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1652.29605515

^{1}TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.533201	0.655586	-0.253341
2	6	0	3.938034	0.244587	-0.446793
3	6	0	4.940595	1.249655	-0.489185
4	6	0	4.612491	2.552129	-0.240151
5	6	0	3.279153	2.952162	0.084348
6	6	0	2.271033	2.044942	0.075453
7	1	0	5.963729	0.983680	-0.744119
8	1	0	5.386557	3.314335	-0.305359
9	1	0	3.080593	3.996780	0.309338
10	1	0	1.242371	2.317336	0.286411

11	7	0	1.614794	-0.255036	-0.401262
12	45	0	-0.389363	-0.077513	-0.117971
13	45	0	-2.804089	0.010988	0.236218
14	8	0	-0.394502	-1.866682	0.924906
15	6	0	-1.500249	-2.326488	1.350902
16	8	0	-2.637951	-1.795551	1.230975
17	8	0	-2.788692	1.812739	-0.798758
18	6	0	-1.704496	2.245334	-1.268544
19	8	0	-0.553756	1.712724	-1.145793
20	8	0	-3.019558	-0.999725	-1.556909
21	6	0	-1.985138	-1.340474	-2.192712
22	8	0	-0.778574	-1.109153	-1.867468
23	8	0	-2.410890	1.012525	2.012089
24	6	0	-1.219778	1.261264	2.329906
25	8	0	-0.173860	0.960918	1.667519
26	6	0	4.203321	-1.174035	-0.568078
27	6	0	4.624219	-1.093243	1.208054
28	6	0	5.635951	-1.689097	-0.700739
29	6	0	6.040550	-1.395092	0.750980
30	1	0	5.572958	-2.758925	-0.915182
31	1	0	6.233497	-1.210187	-1.484953
32	1	0	6.515336	-2.226890	1.281274
33	1	0	6.695282	-0.523256	0.847660
34	6	0	-1.756377	3.505515	-2.086017
35	1	0	-0.864460	4.111322	-1.909217
36	1	0	-1.769198	3.234796	-3.147224
37	1	0	-2.661953	4.070910	-1.858338
38	6	0	-2.173479	-2.107324	-3.471459
39	1	0	-1.648660	-1.597731	-4.284680
40	1	0	-1.720884	-3.098162	-3.365592
41	1	0	-3.233794	-2.207464	-3.708422
42	6	0	-0.979831	1.985510	3.625487
43	1	0	-0.375356	1.355978	4.285626
44	1	0	-0.407664	2.898364	3.434357
45	1	0	-1.926169	2.231088	4.109758
46	6	0	-1.426107	-3.655175	2.049650
47	1	0	-1.264622	-4.439136	1.302402
48	1	0	-0.572262	-3.671543	2.731724
49	1	0	-2.353878	-3.858202	2.587251
50	8	0	3.232121	-1.992588	-0.861512
51	1	0	4.432279	-0.228176	1.845420
52	1	0	4.017326	-1.953019	1.504382
53	1	0	2.267503	-1.339213	-0.701740

Zero-point correction= 0.396785 (Hartree/Particle)
Thermal correction to Energy= 0.429110
Thermal correction to Enthalpy= 0.430054
Thermal correction to Gibbs Free Energy= 0.331883
Sum of electronic and zero-point Energies= -1649.381153
Sum of electronic and thermal Energies= -1649.348827
Sum of electronic and thermal Enthalpies= -1649.347883
Sum of electronic and thermal Free Energies= -1649.446054
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1652.28982672

^{3}INT4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.586339	0.975217	-0.768172
2	6	0	3.941306	0.491937	-0.764991
3	6	0	4.960346	1.331953	-0.341778
4	6	0	4.700955	2.647817	0.044581
5	6	0	3.384576	3.120685	0.064781
6	6	0	2.341529	2.301894	-0.313510
7	1	0	5.984605	0.962769	-0.324100
8	1	0	5.521349	3.295479	0.343217
9	1	0	3.181278	4.140181	0.383261
10	1	0	1.308235	2.641471	-0.301179
11	7	0	1.549093	0.215170	-1.137154
12	45	0	-0.387337	0.127560	-0.377800
13	45	0	-2.559962	-0.265389	0.634452
14	8	0	-0.077000	-1.913456	-0.300092
15	6	0	-0.972465	-2.654869	0.217433
16	8	0	-2.082742	-2.280519	0.682070

17	8	0	-2.889314	1.774134	0.518722
18	6	0	-1.989098	2.518763	0.046668
19	8	0	-0.851914	2.150440	-0.390941
20	8	0	-3.311505	-0.492102	-1.278676
21	6	0	-2.533329	-0.352160	-2.262348
22	8	0	-1.289330	-0.094157	-2.215358
23	8	0	-1.661624	-0.020584	2.482032
24	6	0	-0.420878	0.193145	2.535507
25	8	0	0.372289	0.317525	1.548133
26	6	0	4.218233	-0.928540	-1.124590
27	6	0	2.936299	-2.033594	1.074086
28	6	0	5.086463	-1.719835	-0.174458
29	6	0	4.389961	-1.739656	1.202015
30	1	0	5.164765	-2.730455	-0.590766
31	1	0	6.098894	-1.303913	-0.086405
32	6	0	-2.280355	3.989926	-0.038153
33	1	0	-3.149603	4.244473	0.570364
34	1	0	-1.406903	4.565550	0.278942
35	1	0	-2.484700	4.250790	-1.081860
36	6	0	0.210637	0.294740	3.895159
37	1	0	0.882732	1.156220	3.930938
38	1	0	-0.553424	0.371603	4.670301
39	1	0	0.815999	-0.600950	4.072922
40	6	0	-0.639196	-4.117197	0.293221
41	1	0	-1.522150	-4.700275	0.559652
42	1	0	-0.227967	-4.455373	-0.661705
43	1	0	0.134594	-4.264415	1.054698
44	8	0	3.661791	-1.463828	-2.068442
45	1	0	2.180589	-1.474207	1.620249
46	1	0	2.600257	-2.837363	0.420529
47	1	0	1.834916	-0.680446	-1.542163
48	1	0	4.532963	-0.769318	1.695921
49	1	0	4.904603	-2.482056	1.835363
50	6	0	-3.122498	-0.480674	-3.637368
51	1	0	-3.178412	0.512895	-4.094016
52	1	0	-2.471497	-1.093678	-4.265897
53	1	0	-4.124484	-0.909804	-3.585644

Zero-point correction= 0.398139 (Hartree/Particle)
Thermal correction to Energy= 0.431724
Thermal correction to Enthalpy= 0.432668
Thermal correction to Gibbs Free Energy= 0.331596
Sum of electronic and zero-point Energies= -1649.416990
Sum of electronic and thermal Energies= -1649.383405
Sum of electronic and thermal Enthalpies= -1649.382461
Sum of electronic and thermal Free Energies= -1649.483533
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1652.32644446

[1]INT5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.676741	0.545979	-0.156589
2	6	0	4.090495	0.039801	0.044876
3	6	0	5.135050	1.117233	0.052920
4	6	0	4.821896	2.419387	0.020285
5	6	0	3.440041	2.849138	-0.041230
6	6	0	2.420142	1.969418	-0.111974
7	1	0	6.175533	0.798476	0.108938
8	1	0	5.605786	3.172163	0.051027
9	1	0	3.228317	3.916086	-0.040460
10	1	0	1.382893	2.284365	-0.188621
11	7	0	1.698004	-0.273459	-0.339464
12	45	0	-0.425099	-0.068575	-0.129489
13	45	0	-2.821862	-0.002676	0.248009
14	8	0	-0.382387	-1.891766	0.850388
15	6	0	-1.479111	-2.365599	1.287337
16	8	0	-2.618911	-1.835091	1.197509
17	8	0	-2.847998	1.818369	-0.734815
18	6	0	-1.769108	2.281282	-1.194053
19	8	0	-0.614571	1.756808	-1.097110
20	8	0	-3.048762	-0.964484	-1.569983
21	6	0	-2.018543	-1.281378	-2.227317
22	8	0	-0.810801	-1.060989	-1.902854

23	8	0	-2.419818	0.963695	2.037925
24	6	0	-1.223003	1.203270	2.354299
25	8	0	-0.184511	0.916706	1.680150
26	6	0	4.507785	-0.967803	-1.068005
27	6	0	4.230841	-0.815200	1.329787
28	6	0	5.220072	-2.141173	-0.419474
29	6	0	5.400643	-1.761446	1.045247
30	1	0	4.543820	-3.002892	-0.525992
31	1	0	6.133171	-2.394357	-0.967090
32	1	0	5.398809	-2.626677	1.714779
33	1	0	6.357427	-1.245774	1.195971
34	6	0	-1.844589	3.570702	-1.962054
35	1	0	-0.975592	4.195205	-1.741034
36	1	0	-1.824692	3.343144	-3.033153
37	1	0	-2.770780	4.100348	-1.731753
38	6	0	-2.222248	-2.002395	-3.530092
39	1	0	-1.696255	-1.471019	-4.328401
40	1	0	-1.780459	-3.001409	-3.460943
41	1	0	-3.284660	-2.084196	-3.764522
42	6	0	-0.982268	1.880417	3.674970
43	1	0	-0.580495	1.147915	4.382902
44	1	0	-0.234006	2.668915	3.559137
45	1	0	-1.912911	2.288969	4.072492
46	6	0	-1.391958	-3.708247	1.957868
47	1	0	-1.249966	-4.479323	1.193239
48	1	0	-0.524719	-3.739132	2.622581
49	1	0	-2.307912	-3.921011	2.511642
50	8	0	4.281961	-0.826702	-2.240337
51	1	0	4.374254	-0.193586	2.219573
52	1	0	3.303583	-1.388809	1.474825
53	1	0	1.955154	-1.259569	-0.390117

Zero-point correction= 0.403060 (Hartree/Particle)
Thermal correction to Energy= 0.435918
Thermal correction to Enthalpy= 0.436862
Thermal correction to Gibbs Free Energy= 0.336701
Sum of electronic and zero-point Energies= -1649.475737
Sum of electronic and thermal Energies= -1649.442878
Sum of electronic and thermal Enthalpies= -1649.441934
Sum of electronic and thermal Free Energies= -1649.542096
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1652.39472949

^{1}TS5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.812641	0.509549	-0.762808
2	6	0	-4.151549	-0.017821	-0.840672
3	6	0	-5.239472	0.811342	-0.470191
4	6	0	-5.043066	2.081160	0.007404
5	6	0	-3.728575	2.603217	0.044296
6	6	0	-2.648429	1.858416	-0.347324
7	1	0	-6.247550	0.406932	-0.569640
8	1	0	-5.884910	2.695075	0.314950
9	1	0	-3.573107	3.625173	0.384408
10	1	0	-1.635030	2.247354	-0.308493
11	7	0	-1.733483	-0.313478	-0.813787
12	45	0	0.290962	-0.035747	-0.245890
13	45	0	2.644167	0.087052	0.364298
14	8	0	0.821789	-1.281447	-1.813100
15	6	0	2.058105	-1.516162	-1.998754
16	8	0	3.020079	-1.097511	-1.301255
17	8	0	2.089356	1.261421	1.974172
18	6	0	0.870222	1.547825	2.125078
19	8	0	-0.095831	1.196535	1.378562
20	8	0	2.317311	-1.616334	1.513363
21	6	0	1.165846	-2.124852	1.568258
22	8	0	0.118455	-1.714111	0.974933
23	8	0	2.765171	1.776631	-0.830158
24	6	0	1.739128	2.166640	-1.450199
25	8	0	0.581512	1.641306	-1.419709
26	6	0	-3.058237	-0.825334	0.912936
27	6	0	-4.415424	-1.360116	-1.467881
28	6	0	-3.258753	-2.264322	0.542389

29	6	0	-4.452027	-2.436128	-0.382590
30	1	0	-2.320554	-2.651144	0.135169
31	1	0	-3.417764	-2.749091	1.513844
32	1	0	-4.464853	-3.448837	-0.800406
33	1	0	-5.373307	-2.313598	0.203527
34	6	0	0.499046	2.385714	3.317334
35	1	0	-0.097855	3.243323	2.993904
36	1	0	-0.127306	1.791336	3.990087
37	1	0	1.391721	2.723228	3.846397
38	6	0	1.014873	-3.368747	2.401998
39	1	0	1.673556	-3.319436	3.271854
40	1	0	-0.023529	-3.503718	2.713308
41	1	0	1.315417	-4.235838	1.803799
42	6	0	1.888416	3.367159	-2.343036
43	1	0	1.836798	3.042042	-3.387322
44	1	0	1.061348	4.062430	-2.176510
45	1	0	2.845666	3.860671	-2.166413
46	6	0	2.387827	-2.373962	-3.189346
47	1	0	1.766037	-3.273751	-3.182539
48	1	0	2.151389	-1.821897	-4.104728
49	1	0	3.445153	-2.643428	-3.189401
50	8	0	-2.905224	-0.172761	1.863378
51	1	0	-5.373312	-1.338436	-2.001003
52	1	0	-3.651037	-1.598758	-2.220633
53	1	0	-1.836077	-1.125349	-1.418868

Zero-point correction= 0.401045 (Hartree/Particle)
Thermal correction to Energy= 0.433596
Thermal correction to Enthalpy= 0.434540
Thermal correction to Gibbs Free Energy= 0.336532
Sum of electronic and zero-point Energies= -1649.430588
Sum of electronic and thermal Energies= -1649.398037
Sum of electronic and thermal Enthalpies= -1649.397093
Sum of electronic and thermal Free Energies= -1649.495102
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1652.34676271

[1]INT6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.003592	0.470688	-0.006034
2	6	0	4.241128	0.111452	0.544890
3	6	0	5.260141	1.061344	0.513985
4	6	0	5.056380	2.309584	-0.067815
5	6	0	3.826906	2.625257	-0.635719
6	6	0	2.788821	1.698988	-0.609317
7	1	0	6.229703	0.812824	0.944221
8	1	0	5.866472	3.034908	-0.084733
9	1	0	3.673112	3.595745	-1.101118
10	1	0	1.813893	1.904962	-1.044236
11	7	0	1.963458	-0.541334	0.004425
12	45	0	-0.239987	-0.067435	-0.026874
13	45	0	-2.622803	0.270354	0.172668
14	8	0	-0.284392	-1.138502	1.746021
15	6	0	-1.405533	-1.265403	2.337465
16	8	0	-2.509562	-0.795739	1.955109
17	8	0	-2.558139	1.298922	-1.612979
18	6	0	-1.443253	1.447526	-2.188909
19	8	0	-0.318183	1.020493	-1.783027
20	8	0	-2.873689	-1.504205	-0.862683
21	6	0	-1.854609	-2.150998	-1.232806
22	8	0	-0.641247	-1.831495	-1.033251
23	8	0	-2.205521	2.024824	1.188570
24	6	0	-1.000788	2.339767	1.397173
25	8	0	0.026691	1.694155	1.022814
26	6	0	2.313870	-1.564080	-0.971874
27	6	0	4.463460	-1.265427	1.129228
28	6	0	2.903386	-2.782955	-0.326477
29	6	0	4.332862	-2.436507	0.139346
30	1	0	2.284778	-3.094676	0.528528
31	1	0	2.929841	-3.598225	-1.055252
32	1	0	4.761596	-3.334351	0.601337
33	1	0	4.942086	-2.217041	-0.748450
34	6	0	-1.435066	2.182259	-3.498213

35	1	0	-0.617865	2.908070	-3.512563
36	1	0	-1.247674	1.464930	-4.303805
37	1	0	-2.392441	2.677081	-3.668797
38	6	0	-2.080064	-3.436431	-1.976409
39	1	0	-3.138488	-3.570531	-2.204708
40	1	0	-1.488037	-3.434457	-2.895914
41	1	0	-1.728374	-4.273408	-1.364654
42	6	0	-0.750774	3.588444	2.193537
43	1	0	-0.736607	3.329473	3.257731
44	1	0	0.217613	4.020791	1.933625
45	1	0	-1.556051	4.307929	2.031026
46	6	0	-1.392057	-2.067815	3.607296
47	1	0	-1.159490	-3.111256	3.370887
48	1	0	-0.604378	-1.699301	4.270531
49	1	0	-2.361545	-2.015653	4.104901
50	8	0	2.267825	-1.337465	-2.147926
51	1	0	5.473968	-1.293275	1.555239
52	1	0	3.784504	-1.436722	1.982078
53	1	0	1.934044	-0.961892	0.935154

Zero-point correction= 0.404854 (Hartree/Particle)
Thermal correction to Energy= 0.437322
Thermal correction to Enthalpy= 0.438267
Thermal correction to Gibbs Free Energy= 0.338177
Sum of electronic and zero-point Energies= -1649.514569
Sum of electronic and thermal Energies= -1649.482101
Sum of electronic and thermal Enthalpies= -1649.481157
Sum of electronic and thermal Free Energies= -1649.581246
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1652.43146540

2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.519237	-0.523630	0.519638
2	6	0	-0.572762	0.847392	0.223349
3	6	0	-1.776791	1.367362	-0.246069
4	6	0	-2.885954	0.547247	-0.433428
5	6	0	-2.805918	-0.811144	-0.151503
6	6	0	-1.615055	-1.348977	0.327417
7	1	0	-1.841932	2.429866	-0.477875
8	1	0	-3.814098	0.971875	-0.808458
9	1	0	-3.668192	-1.454384	-0.307564
10	1	0	-1.511314	-2.407376	0.550285
11	7	0	0.739642	-1.061785	0.967989
12	6	0	1.678212	-1.015913	-0.094343
13	6	0	0.641706	1.730235	0.415259
14	6	0	2.658570	0.121785	0.016010
15	6	0	1.888811	1.385444	-0.417320
16	1	0	3.031864	0.243077	1.043037
17	1	0	3.509588	-0.050791	-0.649406
18	1	0	2.578289	2.237869	-0.376541
19	1	0	1.596246	1.265178	-1.469419
20	8	0	1.555299	-1.698519	-1.081964
21	1	0	0.349879	2.760527	0.176085
22	1	0	0.925374	1.750488	1.481931
23	1	0	1.074921	-0.524488	1.763639

Zero-point correction= 0.192432 (Hartree/Particle)
Thermal correction to Energy= 0.201692
Thermal correction to Enthalpy= 0.202636
Thermal correction to Gibbs Free Energy= 0.158020
Sum of electronic and zero-point Energies= -517.121967
Sum of electronic and thermal Energies= -517.112708
Sum of electronic and thermal Enthalpies= -517.111764
Sum of electronic and thermal Free Energies= -517.156379
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -517.44289526

^{1}INT2'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.318834	0.082410	-0.341939

2	45	0	2.583756	-0.175046	0.579775
3	8	0	0.913709	1.938962	-1.044545
4	6	0	2.128121	2.299917	-0.884813
5	8	0	3.029114	1.654426	-0.295166
6	8	0	1.036736	-0.763671	-2.081234
7	6	0	2.227150	-1.214623	-2.106264
8	8	0	3.083533	-1.138398	-1.185594
9	8	0	-0.039616	-1.824843	0.432011
10	6	0	0.847103	-2.410817	1.129692
11	8	0	2.001711	-1.984930	1.395575
12	8	0	-0.217049	0.938111	1.466730
13	6	0	0.676720	1.111950	2.359408
14	8	0	1.892139	0.799804	2.279326
15	7	0	-1.560411	0.004646	-0.834565
16	6	0	-2.462323	0.942285	-0.559824
17	6	0	-3.831043	0.531660	-0.321772
18	6	0	-2.139010	2.337250	-0.526154
19	6	0	-4.775239	1.517263	-0.075912
20	6	0	-3.117378	3.284880	-0.331445
21	1	0	-1.103480	2.611761	-0.711537
22	6	0	-4.431744	2.868093	-0.097397
23	1	0	-5.792362	1.215522	0.155416
24	1	0	-2.873079	4.343916	-0.343053
25	1	0	-5.205170	3.612650	0.082473
26	6	0	-4.217466	-0.920212	-0.217351
27	6	0	-3.788284	-1.931851	-1.315402
28	6	0	-3.453012	-1.789414	0.813246
29	6	0	-3.407907	-2.936340	-0.210819
30	1	0	-2.920960	-1.591491	-1.881610
31	1	0	-4.600379	-2.213574	-1.998600
32	1	0	-2.455258	-1.392175	1.024562
33	1	0	-4.010826	-1.946306	1.742167
34	1	0	-2.437585	-3.428223	-0.326783
35	1	0	-4.181947	-3.690565	-0.037917
36	8	0	-5.597499	-1.065964	0.064996
37	1	0	-6.077801	-0.998936	-0.768037
38	6	0	0.201079	1.731017	3.643174
39	1	0	1.040325	2.172094	4.184034
40	1	0	-0.570634	2.478326	3.444614
41	1	0	-0.243834	0.948301	4.266806
42	6	0	2.487035	3.630752	-1.482215
43	1	0	1.808677	4.400245	-1.102025
44	1	0	3.520058	3.890309	-1.246100
45	1	0	2.353551	3.586887	-2.567537
46	6	0	2.623397	-1.916849	-3.373727
47	1	0	3.696939	-2.111820	-3.384215
48	1	0	2.079556	-2.864673	-3.440228
49	1	0	2.333800	-1.313724	-4.238457
50	6	0	0.450355	-3.756479	1.668828
51	1	0	-0.522031	-3.681349	2.165225
52	1	0	0.336581	-4.456260	0.834428
53	1	0	1.204654	-4.133694	2.361335

Zero-point correction= 0.401828 (Hartree/Particle)
Thermal correction to Energy= 0.434474
Thermal correction to Enthalpy= 0.435418
Thermal correction to Gibbs Free Energy= 0.337384
Sum of electronic and zero-point Energies= -1649.388668
Sum of electronic and thermal Energies= -1649.356021
Sum of electronic and thermal Enthalpies= -1649.355077
Sum of electronic and thermal Free Energies= -1649.453111
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1652.29945429

^{3}INT2'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.355508	0.070172	-0.360367
2	45	0	2.563899	-0.114473	0.618242
3	8	0	0.812726	2.058782	-0.759730
4	6	0	2.004843	2.459205	-0.572007
5	8	0	2.951315	1.792063	-0.072107
6	8	0	1.201090	-0.479919	-2.160861
7	6	0	2.407408	-0.879764	-2.168293

8	8	0	3.201606	-0.892033	-1.186513
9	8	0	0.072605	-1.918257	0.113331
10	6	0	0.931417	-2.497413	0.852028
11	8	0	2.026175	-2.014606	1.249071
12	8	0	-0.324113	0.606772	1.526696
13	6	0	0.528441	0.825782	2.444273
14	8	0	1.778412	0.677259	2.358137
15	7	0	-1.571655	0.319321	-1.005439
16	6	0	-2.635479	1.034529	-0.669056
17	6	0	-3.891499	0.424920	-0.330019
18	6	0	-2.505833	2.456637	-0.657348
19	6	0	-4.944008	1.265225	-0.001534
20	6	0	-3.584414	3.248238	-0.329214
21	1	0	-1.528671	2.867216	-0.901441
22	6	0	-4.808217	2.655134	-0.003860
23	1	0	-5.887645	0.808599	0.284955
24	1	0	-3.480237	4.330454	-0.319240
25	1	0	-5.660600	3.276664	0.260652
26	6	0	-4.046833	-1.072944	-0.255172
27	6	0	-3.438603	-2.000029	-1.337881
28	6	0	-3.204129	-1.843693	0.786567
29	6	0	-3.075519	-2.998646	-0.222421
30	1	0	-2.540047	-1.574003	-1.796429
31	1	0	-4.132449	-2.319609	-2.126063
32	1	0	-2.238443	-1.356694	0.964549
33	1	0	-3.720071	-2.022167	1.735683
34	1	0	-2.095500	-3.478005	-0.298155
35	1	0	-3.851630	-3.756720	-0.080298
36	8	0	-5.397235	-1.432724	-0.024304
37	1	0	-5.875608	-1.313566	-0.853035
38	6	0	-0.026080	1.289707	3.760000
39	1	0	0.775648	1.645596	4.409115
40	1	0	-0.768814	2.074745	3.596480
41	1	0	-0.536777	0.451661	4.245581
42	6	0	2.300112	3.866954	-1.003385
43	1	0	1.579313	4.550585	-0.545619
44	1	0	3.316399	4.149701	-0.725032
45	1	0	2.178231	3.943872	-2.088314
46	6	0	2.916792	-1.404767	-3.478976
47	1	0	2.485299	-2.395678	-3.654783
48	1	0	2.587364	-0.754878	-4.293556
49	1	0	4.004951	-1.484208	-3.464035
50	6	0	0.576280	-3.890496	1.283891
51	1	0	-0.351089	-3.858530	1.865915
52	1	0	0.382326	-4.507815	0.401196
53	1	0	1.377629	-4.329064	1.880275

Zero-point correction= 0.401046 (Hartree/Particle)
Thermal correction to Energy= 0.433487
Thermal correction to Enthalpy= 0.434431
Thermal correction to Gibbs Free Energy= 0.336112
Sum of electronic and zero-point Energies= -1649.400120
Sum of electronic and thermal Energies= -1649.367679
Sum of electronic and thermal Enthalpies= -1649.366735
Sum of electronic and thermal Free Energies= -1649.465054
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1652.30967442

^{3}TS6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	2.608443	-0.129743	0.666428
2	6	0	1.867536	-2.400513	-1.000889
3	6	0	2.086087	-3.739910	-1.648396
4	8	0	2.810013	-1.965510	-0.281182
5	8	0	-0.389303	-0.886643	1.274673
6	6	0	-0.270740	-1.966946	3.369565
7	6	0	0.393185	-1.267560	2.218870
8	8	0	1.627427	-1.078708	2.262273
9	8	0	0.756727	-1.830498	-1.232496
10	8	0	2.237384	1.721482	1.526725
11	8	0	1.370136	0.943920	-2.000810
12	8	0	3.397595	0.799904	-0.995971
13	6	0	3.242923	1.789021	-3.139604

14	6	0	2.626151	1.121412	-1.942630
15	8	0	0.217496	1.890818	0.513368
16	6	0	1.152682	2.310784	1.263199
17	6	0	0.948511	3.660070	1.894797
18	45	0	0.414892	0.041778	-0.408871
19	1	0	-0.798064	-1.226098	3.979983
20	1	0	0.471668	-2.473275	3.988147
21	1	0	2.981601	-3.693795	-2.275305
22	1	0	2.273184	-4.489861	-0.873851
23	1	0	1.674738	4.363604	1.475231
24	1	0	-0.063593	4.026572	1.713516
25	1	0	3.006224	1.211618	-4.038155
26	1	0	4.324091	1.874102	-3.020434
27	7	0	-1.496132	0.200880	-1.196306
28	6	0	-2.486132	0.872309	-0.637734
29	6	0	-3.653575	0.163528	-0.060004
30	6	0	-2.570181	2.287888	-0.774530
31	6	0	-4.675395	0.985145	0.561560
32	6	0	-3.644525	3.001739	-0.309773
33	1	0	-1.725694	2.771155	-1.259014
34	6	0	-4.687606	2.338473	0.386621
35	1	0	-5.441673	0.500867	1.162307
36	1	0	-3.673599	4.081695	-0.426656
37	1	0	-5.485369	2.923615	0.839191
38	6	0	-3.637474	-1.257641	0.197207
39	6	0	-4.945036	-2.007921	0.264302
40	6	0	-4.445515	-0.715869	-1.557553
41	6	0	-5.654608	-1.393581	-0.945104
42	1	0	-4.715269	-3.068418	0.119329
43	1	0	-4.579908	0.214846	-2.114754
44	1	0	-3.748158	-1.376277	-2.087111
45	1	0	-6.411866	-0.657779	-0.659397
46	1	0	-6.131143	-2.125148	-1.604802
47	8	0	-2.574669	-1.999397	0.286777
48	1	0	-1.738508	-1.506443	0.515411
49	1	0	-1.013231	-2.680976	3.000686
50	1	0	1.223637	-4.029883	-2.250473
51	1	0	2.801725	2.782186	-3.267649
52	1	0	1.144247	3.594525	2.968673
53	1	0	-5.452355	-1.910048	1.232949

Zero-point correction= 0.398429 (Hartree/Particle)
Thermal correction to Energy= 0.430856
Thermal correction to Enthalpy= 0.431800
Thermal correction to Gibbs Free Energy= 0.333170
Sum of electronic and zero-point Energies= -1649.340800
Sum of electronic and thermal Energies= -1649.308373
Sum of electronic and thermal Enthalpies= -1649.307429
Sum of electronic and thermal Free Energies= -1649.406060
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1652.25036397

^{1}TS7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.495428	0.592982	-0.427743
2	6	0	3.956506	0.195721	-0.356608
3	6	0	4.944218	1.230995	-0.099418
4	6	0	4.555989	2.524299	0.007415
5	6	0	3.189081	2.940818	-0.124375
6	6	0	2.219421	2.025399	-0.351113
7	1	0	6.000859	0.974838	-0.065738
8	1	0	5.321497	3.284300	0.156289
9	1	0	2.950267	3.998235	-0.046515
10	1	0	1.177879	2.309336	-0.458022
11	7	0	1.631269	-0.356202	-0.390029
12	45	0	-0.360722	-0.107285	-0.125209
13	45	0	-2.791016	0.053809	0.269400
14	8	0	-0.796370	-1.496816	-1.606826
15	6	0	-2.009350	-1.797410	-1.828490
16	8	0	-3.029162	-1.356829	-1.232150
17	8	0	-2.341735	1.456803	1.743580
18	6	0	-1.140578	1.735406	1.988482
19	8	0	-0.109283	1.280830	1.397077

20	8	0	-2.563160	-1.475826	1.655827
21	6	0	-1.423515	-1.984955	1.832090
22	8	0	-0.331906	-1.643515	1.280601
23	8	0	-2.816015	1.566073	-1.159235
24	6	0	-1.742372	1.910117	-1.714548
25	8	0	-0.580293	1.430833	-1.506138
26	6	0	4.372613	-1.093231	-0.786331
27	6	0	-0.871916	2.689960	3.121349
28	1	0	-1.763642	3.279061	3.343681
29	1	0	-0.027049	3.339840	2.879688
30	1	0	-0.603359	2.112132	4.012458
31	6	0	-1.347052	-3.154046	2.778925
32	1	0	-0.348311	-3.237581	3.213082
33	1	0	-1.557225	-4.072121	2.219246
34	1	0	-2.103416	-3.055868	3.560788
35	6	0	-1.811945	3.006528	-2.743568
36	1	0	-2.838294	3.357425	-2.862170
37	1	0	-1.430564	2.633390	-3.698990
38	1	0	-1.167013	3.836976	-2.439751
39	6	0	-2.244460	-2.772317	-2.952047
40	1	0	-1.438503	-3.508980	-2.990608
41	1	0	-2.242559	-2.224232	-3.900495
42	1	0	-3.213588	-3.261716	-2.835926
43	6	0	4.042754	-1.077445	1.081115
44	6	0	5.508142	-1.472240	1.161762
45	6	0	5.710869	-1.656105	-0.348381
46	1	0	5.778350	-2.712151	-0.636901
47	1	0	6.569590	-1.143276	-0.797364
48	1	0	5.691217	-2.373572	1.753580
49	1	0	6.122906	-0.668996	1.577482
50	1	0	3.650914	-0.322678	1.765197
51	1	0	3.293449	-1.875361	0.996117
52	8	0	3.605165	-1.777663	-1.608485
53	1	0	3.864969	-2.707143	-1.648617

Zero-point correction= 0.399718 (Hartree/Particle)
Thermal correction to Energy= 0.432338
Thermal correction to Enthalpy= 0.433282
Thermal correction to Gibbs Free Energy= 0.334521
Sum of electronic and zero-point Energies= -1649.334315
Sum of electronic and thermal Energies= -1649.301696
Sum of electronic and thermal Enthalpies= -1649.300751
Sum of electronic and thermal Free Energies= -1649.399512
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1652.25413538

^{3}TS8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.347544	-0.032175	-0.363777
2	45	0	-2.567646	0.058964	0.616180
3	8	0	-0.868440	-1.882190	-1.146526
4	6	0	-2.068174	-2.284440	-1.012034
5	8	0	-2.990591	-1.702594	-0.379466
6	8	0	-1.135374	0.901224	-2.029486
7	6	0	-2.338093	1.308634	-1.988335
8	8	0	-3.160377	1.139714	-1.045321
9	8	0	0.017530	1.816381	0.496152
10	6	0	-0.852685	2.302471	1.287052
11	8	0	-1.982634	1.813003	1.553181
12	8	0	0.290667	-0.951195	1.379092
13	6	0	-0.573861	-1.263291	2.257532
14	8	0	-1.811982	-1.028325	2.211717
15	7	0	1.632228	-0.055031	-0.992012
16	6	0	2.613454	-0.900840	-0.648375
17	6	0	3.928247	-0.417415	-0.341884
18	6	0	2.352442	-2.298505	-0.579276
19	6	0	4.918138	-1.323243	-0.005483
20	6	0	3.365623	-3.172379	-0.244935
21	1	0	1.342896	-2.633525	-0.805865
22	6	0	4.650048	-2.693096	0.039242
23	1	0	5.908064	-0.943937	0.238465
24	1	0	3.164361	-4.240155	-0.201532
25	1	0	5.442367	-3.389055	0.305068

26	6	0	4.155261	1.064774	-0.321226
27	6	0	3.219911	1.901653	-1.196930
28	6	0	3.588664	1.857526	0.889979
29	6	0	3.029475	2.913957	-0.084591
30	1	0	2.174985	1.078278	-1.194221
31	1	0	3.433796	2.137345	-2.244765
32	1	0	2.789781	1.305548	1.400075
33	1	0	4.353557	2.167147	1.608034
34	1	0	2.010092	3.270095	0.094224
35	1	0	3.704274	3.772370	-0.199145
36	8	0	5.516478	1.413481	-0.464251
37	1	0	5.812665	1.097005	-1.326000
38	6	0	-0.048470	-1.960519	3.479860
39	1	0	-0.851417	-2.502841	3.982546
40	1	0	0.768418	-2.633553	3.208984
41	1	0	0.350487	-1.210064	4.170689
42	6	0	-2.401046	-3.582644	-1.690366
43	1	0	-1.701922	-4.357511	-1.362520
44	1	0	-3.426090	-3.882346	-1.467308
45	1	0	-2.274315	-3.466968	-2.771211
46	6	0	-2.805893	2.089772	-3.182902
47	1	0	-2.405572	3.107123	-3.118169
48	1	0	-2.416532	1.640426	-4.099751
49	1	0	-3.895760	2.138442	-3.207609
50	6	0	-0.472235	3.594455	1.953098
51	1	0	0.505363	3.482951	2.433488
52	1	0	-0.373879	4.376791	1.193084
53	1	0	-1.224685	3.888923	2.686092

Zero-point correction= 0.395201 (Hartree/Particle)
Thermal correction to Energy= 0.427288
Thermal correction to Enthalpy= 0.428232
Thermal correction to Gibbs Free Energy= 0.331262
Sum of electronic and zero-point Energies= -1649.378444
Sum of electronic and thermal Energies= -1649.346356
Sum of electronic and thermal Enthalpies= -1649.345412
Sum of electronic and thermal Free Energies= -1649.442382
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1652.28208708

^{1}TS9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.261441	-0.018540	-0.355348
2	45	0	2.484240	0.023320	0.659082
3	8	0	0.797137	1.805138	-1.216396
4	6	0	1.947119	2.305265	-1.003553
5	8	0	2.856827	1.816566	-0.282387
6	8	0	1.094629	-1.015349	-1.969379
7	6	0	2.340704	-1.269242	-1.945404
8	8	0	3.154080	-0.989408	-1.022805
9	8	0	-0.032376	-1.823490	0.586140
10	6	0	0.880205	-2.296529	1.340370
11	8	0	2.001276	-1.777169	1.569768
12	8	0	-0.441431	0.929220	1.345043
13	6	0	0.386699	1.251014	2.256461
14	8	0	1.629228	1.040867	2.255021
15	7	0	-1.526417	0.068227	-1.322109
16	6	0	-2.508362	0.875021	-0.775059
17	6	0	-3.742506	0.377725	-0.308818
18	6	0	-2.278000	2.265069	-0.734980
19	6	0	-4.718608	1.250023	0.152350
20	6	0	-3.271345	3.114242	-0.275678
21	1	0	-1.322384	2.642734	-1.085197
22	6	0	-4.496307	2.622153	0.170420
23	1	0	-5.655440	0.830683	0.515802
24	1	0	-3.078914	4.185115	-0.264283
25	1	0	-5.262567	3.298808	0.539223
26	6	0	-3.916938	-1.109237	-0.311379
27	6	0	-3.014056	-1.839287	-1.300719
28	6	0	-3.257470	-1.959781	0.804668
29	6	0	-2.751654	-2.929572	-0.282679
30	1	0	-2.000324	-1.104272	-1.457951
31	1	0	-3.280441	-1.997116	-2.352449

32	1	0	-2.428689	-1.423043	1.280678
33	1	0	-3.955185	-2.340587	1.555678
34	1	0	-1.740543	-3.331570	-0.196566
35	1	0	-3.462869	-3.748692	-0.460410
36	8	0	-5.264211	-1.512049	-0.423163
37	1	0	-5.654213	-1.030187	-1.163015
38	6	0	-0.201016	1.930084	3.460450
39	1	0	0.568710	2.493023	3.991617
40	1	0	-1.025850	2.580535	3.160034
41	1	0	-0.603847	1.167633	4.135688
42	6	0	2.224254	3.612696	-1.688565
43	1	0	1.506654	4.362741	-1.341752
44	1	0	3.241132	3.947868	-1.479174
45	1	0	2.079175	3.497618	-2.766664
46	6	0	2.883308	-1.965689	-3.161636
47	1	0	3.920147	-2.266209	-3.003105
48	1	0	2.264520	-2.835850	-3.397663
49	1	0	2.825466	-1.285265	-4.017174
50	6	0	0.560686	-3.615131	1.983994
51	1	0	-0.479849	-3.622416	2.322568
52	1	0	0.673397	-4.410765	1.239184
53	1	0	1.239650	-3.811009	2.815442

Zero-point correction= 0.395325 (Hartree/Particle)
Thermal correction to Energy= 0.427393
Thermal correction to Enthalpy= 0.428338
Thermal correction to Gibbs Free Energy= 0.332188
Sum of electronic and zero-point Energies= -1649.367108
Sum of electronic and thermal Energies= -1649.335039
Sum of electronic and thermal Enthalpies= -1649.334095
Sum of electronic and thermal Free Energies= -1649.430245
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1652.27138063

^{3}INT7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.380006	0.076792	-0.373501
2	45	0	2.578346	-0.158841	0.633435
3	8	0	0.982235	1.936630	-1.060198
4	6	0	2.190157	2.289061	-0.872024
5	8	0	3.076777	1.638225	-0.256042
6	8	0	1.149438	-0.812219	-2.072211
7	6	0	2.338598	-1.259684	-2.039425
8	8	0	3.153376	-1.168175	-1.080323
9	8	0	-0.079763	-1.799124	0.382453
10	6	0	0.760250	-2.368424	1.151819
11	8	0	1.903568	-1.942888	1.459845
12	8	0	-0.248645	0.938922	1.401540
13	6	0	0.610867	1.156842	2.312558
14	8	0	1.837918	0.867952	2.274882
15	7	0	-1.605479	0.080839	-1.026963
16	6	0	-2.592522	0.924812	-0.695455
17	6	0	-3.929055	0.489392	-0.390657
18	6	0	-2.283536	2.313935	-0.630141
19	6	0	-4.875226	1.449369	-0.071274
20	6	0	-3.257756	3.238180	-0.323447
21	1	0	-1.258270	2.602997	-0.852154
22	6	0	-4.560450	2.810520	-0.047438
23	1	0	-5.875145	1.116770	0.194129
24	1	0	-3.013005	4.297088	-0.294933
25	1	0	-5.331549	3.535479	0.203062
26	6	0	-4.274371	-0.977163	-0.278030
27	6	0	-3.683310	-1.988838	-1.230489
28	6	0	-3.583435	-1.778529	0.864793
29	6	0	-3.233742	-2.905366	-0.136884
30	1	0	-1.926660	-0.879852	-1.186079
31	1	0	-3.837887	-2.129211	-2.299931
32	1	0	-2.692275	-1.276878	1.259459
33	1	0	-4.270714	-2.025192	1.678685
34	1	0	-2.175335	-3.202361	-0.153218
35	1	0	-3.845649	-3.813012	-0.030231
36	8	0	-5.677132	-1.176478	-0.147726
37	1	0	-6.082119	-0.961009	-0.996539

38	6	0	0.094183	1.799469	3.568430
39	1	0	0.906396	2.298391	4.100536
40	1	0	-0.708665	2.502139	3.334193
41	1	0	-0.318787	1.020749	4.218603
42	6	0	2.581055	3.616749	-1.455852
43	1	0	1.910860	4.393503	-1.075834
44	1	0	3.615266	3.858465	-1.206281
45	1	0	2.457215	3.584192	-2.542599
46	6	0	2.798582	-1.981546	-3.274071
47	1	0	2.281445	-2.944478	-3.338467
48	1	0	2.526594	-1.404967	-4.162187
49	1	0	3.875911	-2.151372	-3.241789
50	6	0	0.317520	-3.683306	1.729381
51	1	0	-0.668574	-3.566819	2.190742
52	1	0	0.215399	-4.416037	0.921798
53	1	0	1.039035	-4.047858	2.462197

Zero-point correction= 0.399157 (Hartree/Particle)
Thermal correction to Energy= 0.432111
Thermal correction to Enthalpy= 0.433055
Thermal correction to Gibbs Free Energy= 0.333960
Sum of electronic and zero-point Energies= -1649.389656
Sum of electronic and thermal Energies= -1649.356703
Sum of electronic and thermal Enthalpies= -1649.355759
Sum of electronic and thermal Free Energies= -1649.454853
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1652.29876139

[1]INT8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.450245	-1.658507	-0.266659
2	6	0	0.705387	-0.897225	-0.113583
3	6	0	0.400309	0.466178	-0.005244
4	6	0	2.024559	-1.332756	-0.046686
5	6	0	1.398886	1.407240	0.160393
6	6	0	3.024316	-0.375399	0.124055
7	1	0	2.271521	-2.388959	-0.134097
8	6	0	2.727717	0.981623	0.225543
9	1	0	1.140807	2.463193	0.226630
10	1	0	4.061602	-0.700389	0.171477
11	1	0	3.528066	1.705772	0.352995
12	6	0	-1.082563	0.622847	-0.127467
13	6	0	-1.582037	-0.789680	-0.582842
14	6	0	-1.948412	0.466848	1.144867
15	6	0	-2.673907	-0.730230	0.496872
16	1	0	-0.372322	-2.541326	-0.751519
17	1	0	-1.912739	-0.887328	-1.627857
18	1	0	-1.348848	0.191414	2.018070
19	1	0	-2.550792	1.348951	1.381193
20	1	0	-2.795005	-1.634228	1.101133
21	1	0	-3.642776	-0.444408	0.073402
22	8	0	-1.524943	1.726732	-0.866200
23	1	0	-0.993797	1.766316	-1.670657

Zero-point correction= 0.191266 (Hartree/Particle)
Thermal correction to Energy= 0.200683
Thermal correction to Enthalpy= 0.201627
Thermal correction to Gibbs Free Energy= 0.156992
Sum of electronic and zero-point Energies= -517.092167
Sum of electronic and thermal Energies= -517.082751
Sum of electronic and thermal Enthalpies= -517.081806
Sum of electronic and thermal Free Energies= -517.126442
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -517.40995898

3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.333137	-0.005386	0.027499
2	6	0	0.140400	0.735805	0.080761
3	6	0	0.259536	2.122081	-0.003533
4	6	0	1.491639	2.752461	-0.143337

5	6	0	2.653041	1.994774	-0.199651
6	6	0	2.574100	0.612325	-0.110702
7	1	0	-0.637105	2.733193	0.048093
8	1	0	1.540632	3.836463	-0.203324
9	1	0	3.623156	2.472889	-0.307863
10	1	0	3.479428	0.008523	-0.145615
11	7	0	1.214697	-1.424439	0.137889
12	7	0	2.235078	-2.103197	0.031987
13	7	0	3.109408	-2.828993	-0.050126
14	8	0	-1.224183	-0.814923	1.348840
15	6	0	-1.207438	0.040989	0.214618
16	6	0	-2.412406	0.958881	0.396994
17	6	0	-1.616306	-0.735348	-1.047731
18	6	0	-3.608375	0.034481	0.163848
19	1	0	-2.392466	1.742775	-0.371493
20	1	0	-2.407979	1.439959	1.381916
21	6	0	-3.109535	-1.027691	-0.843444
22	1	0	-1.007398	-1.634918	-1.194029
23	1	0	-1.454439	-0.088280	-1.921862
24	1	0	-3.892049	-0.443989	1.106414
25	1	0	-4.483380	0.583704	-0.199427
26	1	0	-3.250821	-2.033962	-0.435039
27	1	0	-3.655553	-0.991348	-1.792353
28	1	0	-0.569591	-1.509456	1.193672

Zero-point correction= 0.228965 (Hartree/Particle)
Thermal correction to Energy= 0.242057
Thermal correction to Enthalpy= 0.243001
Thermal correction to Gibbs Free Energy= 0.188724
Sum of electronic and zero-point Energies= -665.748839
Sum of electronic and thermal Energies= -665.735747
Sum of electronic and thermal Enthalpies= -665.734803
Sum of electronic and thermal Free Energies= -665.789080
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -666.13348662

INT9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.616511	0.210123	0.352056
2	45	0	2.418383	-0.809238	-0.879512
3	8	0	1.435807	2.053439	-0.054243
4	6	0	2.535131	2.087438	-0.693691
5	8	0	3.177299	1.094338	-1.136193
6	8	0	-0.460252	0.252130	-1.412565
7	6	0	0.088002	-0.172061	-2.476395
8	8	0	1.268772	-0.608101	-2.591061
9	8	0	-0.108526	-1.698528	0.702312
10	6	0	0.464383	-2.693626	0.146651
11	8	0	1.513926	-2.646364	-0.547159
12	8	0	1.790353	0.111586	2.042728
13	6	0	2.923434	-0.458517	1.957117
14	8	0	3.434427	-0.958549	0.915467
15	6	0	-2.130776	1.743721	0.583631
16	6	0	-3.183133	0.925567	0.161007
17	6	0	-4.054443	1.487856	-0.781928
18	6	0	-3.908530	2.778483	-1.266031
19	6	0	-2.856008	3.570786	-0.816600
20	6	0	-1.963029	3.042985	0.098866
21	1	0	-4.884557	0.882327	-1.145462
22	1	0	-4.617503	3.166293	-1.993673
23	1	0	-2.721650	4.582852	-1.189471
24	1	0	-1.095072	3.615041	0.422864
25	7	0	-1.096491	1.217142	1.439959
26	7	0	-0.665062	1.970851	2.325467
27	7	0	-0.193213	2.561550	3.172754
28	8	0	-2.681792	-0.915558	1.719598
29	6	0	-3.445441	-0.512145	0.605912
30	6	0	-4.920677	-0.745900	1.037265
31	6	0	-3.238678	-1.515547	-0.550513
32	6	0	-5.374236	-2.039756	0.340986
33	1	0	-5.573636	0.099999	0.800965
34	1	0	-4.911152	-0.849852	2.126868
35	6	0	-4.080509	-2.708881	-0.121218

36	1	0	-2.171570	-1.721714	-0.706805
37	1	0	-3.628437	-1.095108	-1.489390
38	1	0	-5.989403	-2.677289	0.984881
39	1	0	-5.983766	-1.794553	-0.541689
40	1	0	-3.590107	-3.212394	0.722872
41	1	0	-4.232277	-3.448641	-0.915668
42	6	0	3.111849	3.451464	-0.936630
43	1	0	4.039319	3.382719	-1.506774
44	1	0	2.383026	4.061305	-1.478758
45	1	0	3.297849	3.942921	0.023148
46	6	0	-0.777598	-0.184064	-3.701797
47	1	0	-0.175476	-0.022253	-4.598372
48	1	0	-1.249399	-1.170036	-3.783460
49	1	0	-1.565023	0.568090	-3.614886
50	6	0	-0.211626	-4.020935	0.317809
51	1	0	0.493370	-4.836907	0.149793
52	1	0	-0.662902	-4.092187	1.310819
53	1	0	-1.019118	-4.097965	-0.420894
54	6	0	3.711269	-0.555331	3.230433
55	1	0	3.255128	-1.314033	3.874674
56	1	0	4.745339	-0.834295	3.022117
57	1	0	3.668613	0.396807	3.765536
58	1	0	-1.794847	-1.182109	1.428692

Zero-point correction= 0.443015 (Hartree/Particle)
Thermal correction to Energy= 0.478283
Thermal correction to Enthalpy= 0.479227
Thermal correction to Gibbs Free Energy= 0.375389
Sum of electronic and zero-point Energies= -1798.130084
Sum of electronic and thermal Energies= -1798.094816
Sum of electronic and thermal Enthalpies= -1798.093872
Sum of electronic and thermal Free Energies= -1798.197711
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1801.11726558

TS10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.627901	0.269200	0.332480
2	45	0	2.361312	-0.890939	-0.911232
3	8	0	1.483857	2.054731	-0.240366
4	6	0	2.593672	2.010134	-0.864734
5	8	0	3.201739	0.973071	-1.243919
6	8	0	-0.496895	0.204502	-1.409782
7	6	0	0.024488	-0.247400	-2.476841
8	8	0	1.195970	-0.696951	-2.610594
9	8	0	-0.099757	-1.607704	0.848821
10	6	0	0.379752	-2.640062	0.276588
11	8	0	1.374584	-2.668988	-0.496596
12	8	0	1.873097	0.252390	1.960403
13	6	0	2.956720	-0.418311	1.896719
14	8	0	3.397950	-1.020235	0.882903
15	6	0	-1.973624	1.666739	0.645018
16	6	0	-3.180649	1.022848	0.277901
17	6	0	-3.998943	1.707803	-0.632481
18	6	0	-3.706981	2.982013	-1.086534
19	6	0	-2.538921	3.626546	-0.669131
20	6	0	-1.668919	2.954977	0.160211
21	1	0	-4.908483	1.222692	-0.983598
22	1	0	-4.392211	3.480207	-1.768559
23	1	0	-2.306722	4.630633	-1.014670
24	1	0	-0.720961	3.395197	0.463023
25	7	0	-1.035158	0.936243	1.363786
26	7	0	-0.488428	1.833044	2.687244
27	7	0	0.250827	1.788869	3.524297
28	8	0	-2.964723	-0.898242	1.822527
29	6	0	-3.572183	-0.404507	0.652169
30	6	0	-5.098148	-0.580905	0.907114
31	6	0	-3.280928	-1.362985	-0.530387
32	6	0	-5.570680	-1.693323	-0.037136
33	1	0	-5.667841	0.346723	0.795776
34	1	0	-5.192297	-0.890150	1.953037
35	6	0	-4.297802	-2.478900	-0.339926
36	1	0	-2.227882	-1.669209	-0.516379

37	1	0	-3.460920	-0.850614	-1.487638
38	1	0	-6.374044	-2.300706	0.393735
39	1	0	-5.958714	-1.262306	-0.973169
40	1	0	-4.017550	-3.084312	0.532832
41	1	0	-4.386139	-3.146172	-1.204721
42	6	0	3.245503	3.333097	-1.145122
43	1	0	3.909871	3.253116	-2.007561
44	1	0	2.488868	4.103803	-1.307640
45	1	0	3.842403	3.623183	-0.273701
46	6	0	-0.873392	-0.274606	-3.679211
47	1	0	-0.290307	-0.154189	-4.594678
48	1	0	-1.370072	-1.250961	-3.718785
49	1	0	-1.640863	0.498598	-3.596076
50	6	0	-0.340404	-3.931269	0.533826
51	1	0	0.377671	-4.726997	0.747746
52	1	0	-1.053811	-3.818146	1.353110
53	1	0	-0.884034	-4.213597	-0.374978
54	6	0	3.751827	-0.501039	3.165733
55	1	0	3.326852	-1.288209	3.797522
56	1	0	4.791873	-0.749292	2.947066
57	1	0	3.682673	0.440187	3.716243
58	1	0	-2.001535	-0.884039	1.708772

Zero-point correction= 0.439725 (Hartree/Particle)
Thermal correction to Energy= 0.474747
Thermal correction to Enthalpy= 0.475691
Thermal correction to Gibbs Free Energy= 0.374538
Sum of electronic and zero-point Energies= -1798.085924
Sum of electronic and thermal Energies= -1798.050901
Sum of electronic and thermal Enthalpies= -1798.049957
Sum of electronic and thermal Free Energies= -1798.151111
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1801.06981576

[1]INT10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.470388	0.040769	-0.133223
2	45	0	-2.864525	-0.341038	0.227995
3	8	0	-0.486510	1.223506	1.566173
4	6	0	-1.583698	1.376359	2.199313
5	8	0	-2.698781	0.878987	1.901286
6	8	0	-0.151018	-1.639629	1.039606
7	6	0	-1.144550	-2.267581	1.526918
8	8	0	-2.361944	-1.979922	1.381334
9	8	0	-0.629210	-1.177013	-1.798653
10	6	0	-1.757089	-1.690499	-2.087426
11	8	0	-2.839947	-1.532725	-1.462945
12	8	0	-0.998243	1.692760	-1.265320
13	6	0	-2.235307	1.960569	-1.432745
14	8	0	-3.209327	1.327439	-0.955209
15	7	0	1.452377	0.156888	-0.419009
16	6	0	2.236449	1.208293	-0.219894
17	6	0	3.671472	0.979215	-0.220212
18	6	0	1.738961	2.541277	-0.036480
19	6	0	4.503821	2.073283	-0.050954
20	6	0	2.605336	3.600019	0.101875
21	1	0	0.663417	2.682541	-0.052272
22	6	0	3.983280	3.359992	0.095342
23	1	0	5.582322	1.941538	-0.050368
24	1	0	2.228545	4.612979	0.215171
25	1	0	4.671582	4.196157	0.203379
26	6	0	4.197549	-0.439126	-0.336942
27	6	0	5.712561	-0.587297	-0.448155
28	8	0	3.662216	-1.080263	-1.472873
29	1	0	2.697464	-1.078982	-1.340022
30	6	0	5.937406	-2.076493	-0.180261
31	1	0	5.831265	-2.634192	-1.115888
32	1	0	6.942176	-2.274818	0.207811
33	6	0	3.907475	-1.254446	0.938765
34	1	0	4.172407	-0.651506	1.820486
35	1	0	2.839735	-1.494418	1.015200
36	6	0	4.821206	-2.481757	0.810758
37	1	0	5.221640	-2.781667	1.785376

38	1	0	4.258605	-3.336770	0.421891
39	1	0	6.084268	-0.250089	-1.422883
40	1	0	6.200493	0.007025	0.336526
41	6	0	-2.527588	3.146100	-2.307234
42	1	0	-3.586815	3.403092	-2.259747
43	1	0	-1.912970	3.997937	-2.003700
44	1	0	-2.258087	2.901791	-3.339844
45	6	0	-1.503326	2.225714	3.436079
46	1	0	-0.984083	1.664522	4.219841
47	1	0	-0.916814	3.126148	3.235590
48	1	0	-2.503562	2.487745	3.784550
49	6	0	-0.807368	-3.485687	2.338469
50	1	0	0.038512	-3.273952	2.997260
51	1	0	-1.674840	-3.810627	2.915417
52	1	0	-0.504258	-4.290656	1.661011
53	6	0	-1.781262	-2.551904	-3.317636
54	1	0	-0.897930	-3.194788	-3.341048
55	1	0	-2.694999	-3.147914	-3.347269
56	1	0	-1.743503	-1.908511	-4.202805

Zero-point correction= 0.431859 (Hartree/Particle)
Thermal correction to Energy= 0.465434
Thermal correction to Enthalpy= 0.466378
Thermal correction to Gibbs Free Energy= 0.366011
Sum of electronic and zero-point Energies= -1688.675850
Sum of electronic and thermal Energies= -1688.642275
Sum of electronic and thermal Enthalpies= -1688.641331
Sum of electronic and thermal Free Energies= -1688.741699
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1691.62732338

^{3}INT10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.489267	0.078379	-0.104306
2	45	0	-2.860641	-0.323541	0.179420
3	8	0	-0.642165	1.485598	1.411207
4	6	0	-1.771571	1.675507	1.964618
5	8	0	-2.857002	1.103473	1.673131
6	8	0	-0.149844	-1.403683	1.298889
7	6	0	-1.148268	-1.996529	1.817278
8	8	0	-2.364381	-1.769358	1.572457
9	8	0	-0.497270	-1.355035	-1.590063
10	6	0	-1.595024	-1.927831	-1.882073
11	8	0	-2.713728	-1.725998	-1.334301
12	8	0	-0.999527	1.532131	-1.490690
13	6	0	-2.227309	1.735108	-1.749882
14	8	0	-3.213228	1.143031	-1.231360
15	7	0	1.474381	0.524322	-0.290093
16	6	0	2.452548	1.394598	-0.156343
17	6	0	3.818929	0.935571	-0.173151
18	6	0	2.159230	2.784570	-0.008751
19	6	0	4.813474	1.889325	-0.058588
20	6	0	3.190297	3.691099	0.109485
21	1	0	1.113137	3.079556	0.010233
22	6	0	4.517152	3.250265	0.080657
23	1	0	5.855535	1.579351	-0.082903
24	1	0	2.970091	4.749959	0.221588
25	1	0	5.328719	3.968953	0.165590
26	6	0	4.069730	-0.555863	-0.294956
27	6	0	5.530981	-0.967346	-0.441891
28	8	0	3.414393	-1.084997	-1.437806
29	1	0	2.460210	-1.094842	-1.272164
30	6	0	5.510206	-2.475189	-0.178649
31	1	0	5.334179	-3.010284	-1.117116
32	1	0	6.464693	-2.831255	0.223793
33	6	0	3.659187	-1.332640	0.966213
34	1	0	4.053448	-0.804654	1.846627
35	1	0	2.568650	-1.385234	1.083111
36	6	0	4.330776	-2.702689	0.795773
37	1	0	4.659581	-3.106263	1.759739
38	1	0	3.622838	-3.425135	0.375301
39	1	0	5.931293	-0.692908	-1.424761
40	1	0	6.128120	-0.460831	0.328284

41	6	0	-2.508559	2.778658	-2.792053
42	1	0	-3.578984	2.978831	-2.858499
43	1	0	-1.961960	3.695033	-2.553189
44	1	0	-2.139789	2.423592	-3.759597
45	6	0	-1.793443	2.666501	3.092137
46	1	0	-1.330389	2.209410	3.972839
47	1	0	-1.202310	3.547590	2.830171
48	1	0	-2.819936	2.947213	3.333512
49	6	0	-0.825666	-3.076836	2.808213
50	1	0	-0.149656	-2.684470	3.572997
51	1	0	-1.737547	-3.461820	3.266978
52	1	0	-0.299742	-3.888102	2.295000
53	6	0	-1.536594	-2.919754	-3.006566
54	1	0	-0.636495	-3.533176	-2.918793
55	1	0	-2.431692	-3.543920	-3.014493
56	1	0	-1.471234	-2.375022	-3.954261

Zero-point correction= 0.429864 (Hartree/Particle)
Thermal correction to Energy= 0.463940
Thermal correction to Enthalpy= 0.464884
Thermal correction to Gibbs Free Energy= 0.361212
Sum of electronic and zero-point Energies= -1688.682760
Sum of electronic and thermal Energies= -1688.648684
Sum of electronic and thermal Enthalpies= -1688.647740
Sum of electronic and thermal Free Energies= -1688.751412
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1691.63225001

^{3}TS11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.572429	0.040993	-0.359166
2	45	0	-2.759693	-0.251517	0.646720
3	8	0	0.072396	0.723751	1.490892
4	6	0	-0.780796	0.888747	2.418705
5	8	0	-2.015470	0.637262	2.358706
6	8	0	-0.120906	-1.886892	0.214249
7	6	0	-0.958564	-2.513530	0.936620
8	8	0	-2.085670	-2.092362	1.317524
9	8	0	-1.370160	-0.668793	-2.119004
10	6	0	-2.558044	-1.120444	-2.111129
11	8	0	-3.352854	-1.123717	-1.130081
12	8	0	-1.169758	1.966921	-0.862172
13	6	0	-2.378302	2.305293	-0.655160
14	8	0	-3.269345	1.608599	-0.097300
15	7	0	1.367777	0.248405	-1.016191
16	6	0	2.329689	1.107226	-0.677360
17	6	0	3.688214	0.646294	-0.605566
18	6	0	2.031256	2.468593	-0.392398
19	6	0	4.686183	1.556431	-0.318801
20	6	0	3.055902	3.346316	-0.104875
21	1	0	0.989223	2.776029	-0.436233
22	6	0	4.381827	2.901944	-0.078997
23	1	0	5.724032	1.229083	-0.275204
24	1	0	2.832144	4.392138	0.090964
25	1	0	5.185040	3.603666	0.132936
26	6	0	3.866166	-0.860702	-0.714714
27	6	0	5.301853	-1.281963	-1.122891
28	8	0	2.969118	-1.365172	-1.637729
29	1	0	1.851633	-0.727073	-1.368140
30	6	0	6.073659	-1.521595	0.191940
31	1	0	6.452673	-2.549813	0.217539
32	1	0	6.950354	-0.868418	0.280545
33	6	0	3.712457	-1.494743	0.685099
34	1	0	2.862006	-1.077567	1.240326
35	1	0	3.511100	-2.561823	0.512470
36	6	0	5.069618	-1.291139	1.337397
37	1	0	5.150036	-0.262970	1.715794
38	1	0	5.242098	-1.956460	2.189812
39	1	0	5.204564	-2.208484	-1.698887
40	1	0	5.760621	-0.540837	-1.785816
41	6	0	-0.571369	-3.904146	1.348119
42	1	0	-0.959741	-4.609862	0.605979
43	1	0	0.515010	-4.006441	1.383322

44	1	0	-1.019708	-4.148209	2.313601
45	6	0	-3.051039	-1.687835	-3.410070
46	1	0	-3.124485	-0.881744	-4.146902
47	1	0	-2.327825	-2.412733	-3.793621
48	1	0	-4.028690	-2.154407	-3.279480
49	6	0	-0.245736	1.413754	3.720001
50	1	0	0.247952	0.594617	4.253639
51	1	0	0.503350	2.187828	3.536316
52	1	0	-1.058072	1.798145	4.339238
53	6	0	-2.777035	3.664351	-1.154149
54	1	0	-3.718251	3.978340	-0.700009
55	1	0	-1.986446	4.389373	-0.945029
56	1	0	-2.902000	3.618509	-2.241063

Zero-point correction= 0.424636 (Hartree/Particle)
Thermal correction to Energy= 0.457732
Thermal correction to Enthalpy= 0.458676
Thermal correction to Gibbs Free Energy= 0.358528
Sum of electronic and zero-point Energies= -1688.658617
Sum of electronic and thermal Energies= -1688.625522
Sum of electronic and thermal Enthalpies= -1688.624578
Sum of electronic and thermal Free Energies= -1688.724726
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1691.60079816

^{3}TS12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.573537	0.140699	-0.369610
2	45	0	-2.712123	-0.410952	0.647502
3	8	0	0.082068	0.709446	1.517481
4	6	0	-0.745693	0.683409	2.481742
5	8	0	-1.946206	0.300801	2.435529
6	8	0	0.016797	-1.808636	0.024912
7	6	0	-0.775224	-2.572398	0.665144
8	8	0	-1.936515	-2.289020	1.060249
9	8	0	-1.361719	-0.473046	-2.175802
10	6	0	-2.532852	-0.965718	-2.194020
11	8	0	-3.318089	-1.082041	-1.213134
12	8	0	-1.306540	2.049351	-0.691960
13	6	0	-2.515724	2.297394	-0.381387
14	8	0	-3.330626	1.504678	0.162381
15	7	0	1.337513	0.388550	-1.141161
16	6	0	2.306715	1.233429	-0.767864
17	6	0	3.691838	0.840462	-0.709468
18	6	0	1.943738	2.551419	-0.374015
19	6	0	4.622301	1.783186	-0.298313
20	6	0	2.904161	3.463630	0.009306
21	1	0	0.886260	2.804619	-0.412649
22	6	0	4.248801	3.086388	0.042092
23	1	0	5.672434	1.509214	-0.227372
24	1	0	2.615096	4.474387	0.286284
25	1	0	5.010707	3.799432	0.347762
26	6	0	4.089508	-0.588302	-0.998239
27	6	0	5.549223	-0.999439	-0.768921
28	8	0	3.446918	-1.229115	-1.893187
29	1	0	1.713113	-0.466262	-1.563580
30	6	0	5.773284	-1.371966	0.690752
31	1	0	6.727729	-1.888065	0.844266
32	1	0	5.782398	-0.473621	1.325687
33	6	0	3.353668	-1.479667	0.636406
34	1	0	3.102188	-0.601596	1.237246
35	1	0	2.468138	-2.011789	0.286036
36	6	0	4.571314	-2.239236	1.050882
37	1	0	4.535247	-2.469688	2.125754
38	1	0	4.625821	-3.194516	0.512133
39	1	0	5.690672	-1.884780	-1.400606
40	1	0	6.242938	-0.231769	-1.131607
41	6	0	-3.015823	3.669420	-0.732310
42	1	0	-3.897627	3.918011	-0.138946
43	1	0	-2.226969	4.410790	-0.584808
44	1	0	-3.290474	3.682360	-1.792467
45	6	0	-0.225960	1.129019	3.820050
46	1	0	0.646280	1.774839	3.701885

47	1	0	-1.016067	1.641366	4.373701
48	1	0	0.066658	0.245883	4.398149
49	6	0	-0.239471	-3.938875	0.987668
50	1	0	-1.032833	-4.584578	1.367428
51	1	0	0.218603	-4.377593	0.096794
52	1	0	0.543947	-3.844333	1.747808
53	6	0	-3.008399	-1.480230	-3.522517
54	1	0	-4.096039	-1.570571	-3.529527
55	1	0	-2.667066	-0.822110	-4.324987
56	1	0	-2.570155	-2.468979	-3.695115

Zero-point correction= 0.427629 (Hartree/Particle)
Thermal correction to Energy= 0.461226
Thermal correction to Enthalpy= 0.462170
Thermal correction to Gibbs Free Energy= 0.360203
Sum of electronic and zero-point Energies= -1688.657870
Sum of electronic and thermal Energies= -1688.624274
Sum of electronic and thermal Enthalpies= -1688.623329
Sum of electronic and thermal Free Energies= -1688.725296
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1691.60450871

^{1}TS13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.568749	-0.002304	-0.121420
2	45	0	-2.962603	-0.245102	0.214935
3	8	0	-0.511848	1.098865	1.635999
4	6	0	-1.595625	1.275187	2.279380
5	8	0	-2.738405	0.853819	1.958030
6	8	0	-0.329865	-1.754902	0.944003
7	6	0	-1.359831	-2.351488	1.391175
8	8	0	-2.559290	-1.987118	1.255652
9	8	0	-0.788397	-1.104732	-1.850424
10	6	0	-1.942514	-1.528656	-2.171231
11	8	0	-3.019058	-1.330153	-1.543902
12	8	0	-0.973064	1.743011	-1.167603
13	6	0	-2.186745	2.098160	-1.314973
14	8	0	-3.202816	1.510246	-0.857999
15	7	0	1.469913	0.054460	-0.374423
16	6	0	2.344419	1.022823	-0.245264
17	6	0	3.772292	0.738638	-0.363628
18	6	0	1.909859	2.378112	0.006272
19	6	0	4.667338	1.816070	-0.209209
20	6	0	2.821858	3.377962	0.115735
21	1	0	0.841363	2.549350	0.094775
22	6	0	4.212235	3.093310	0.000016
23	1	0	5.737323	1.628875	-0.279346
24	1	0	2.500348	4.400651	0.293965
25	1	0	4.927991	3.909500	0.071121
26	6	0	4.230107	-0.659230	-0.533142
27	6	0	5.635718	-0.892350	-1.168807
28	6	0	6.559878	-1.465136	-0.086752
29	1	0	7.249102	-2.221985	-0.476525
30	1	0	7.175996	-0.665712	0.352765
31	6	0	4.600259	-0.890305	1.139297
32	6	0	5.612083	-2.001968	0.976702
33	1	0	6.109306	-2.228513	1.929058
34	1	0	5.100381	-2.903636	0.620730
35	1	0	5.446110	-1.628556	-1.955383
36	1	0	6.047819	0.002543	-1.648981
37	1	0	5.051227	-0.006557	1.603715
38	1	0	3.647237	-1.142240	1.610968
39	6	0	-1.095198	-3.612172	2.163186
40	1	0	-0.535874	-3.366423	3.071336
41	1	0	-2.031984	-4.104500	2.428756
42	1	0	-0.468117	-4.280799	1.566835
43	6	0	-2.010038	-2.370532	-3.412547
44	1	0	-1.299718	-2.003504	-4.156709
45	1	0	-1.725718	-3.396836	-3.157092
46	1	0	-3.025891	-2.377967	-3.811983
47	6	0	-1.477131	2.042426	3.565807
48	1	0	-1.104769	1.368459	4.344638
49	1	0	-0.753786	2.854106	3.456998

50	1	0	-2.451018	2.428498	3.871765
51	6	0	-2.416906	3.329040	-2.144569
52	1	0	-1.617000	4.055254	-1.982638
53	1	0	-2.400963	3.046041	-3.202540
54	1	0	-3.390833	3.765496	-1.915858
55	1	0	1.965215	-0.856449	-0.571264
56	8	0	3.364666	-1.588089	-0.832627

Zero-point correction= 0.428966 (Hartree/Particle)
Thermal correction to Energy= 0.462014
Thermal correction to Enthalpy= 0.462959
Thermal correction to Gibbs Free Energy= 0.363224
Sum of electronic and zero-point Energies= -1688.655287
Sum of electronic and thermal Energies= -1688.622239
Sum of electronic and thermal Enthalpies= -1688.621294
Sum of electronic and thermal Free Energies= -1688.721029
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1691.60625692

^{1}TS14

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.385802	0.073282	0.281760
2	45	0	-2.720909	-0.106223	-0.403349
3	8	0	-0.607073	2.129046	0.119381
4	6	0	-1.719127	2.603977	-0.271123
5	8	0	-2.753668	1.952701	-0.581626
6	8	0	-1.046855	0.168685	2.236243
7	6	0	-2.297855	0.164200	2.455153
8	8	0	-3.218946	0.073012	1.596474
9	8	0	-0.304595	-2.004290	0.385855
10	6	0	-1.381031	-2.649573	0.157391
11	8	0	-2.493780	-2.164150	-0.166907
12	8	0	0.130289	-0.078766	-1.728652
13	6	0	-0.797213	-0.202111	-2.589974
14	8	0	-2.034104	-0.261305	-2.363975
15	7	0	1.659709	-0.040659	0.835142
16	6	0	2.756777	0.755448	0.817040
17	6	0	4.082491	0.198204	0.907421
18	6	0	2.620216	2.130463	0.496401
19	6	0	5.176198	1.023248	0.572614
20	6	0	3.718686	2.880609	0.155111
21	1	0	1.611902	2.536560	0.464054
22	6	0	5.014978	2.326728	0.156935
23	1	0	6.178394	0.600663	0.656605
24	1	0	3.583868	3.924083	-0.124135
25	1	0	5.874671	2.930915	-0.119330
26	6	0	2.791017	-1.762152	-1.202010
27	6	0	3.914870	-2.506952	-0.487185
28	6	0	4.352625	-1.111170	1.616252
29	6	0	3.825110	-2.428482	1.026682
30	1	0	5.444605	-1.204722	1.693629
31	1	0	3.989547	-1.030699	2.652652
32	6	0	-2.708866	0.304124	3.894427
33	1	0	-3.762380	0.048876	4.021055
34	1	0	-2.079162	-0.328814	4.525086
35	1	0	-2.550080	1.340816	4.209312
36	6	0	-1.300350	-4.141978	0.326083
37	1	0	-1.367832	-4.381030	1.392872
38	1	0	-2.125592	-4.631197	-0.194422
39	1	0	-0.339564	-4.516972	-0.036688
40	6	0	-1.803793	4.103178	-0.342865
41	1	0	-0.878166	4.513612	-0.754336
42	1	0	-2.662569	4.409334	-0.942785
43	1	0	-1.919983	4.500548	0.671084
44	6	0	-0.368267	-0.266339	-4.030482
45	1	0	-0.663171	0.662923	-4.528431
46	1	0	0.714916	-0.384258	-4.114189
47	1	0	-0.886181	-1.085236	-4.536883
48	1	0	1.812989	-0.941151	1.280454
49	6	0	2.898641	-0.289335	-1.218515
50	8	0	2.956422	0.633922	-1.905380
51	1	0	2.801244	-1.986775	-2.279108
52	1	0	1.798280	-2.029459	-0.819904

53	1	0	3.840940	-3.550884	-0.814028
54	1	0	4.889371	-2.134976	-0.835431
55	1	0	4.417317	-3.244160	1.460064
56	1	0	2.788483	-2.634424	1.330852

Zero-point correction= 0.429570 (Hartree/Particle)
Thermal correction to Energy= 0.463321
Thermal correction to Enthalpy= 0.464265
Thermal correction to Gibbs Free Energy= 0.363510
Sum of electronic and zero-point Energies= -1688.676316
Sum of electronic and thermal Energies= -1688.642565
Sum of electronic and thermal Enthalpies= -1688.641621
Sum of electronic and thermal Free Energies= -1688.742376
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1691.63089601

^{3}INT11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.590762	0.106530	-0.346509
2	45	0	-2.768262	-0.334178	0.639324
3	8	0	0.140768	0.368237	1.578395
4	6	0	-0.659540	0.222747	2.556297
5	8	0	-1.887550	-0.054255	2.491461
6	8	0	-0.208670	-1.923059	-0.216278
7	6	0	-1.108472	-2.686803	0.258568
8	8	0	-2.238957	-2.338572	0.693485
9	8	0	-1.459851	-0.190004	-2.192974
10	6	0	-2.699676	-0.463053	-2.254486
11	8	0	-3.494609	-0.586876	-1.282188
12	8	0	-1.127239	2.111093	-0.414396
13	6	0	-2.272964	2.454521	0.019573
14	8	0	-3.150366	1.694320	0.509710
15	7	0	1.359978	0.242503	-1.071667
16	6	0	2.365520	1.065299	-0.745420
17	6	0	3.741463	0.637074	-0.701536
18	6	0	2.051476	2.417471	-0.428862
19	6	0	4.710485	1.587739	-0.425978
20	6	0	3.048417	3.329622	-0.156883
21	1	0	1.000512	2.697830	-0.445975
22	6	0	4.384342	2.923068	-0.168117
23	1	0	5.757541	1.295964	-0.389424
24	1	0	2.794697	4.364346	0.059911
25	1	0	5.177204	3.637759	0.039352
26	6	0	4.090648	-0.839393	-0.843788
27	6	0	5.593799	-1.184785	-0.784478
28	8	0	3.453743	-1.446934	-1.869857
29	1	0	1.685839	-0.646643	-1.458570
30	6	0	5.989578	-1.258104	0.701079
31	1	0	6.568458	-2.167998	0.894415
32	1	0	6.624932	-0.417953	1.004969
33	6	0	3.588563	-1.611242	0.460676
34	1	0	2.572108	-1.308970	0.732641
35	1	0	3.591067	-2.680060	0.213278
36	6	0	4.663542	-1.260355	1.480842
37	1	0	4.456853	-0.266312	1.896958
38	1	0	4.656981	-1.967624	2.317522
39	1	0	5.678606	-2.168532	-1.259672
40	1	0	6.200116	-0.494656	-1.381156
41	6	0	-0.787551	-4.154327	0.270560
42	1	0	-1.109472	-4.592243	-0.680378
43	1	0	0.289274	-4.309372	0.367939
44	1	0	-1.328506	-4.653564	1.077052
45	6	0	-3.255554	-0.652319	-3.636983
46	1	0	-3.110657	0.266242	-4.213508
47	1	0	-2.700126	-1.444789	-4.147237
48	1	0	-4.316330	-0.903907	-3.595265
49	6	0	-0.058544	0.402335	3.922136
50	1	0	0.742812	-0.329291	4.064280
51	1	0	0.393016	1.396194	3.994946
52	1	0	-0.817105	0.277682	4.696347
53	6	0	-2.607782	3.914684	-0.093613
54	1	0	-3.482738	4.155468	0.512370
55	1	0	-1.750798	4.521758	0.209410

56	1	0	-2.822694	4.148658	-1.141599

Zero-point correction= 0.430242 (Hartree/Particle)
Thermal correction to Energy= 0.463746
Thermal correction to Enthalpy= 0.464691
Thermal correction to Gibbs Free Energy= 0.363940
Sum of electronic and zero-point Energies= -1688.663756
Sum of electronic and thermal Energies= -1688.630252
Sum of electronic and thermal Enthalpies= -1688.629308
Sum of electronic and thermal Free Energies= -1688.730058
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1691.61141158

^{3}INT12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.552179	0.155815	-0.385701
2	45	0	-2.686084	-0.395477	0.639648
3	8	0	0.204508	0.390172	1.527391
4	6	0	-0.546832	0.138748	2.522073
5	8	0	-1.764841	-0.183423	2.482983
6	8	0	-0.100749	-1.862232	-0.320845
7	6	0	-0.963462	-2.674985	0.145486
8	8	0	-2.101807	-2.382603	0.597864
9	8	0	-1.453106	-0.123590	-2.219351
10	6	0	-2.689193	-0.416210	-2.258077
11	8	0	-3.455116	-0.588256	-1.269242
12	8	0	-1.161842	2.140085	-0.383003
13	6	0	-2.294882	2.431236	0.118651
14	8	0	-3.128933	1.624447	0.609150
15	7	0	1.366496	0.386628	-1.152204
16	6	0	2.355585	1.201838	-0.771595
17	6	0	3.749331	0.833462	-0.846788
18	6	0	2.017800	2.474135	-0.228671
19	6	0	4.701560	1.745363	-0.408930
20	6	0	2.997553	3.355910	0.176001
21	1	0	0.961445	2.725550	-0.171660
22	6	0	4.346256	3.001923	0.082564
23	1	0	5.755452	1.478807	-0.449787
24	1	0	2.718105	4.330994	0.567598
25	1	0	5.120015	3.696141	0.400431
26	6	0	4.153330	-0.524330	-1.302940
27	6	0	5.464309	-1.097847	-0.813093
28	8	0	3.434243	-1.201524	-2.026770
29	6	0	5.455734	-1.407405	0.689157
30	1	0	6.395503	-1.917706	0.936719
31	1	0	5.445175	-0.471926	1.268362
32	6	0	2.988140	-1.501627	1.179696
33	6	0	4.258593	-2.270857	1.104697
34	1	0	4.486802	-2.725107	2.084939
35	1	0	4.155278	-3.108948	0.400204
36	1	0	5.610504	-2.024329	-1.380746
37	1	0	6.302180	-0.430658	-1.054161
38	1	0	2.939249	-0.612840	1.809084
39	1	0	2.047884	-1.876862	0.780699
40	6	0	-0.553226	-4.119446	0.149351
41	1	0	-1.343843	-4.744542	0.566840
42	1	0	-0.323822	-4.434939	-0.872806
43	1	0	0.363908	-4.233114	0.736551
44	6	0	-3.294571	-0.539864	-3.626595
45	1	0	-3.575655	0.458667	-3.978129
46	1	0	-2.564658	-0.949078	-4.328550
47	1	0	-4.191945	-1.160478	-3.590581
48	6	0	0.111919	0.231183	3.869151
49	1	0	-0.613113	0.064876	4.667243
50	1	0	0.907392	-0.519667	3.926395
51	1	0	0.582768	1.212022	3.982868
52	6	0	-2.649781	3.890813	0.137747
53	1	0	-2.100645	4.380571	0.949041
54	1	0	-2.346599	4.362855	-0.800123
55	1	0	-3.719956	4.020985	0.307344
56	1	0	1.717134	-0.459729	-1.612647

Zero-point correction= 0.427721 (Hartree/Particle)

Thermal correction to Energy= 0.462180
Thermal correction to Enthalpy= 0.463125
Thermal correction to Gibbs Free Energy= 0.360620
Sum of electronic and zero-point Energies= -1688.676107
Sum of electronic and thermal Energies= -1688.641648
Sum of electronic and thermal Enthalpies= -1688.640704
Sum of electronic and thermal Free Energies= -1688.743208
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1691.62339797

[1]INT13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.583667	0.014962	-0.267585
2	45	0	-2.883624	-0.220689	0.473997
3	8	0	-0.073902	0.534181	1.675410
4	6	0	-0.995286	0.556646	2.550867
5	8	0	-2.214692	0.288034	2.373267
6	8	0	-0.288991	-1.974280	0.209208
7	6	0	-1.277130	-2.640025	0.654558
8	8	0	-2.443670	-2.210208	0.861889
9	8	0	-1.218877	-0.531155	-2.155225
10	6	0	-2.453761	-0.759026	-2.340334
11	8	0	-3.372224	-0.707345	-1.474050
12	8	0	-1.024481	2.002185	-0.690797
13	6	0	-2.196237	2.434980	-0.453230
14	8	0	-3.158565	1.780036	0.030940
15	7	0	1.502069	-0.007540	-0.751241
16	6	0	2.448015	0.814268	-0.455953
17	6	0	3.854615	0.315932	-0.161320
18	6	0	2.143840	2.218884	-0.290206
19	6	0	4.868623	1.424607	-0.060451
20	6	0	3.129352	3.117613	-0.089256
21	1	0	1.098576	2.505869	-0.384625
22	6	0	4.517799	2.717386	-0.009661
23	1	0	5.917132	1.141042	0.010134
24	1	0	2.886618	4.174475	-0.004379
25	1	0	5.281134	3.484256	0.098901
26	6	0	4.375204	-0.646138	-1.252724
27	6	0	5.677065	-1.359498	-0.941806
28	8	0	3.796045	-0.821629	-2.299009
29	6	0	5.917434	-1.599420	0.550176
30	1	0	6.536557	-2.493347	0.685139
31	1	0	6.477214	-0.770717	1.006849
32	6	0	3.783477	-0.446149	1.222486
33	6	0	4.574754	-1.749411	1.250296
34	1	0	4.698263	-2.075211	2.289600
35	1	0	3.999427	-2.541988	0.744755
36	1	0	5.625961	-2.305560	-1.493856
37	1	0	6.491204	-0.786059	-1.407163
38	1	0	4.153405	0.239979	1.996091
39	1	0	2.728145	-0.642879	1.451113
40	6	0	-1.028471	-4.095296	0.936190
41	1	0	-1.632734	-4.419873	1.786265
42	1	0	-1.334457	-4.680853	0.062626
43	1	0	0.031850	-4.278847	1.121646
44	6	0	-2.861794	-1.097193	-3.746373
45	1	0	-3.064682	-0.166858	-4.287717
46	1	0	-2.052557	-1.618329	-4.262357
47	1	0	-3.773607	-1.697938	-3.742380
48	6	0	-0.585762	0.979890	3.934277
49	1	0	-1.264719	0.555794	4.676730
50	1	0	0.446334	0.684925	4.136654
51	1	0	-0.645532	2.071718	4.000157
52	6	0	-2.453344	3.871061	-0.815043
53	1	0	-1.616916	4.496385	-0.491950
54	1	0	-2.522954	3.954464	-1.904709
55	1	0	-3.387101	4.218611	-0.369936
56	1	0	1.801552	-0.971797	-0.895481

Zero-point correction= 0.432152 (Hartree/Particle)
Thermal correction to Energy= 0.466128
Thermal correction to Enthalpy= 0.467072
Thermal correction to Gibbs Free Energy= 0.364787

Sum of electronic and zero-point Energies= -1688.726252
Sum of electronic and thermal Energies= -1688.692276
Sum of electronic and thermal Enthalpies= -1688.691332
Sum of electronic and thermal Free Energies= -1688.793617
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1691.68148315

[1]INT14

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.432515	-1.240695	0.533632
2	6	0	-0.818083	-0.616943	0.253244
3	6	0	-0.839639	0.737139	-0.122463
4	6	0	-1.994679	-1.333946	0.435135
5	6	0	-2.090636	1.322265	-0.325490
6	6	0	-3.226668	-0.723255	0.238794
7	1	0	-1.923003	-2.380067	0.723807
8	6	0	-3.271421	0.610506	-0.147884
9	1	0	-2.135331	2.369886	-0.620952
10	1	0	-4.144579	-1.287932	0.381346
11	1	0	-4.228241	1.101849	-0.307995
12	6	0	2.786189	-0.754281	0.295658
13	6	0	2.835105	0.784621	0.253481
14	6	0	0.407872	1.558175	-0.354748
15	6	0	1.552421	1.508109	0.691785
16	1	0	0.816635	1.284075	-1.338884
17	1	0	0.081895	2.600579	-0.455432
18	1	0	0.691787	-1.252136	1.511946
19	6	0	1.483099	-1.127798	-0.359081
20	8	0	1.330707	-1.138146	-1.563944
21	1	0	3.628017	-1.177674	-0.259944
22	1	0	2.839944	-1.108330	1.334480
23	1	0	3.675232	1.125218	0.871429
24	1	0	3.063879	1.084875	-0.778585
25	1	0	1.835272	2.543086	0.920050
26	1	0	1.183875	1.099053	1.644276

Zero-point correction= 0.221561 (Hartree/Particle)
Thermal correction to Energy= 0.231870
Thermal correction to Enthalpy= 0.232814
Thermal correction to Gibbs Free Energy= 0.186190
Sum of electronic and zero-point Energies= -556.383648
Sum of electronic and thermal Energies= -556.373340
Sum of electronic and thermal Enthalpies= -556.372396
Sum of electronic and thermal Free Energies= -556.419020
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -556.74101334

[3]TS15

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.538843	0.045994	-0.528517
2	45	0	2.503843	-0.252500	0.907562
3	8	0	0.658729	2.069399	-0.090003
4	6	0	1.641743	2.498578	0.590306
5	8	0	2.572684	1.813380	1.096451
6	8	0	1.849185	0.313081	-2.104780
7	6	0	3.091739	0.145171	-1.903162
8	8	0	3.654098	-0.135378	-0.808543
9	8	0	0.574092	-2.005762	-0.861314
10	6	0	1.408527	-2.710936	-0.209760
11	8	0	2.270331	-2.296750	0.610498
12	8	0	-0.626349	-0.251163	1.190408
13	6	0	-0.041959	-0.320957	2.318841
14	8	0	1.197832	-0.327524	2.527676
15	7	0	-1.174877	0.250129	-1.692899
16	6	0	-2.091174	1.021493	-1.126196
17	6	0	-3.104647	0.392891	-0.237322
18	6	0	-2.187515	2.420684	-1.337702
19	6	0	-3.708393	1.279172	0.748920
20	6	0	-3.007468	3.201507	-0.559284
21	1	0	-1.524266	2.853300	-2.082017
22	6	0	-3.704745	2.625142	0.538898

23	1	0	-4.187215	0.859004	1.629384
24	1	0	-3.047509	4.275900	-0.717868
25	1	0	-4.207100	3.276755	1.250493
26	6	0	-3.138828	-1.027139	-0.070338
27	6	0	-4.106878	-1.680528	0.864749
28	8	0	-2.383424	-1.866062	-0.718879
29	6	0	-5.543852	-1.327654	0.456831
30	1	0	-6.243188	-2.103995	0.783676
31	1	0	-5.866516	-0.387057	0.918933
32	6	0	-4.450579	-0.170794	-1.453483
33	6	0	-5.515049	-1.181531	-1.059359
34	1	0	-6.491989	-0.877758	-1.455122
35	1	0	-5.268705	-2.156115	-1.503117
36	1	0	-3.936564	-2.759217	0.785665
37	1	0	-3.876102	-1.381680	1.896078
38	1	0	-4.836117	0.850387	-1.522389
39	1	0	-3.877238	-0.424016	-2.349554
40	6	0	3.978499	0.329661	-3.102976
41	1	0	3.502112	-0.091063	-3.991728
42	1	0	4.117774	1.402030	-3.276624
43	1	0	4.954413	-0.128114	-2.931047
44	6	0	1.365596	-4.189476	-0.478757
45	1	0	0.329470	-4.530666	-0.546948
46	1	0	1.842023	-4.385386	-1.445256
47	1	0	1.903471	-4.735721	0.298118
48	6	0	1.710464	3.988008	0.786392
49	1	0	2.384283	4.411854	0.034042
50	1	0	0.723100	4.438051	0.662664
51	1	0	2.122801	4.217382	1.771722
52	6	0	-0.950795	-0.427622	3.513411
53	1	0	-1.364022	-1.441458	3.560405
54	1	0	-0.400969	-0.229137	4.435059
55	1	0	-1.784016	0.274072	3.406226
56	1	0	-1.670244	-1.385238	-1.229717

Zero-point correction= 0.427973 (Hartree/Particle)
Thermal correction to Energy= 0.461207
Thermal correction to Enthalpy= 0.462151
Thermal correction to Gibbs Free Energy= 0.362439
Sum of electronic and zero-point Energies= -1688.608867
Sum of electronic and thermal Energies= -1688.575633
Sum of electronic and thermal Enthalpies= -1688.574689
Sum of electronic and thermal Free Energies= -1688.674401
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1691.55587089

^{1}TS16

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.522725	-0.050433	-0.121057
2	45	0	-2.961996	-0.118875	0.238968
3	8	0	-0.425842	1.336842	1.423480
4	6	0	-1.506244	1.698401	1.990264
5	8	0	-2.672900	1.310510	1.725047
6	8	0	-0.366597	-1.590992	1.271115
7	6	0	-1.425140	-2.014694	1.827935
8	8	0	-2.606131	-1.620991	1.630047
9	8	0	-0.806659	-1.439350	-1.637674
10	6	0	-1.980759	-1.862685	-1.868903
11	8	0	-3.043812	-1.538801	-1.274053
12	8	0	-0.852348	1.492359	-1.474301
13	6	0	-2.051739	1.848198	-1.710819
14	8	0	-3.099410	1.390081	-1.186887
15	7	0	1.492836	-0.174169	-0.346540
16	6	0	2.321546	0.798988	-0.338577
17	6	0	3.814557	0.457526	-0.294056
18	6	0	1.984731	2.217981	-0.246545
19	6	0	4.748580	1.558926	-0.021346
20	6	0	2.908274	3.177440	-0.025739
21	1	0	0.927207	2.447484	-0.336634
22	6	0	4.297428	2.825188	0.102223
23	1	0	5.815571	1.362267	0.041023
24	1	0	2.619080	4.221416	0.062683
25	1	0	5.024032	3.616975	0.277605

26	6	0	4.312540	-0.700251	-0.944862
27	6	0	5.776621	-1.049141	-0.948807
28	8	0	3.491314	-1.473037	-1.614899
29	6	0	6.265058	-1.273100	0.488284
30	1	0	7.108019	-1.970912	0.511186
31	1	0	6.614864	-0.333657	0.932116
32	6	0	3.891421	-0.833645	1.060535
33	6	0	5.054657	-1.791534	1.249894
34	1	0	5.267197	-1.917246	2.317791
35	1	0	4.780055	-2.782880	0.859535
36	1	0	5.909834	-1.967892	-1.536421
37	1	0	6.333578	-0.258901	-1.467866
38	1	0	3.879368	-0.039703	1.811917
39	1	0	2.891965	-1.270964	0.945945
40	6	0	-1.256809	-3.115024	2.843534
41	1	0	-1.645866	-2.775859	3.808527
42	1	0	-1.855202	-3.979630	2.540674
43	1	0	-0.208946	-3.403008	2.944523
44	6	0	-2.099161	-2.855002	-2.996083
45	1	0	-1.357068	-3.648423	-2.870318
46	1	0	-3.105199	-3.276194	-3.035100
47	1	0	-1.878805	-2.349586	-3.942135
48	6	0	-1.343914	2.692440	3.110060
49	1	0	-2.315148	3.070027	3.434385
50	1	0	-0.844763	2.203073	3.952966
51	1	0	-0.702123	3.516745	2.786128
52	6	0	-2.214929	2.921827	-2.753940
53	1	0	-1.449275	3.691685	-2.626563
54	1	0	-2.073257	2.478109	-3.745244
55	1	0	-3.213485	3.359412	-2.700219
56	1	0	3.919718	-2.298295	-1.880006

Zero-point correction= 0.428795 (Hartree/Particle)
Thermal correction to Energy= 0.462487
Thermal correction to Enthalpy= 0.463432
Thermal correction to Gibbs Free Energy= 0.362655
Sum of electronic and zero-point Energies= -1688.600744
Sum of electronic and thermal Energies= -1688.567052
Sum of electronic and thermal Enthalpies= -1688.566108
Sum of electronic and thermal Free Energies= -1688.666885
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1691.56024929

^{1}INT10`

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.398360	0.121368	-0.332944
2	45	0	2.652296	-0.255209	0.574616
3	8	0	1.113227	1.888252	-1.142340
4	6	0	2.335568	2.205571	-0.951984
5	8	0	3.188139	1.546501	-0.308066
6	8	0	1.015898	-0.878863	-2.031418
7	6	0	2.200217	-1.343623	-2.079630
8	8	0	3.088103	-1.244399	-1.191160
9	8	0	-0.093147	-1.703946	0.560912
10	6	0	0.784911	-2.360745	1.205540
11	8	0	1.984906	-2.031957	1.394325
12	8	0	-0.043637	1.118242	1.427736
13	6	0	0.854820	1.215928	2.327924
14	8	0	2.025414	0.760087	2.276422
15	7	0	-1.479008	0.158745	-0.835687
16	6	0	-2.315177	1.157122	-0.572063
17	6	0	-3.699773	0.825175	-0.313920
18	6	0	-1.909682	2.529625	-0.561348
19	6	0	-4.582019	1.860600	-0.051270
20	6	0	-2.831374	3.531443	-0.359900
21	1	0	-0.863835	2.741778	-0.770388
22	6	0	-4.160923	3.190218	-0.091673
23	1	0	-5.610239	1.616631	0.199784
24	1	0	-2.530997	4.575586	-0.388666
25	1	0	-4.887077	3.978500	0.098693
26	6	0	-4.149985	-0.616752	-0.203397
27	6	0	-3.806809	-1.510893	-1.434083
28	8	0	-5.548740	-0.673627	0.055326

29	1	0	-6.010153	-0.556291	-0.782291
30	6	0	-3.071369	-2.735865	-0.876919
31	1	0	-3.296341	-3.650434	-1.437281
32	1	0	-1.990095	-2.553966	-0.927512
33	6	0	-3.492754	-1.332464	0.995219
34	1	0	-2.456808	-0.991607	1.112133
35	1	0	-4.050433	-1.106469	1.911357
36	6	0	-3.496905	-2.799676	0.587653
37	1	0	-2.822634	-3.406453	1.203865
38	1	0	-4.510155	-3.213796	0.682983
39	1	0	-4.757985	-1.810502	-1.897298
40	1	0	-3.215667	-0.985027	-2.187839
41	6	0	2.768092	3.499107	-1.581720
42	1	0	2.651988	3.428755	-2.667614
43	1	0	2.120423	4.311241	-1.238179
44	1	0	3.807593	3.717749	-1.333196
45	6	0	2.547336	-2.092718	-3.334645
46	1	0	1.959509	-3.015224	-3.374046
47	1	0	2.273405	-1.495575	-4.208767
48	1	0	3.611039	-2.334959	-3.354877
49	6	0	0.308074	-3.655976	1.799821
50	1	0	-0.438888	-3.443509	2.572148
51	1	0	-0.183174	-4.254078	1.025992
52	1	0	1.140380	-4.209278	2.237785
53	6	0	0.438960	1.936693	3.579036
54	1	0	-0.147659	2.823092	3.324466
55	1	0	-0.202002	1.277186	4.173410
56	1	0	1.314805	2.209371	4.170159

Zero-point correction= 0.432169 (Hartree/Particle)
Thermal correction to Energy= 0.465365
Thermal correction to Enthalpy= 0.466309
Thermal correction to Gibbs Free Energy= 0.367691
Sum of electronic and zero-point Energies= -1688.671809
Sum of electronic and thermal Energies= -1688.638614
Sum of electronic and thermal Enthalpies= -1688.637669
Sum of electronic and thermal Free Energies= -1688.736287
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1691.62197536

^{3}INT10'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.425084	0.078503	-0.321606
2	45	0	2.671427	-0.134878	0.565327
3	8	0	1.022138	1.908362	-1.107674
4	6	0	2.248746	2.236119	-1.033428
5	8	0	3.164704	1.593165	-0.451625
6	8	0	1.094244	-0.884350	-2.020856
7	6	0	2.272903	-1.359533	-2.028391
8	8	0	3.135335	-1.247148	-1.112592
9	8	0	0.007882	-1.751766	0.545725
10	6	0	0.879875	-2.287385	1.301020
11	8	0	2.040211	-1.851809	1.530468
12	8	0	-0.082180	1.026617	1.447901
13	6	0	0.835896	1.295805	2.285732
14	8	0	2.056977	0.993978	2.186505
15	7	0	-1.507476	0.393428	-0.914834
16	6	0	-2.506143	1.209506	-0.610957
17	6	0	-3.812838	0.705766	-0.288949
18	6	0	-2.263565	2.616112	-0.616738
19	6	0	-4.798540	1.626993	0.021801
20	6	0	-3.281826	3.493198	-0.312544
21	1	0	-1.255482	2.945285	-0.859732
22	6	0	-4.551731	3.002122	0.007147
23	1	0	-5.778098	1.249378	0.302240
24	1	0	-3.094379	4.564235	-0.315977
25	1	0	-5.354090	3.692980	0.255673
26	6	0	-4.075790	-0.785405	-0.218326
27	6	0	-3.610174	-1.594802	-1.463392
28	8	0	-5.456175	-1.031703	0.022315
29	1	0	-5.932078	-0.864109	-0.798892
30	6	0	-2.851011	-2.816152	-0.917718
31	1	0	-3.052783	-3.727386	-1.491608

32	1	0	-1.770343	-2.623268	-0.962706
33	6	0	-3.347500	-1.449208	0.961404
34	1	0	-2.332105	-1.042126	1.059125
35	1	0	-3.896926	-1.255526	1.889725
36	6	0	-3.276463	-2.912641	0.546463
37	1	0	-2.584314	-3.502347	1.158840
38	1	0	-4.272847	-3.366296	0.631666
39	1	0	-4.503603	-1.898694	-2.025687
40	1	0	-2.988579	-1.001743	-2.142254
41	6	0	2.627624	3.513288	-1.726453
42	1	0	2.507919	3.383201	-2.806687
43	1	0	1.951012	4.315348	-1.418426
44	1	0	3.660964	3.781664	-1.501570
45	6	0	2.655001	-2.138999	-3.253021
46	1	0	2.075684	-3.067373	-3.280265
47	1	0	2.394446	-1.567360	-4.147953
48	1	0	3.720680	-2.372780	-3.245200
49	6	0	0.457425	-3.555678	1.983750
50	1	0	-0.325745	-3.324417	2.713943
51	1	0	0.025274	-4.241576	1.248493
52	1	0	1.303408	-4.023048	2.490073
53	6	0	0.400891	2.040556	3.514658
54	1	0	-0.197723	2.909311	3.227173
55	1	0	-0.239128	1.390220	4.119436
56	1	0	1.266408	2.348568	4.103270

Zero-point correction= 0.430826 (Hartree/Particle)
Thermal correction to Energy= 0.464255
Thermal correction to Enthalpy= 0.465199
Thermal correction to Gibbs Free Energy= 0.364675
Sum of electronic and zero-point Energies= -1688.683004
Sum of electronic and thermal Energies= -1688.649575
Sum of electronic and thermal Enthalpies= -1688.648631
Sum of electronic and thermal Free Energies= -1688.749156
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1691.63192004

^{3}TS17

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.439445	0.137664	-0.356907
2	45	0	2.637815	-0.227231	0.609481
3	8	0	1.242318	1.746508	-1.379128
4	6	0	2.481405	1.998333	-1.243484
5	8	0	3.303264	1.373261	-0.519322
6	8	0	0.977629	-1.137209	-1.890398
7	6	0	2.132888	-1.666757	-1.862303
8	8	0	3.020713	-1.493849	-0.981747
9	8	0	-0.215747	-1.498956	0.747797
10	6	0	0.608681	-2.093017	1.513658
11	8	0	1.825246	-1.809510	1.672996
12	8	0	0.031736	1.375494	1.252033
13	6	0	0.936077	1.566727	2.124325
14	8	0	2.095084	1.068034	2.130179
15	7	0	-1.511969	0.369794	-1.016610
16	6	0	-2.475819	1.234118	-0.671767
17	6	0	-3.796518	0.763355	-0.372857
18	6	0	-2.197163	2.626455	-0.602159
19	6	0	-4.776952	1.680806	-0.041868
20	6	0	-3.201886	3.513379	-0.274738
21	1	0	-1.184407	2.951546	-0.827805
22	6	0	-4.492755	3.047831	0.002001
23	1	0	-5.771785	1.312172	0.199076
24	1	0	-2.989650	4.578990	-0.232845
25	1	0	-5.278469	3.752980	0.263182
26	6	0	-4.040177	-0.724032	-0.311954
27	6	0	-3.175997	-1.509347	-1.288505
28	8	0	-5.416477	-1.042199	-0.473125
29	1	0	-5.674581	-0.786158	-1.366264
30	6	0	-2.836641	-2.853214	-0.674710
31	1	0	-3.206441	-3.688484	-1.281714
32	1	0	-1.744719	-2.966653	-0.603891
33	6	0	-3.617032	-1.327437	1.034108
34	1	0	-2.646149	-0.901380	1.324990

35	1	0	-4.355538	-1.091580	1.808754
36	6	0	-3.468216	-2.815079	0.728819
37	1	0	-2.861688	-3.338048	1.476454
38	1	0	-4.458279	-3.285326	0.708971
39	1	0	-3.482432	-1.470030	-2.339944
40	1	0	-2.115905	-0.739859	-1.259473
41	6	0	2.996670	3.172788	-2.025907
42	1	0	2.664742	3.097709	-3.065003
43	1	0	2.572059	4.093639	-1.613111
44	1	0	4.085436	3.221316	-1.975052
45	6	0	2.449178	-2.610812	-2.986981
46	1	0	1.960152	-3.571331	-2.792701
47	1	0	2.050512	-2.220589	-3.926615
48	1	0	3.526124	-2.771387	-3.060414
49	6	0	0.055090	-3.253454	2.291296
50	1	0	-0.834364	-2.933031	2.843937
51	1	0	-0.257687	-4.038870	1.594610
52	1	0	0.803144	-3.650637	2.979174
53	6	0	0.574496	2.457601	3.278535
54	1	0	-0.270938	3.098925	3.022558
55	1	0	0.294686	1.832068	4.132844
56	1	0	1.441158	3.053949	3.573396

Zero-point correction= 0.424585 (Hartree/Particle)
Thermal correction to Energy= 0.457777
Thermal correction to Enthalpy= 0.458721
Thermal correction to Gibbs Free Energy= 0.358540
Sum of electronic and zero-point Energies= -1688.664334
Sum of electronic and thermal Energies= -1688.631142
Sum of electronic and thermal Enthalpies= -1688.630198
Sum of electronic and thermal Free Energies= -1688.730380
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1691.60714159

^{1}TS18

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.357230	0.126826	-0.348624
2	45	0	2.575100	-0.212063	0.632217
3	8	0	1.252885	1.566899	-1.547069
4	6	0	2.502800	1.783972	-1.448866
5	8	0	3.304924	1.223428	-0.655877
6	8	0	0.813148	-1.345385	-1.731412
7	6	0	1.961307	-1.893867	-1.671049
8	8	0	2.869588	-1.654799	-0.831501
9	8	0	-0.323596	-1.330978	0.947785
10	6	0	0.489507	-1.880183	1.763447
11	8	0	1.716292	-1.635960	1.873468
12	8	0	0.031934	1.542145	1.129709
13	6	0	0.952684	1.781339	1.975162
14	8	0	2.095475	1.252088	2.017908
15	7	0	-1.389987	0.393657	-1.290768
16	6	0	-2.346729	1.218549	-0.753362
17	6	0	-3.641917	0.766355	-0.406807
18	6	0	-2.044036	2.593366	-0.637317
19	6	0	-4.606489	1.682685	-0.014128
20	6	0	-3.037509	3.485305	-0.272509
21	1	0	-1.039651	2.924517	-0.882966
22	6	0	-4.322490	3.043362	0.040137
23	1	0	-5.587471	1.302844	0.267109
24	1	0	-2.798683	4.545398	-0.221912
25	1	0	-5.087803	3.750841	0.348246
26	6	0	-3.885881	-0.718964	-0.335366
27	6	0	-2.981000	-1.490436	-1.280132
28	8	0	-5.248288	-1.045544	-0.580292
29	1	0	-5.494843	-0.661565	-1.430265
30	6	0	-2.609287	-2.814384	-0.633070
31	1	0	-2.895000	-3.660704	-1.268870
32	1	0	-1.522210	-2.873560	-0.488877
33	6	0	-3.546129	-1.323637	1.029886
34	1	0	-2.611388	-0.876886	1.395711
35	1	0	-4.347369	-1.112160	1.746829
36	6	0	-3.341899	-2.804683	0.721777
37	1	0	-2.781884	-3.328604	1.504048

38	1	0	-4.317214	-3.295242	0.621278
39	1	0	-3.332314	-1.512307	-2.319168
40	1	0	-1.984749	-0.810249	-1.433300
41	6	0	3.057597	2.806503	-2.398796
42	1	0	4.095398	3.036711	-2.152873
43	1	0	3.001155	2.412405	-3.418523
44	1	0	2.446574	3.712666	-2.366875
45	6	0	2.244112	-2.918918	-2.732717
46	1	0	2.361930	-2.410655	-3.695270
47	1	0	3.156263	-3.471192	-2.501036
48	1	0	1.395231	-3.601402	-2.827032
49	6	0	-0.104038	-2.934286	2.653300
50	1	0	-1.019718	-2.557121	3.119815
51	1	0	-0.378366	-3.802800	2.043348
52	1	0	0.613438	-3.241373	3.415720
53	6	0	0.622350	2.783181	3.044889
54	1	0	1.508609	3.373454	3.289133
55	1	0	-0.202379	3.426264	2.731431
56	1	0	0.320915	2.244062	3.949351

Zero-point correction= 0.426472 (Hartree/Particle)
Thermal correction to Energy= 0.459191
Thermal correction to Enthalpy= 0.460136
Thermal correction to Gibbs Free Energy= 0.362827
Sum of electronic and zero-point Energies= -1688.654185
Sum of electronic and thermal Energies= -1688.621465
Sum of electronic and thermal Enthalpies= -1688.620521
Sum of electronic and thermal Free Energies= -1688.717829
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1691.59864726

^{3}INT15

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.485920	0.138352	-0.337679
2	45	0	2.689727	-0.310397	0.577611
3	8	0	1.223053	1.950267	-1.017948
4	6	0	2.449156	2.223229	-0.814164
5	8	0	3.291586	1.502560	-0.214168
6	8	0	1.100235	-0.783405	-2.083145
7	6	0	2.273599	-1.268899	-2.131739
8	8	0	3.143400	-1.233495	-1.218133
9	8	0	-0.118470	-1.705198	0.401598
10	6	0	0.719949	-2.396703	1.066345
11	8	0	1.917622	-2.094917	1.307775
12	8	0	0.006208	1.025949	1.471030
13	6	0	0.896884	1.093420	2.375561
14	8	0	2.076651	0.651993	2.306239
15	7	0	-1.504209	0.298767	-0.940706
16	6	0	-2.438172	1.210575	-0.642316
17	6	0	-3.809797	0.867881	-0.376100
18	6	0	-2.036800	2.575837	-0.582515
19	6	0	-4.698634	1.891651	-0.097732
20	6	0	-2.955651	3.566393	-0.315056
21	1	0	-0.988008	2.791278	-0.777842
22	6	0	-4.292139	3.229395	-0.077514
23	1	0	-5.727418	1.627308	0.133258
24	1	0	-2.642620	4.607168	-0.289099
25	1	0	-5.020653	4.007368	0.139336
26	6	0	-4.252156	-0.578996	-0.257184
27	6	0	-3.769825	-1.517901	-1.326117
28	8	0	-5.680372	-0.667604	-0.172755
29	1	0	-6.032589	-0.518035	-1.058262
30	6	0	-3.356995	-2.832622	-0.753008
31	1	0	-3.780305	-3.691652	-1.290713
32	1	0	-2.257735	-2.951729	-0.802974
33	6	0	-3.726011	-1.250186	1.023988
34	1	0	-2.681182	-0.952028	1.191436
35	1	0	-4.321727	-0.933325	1.886998
36	6	0	-3.806676	-2.742965	0.712257
37	1	0	-3.190985	-3.351749	1.382948
38	1	0	-4.845924	-3.079698	0.803568
39	1	0	-3.840564	-1.291136	-2.389219
40	1	0	-1.883906	-0.640842	-1.079999

41	6	0	2.919338	3.546022	-1.348769
42	1	0	2.692233	3.609912	-2.416888
43	1	0	2.372177	4.352804	-0.851150
44	1	0	3.990443	3.670051	-1.182918
45	6	0	2.642233	-1.977813	-3.403926
46	1	0	2.262158	-3.004078	-3.359412
47	1	0	2.176282	-1.484689	-4.260100
48	1	0	3.727161	-2.013866	-3.518284
49	6	0	0.200530	-3.693565	1.619925
50	1	0	-0.567762	-3.480938	2.371085
51	1	0	-0.273166	-4.274091	0.822150
52	1	0	1.007909	-4.268056	2.076512
53	6	0	0.482308	1.739704	3.667023
54	1	0	-0.291009	2.489968	3.489379
55	1	0	0.067220	0.971943	4.328793
56	1	0	1.349126	2.182824	4.161669

Zero-point correction= 0.429166 (Hartree/Particle)
Thermal correction to Energy= 0.463040
Thermal correction to Enthalpy= 0.463985
Thermal correction to Gibbs Free Energy= 0.362228
Sum of electronic and zero-point Energies= -1688.677976
Sum of electronic and thermal Energies= -1688.644101
Sum of electronic and thermal Enthalpies= -1688.643157
Sum of electronic and thermal Free Energies= -1688.744913
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1691.62713915

4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.148324	1.700644	0.202782
2	6	0	0.994889	0.920868	0.061815
3	6	0	0.674112	-0.441175	0.058296
4	6	0	2.314870	1.336186	-0.088034
5	6	0	1.654349	-1.403412	-0.101043
6	6	0	3.296307	0.358584	-0.241652
7	1	0	2.574815	2.392849	-0.079369
8	6	0	2.982026	-0.999300	-0.250472
9	1	0	1.381037	-2.457911	-0.089701
10	1	0	4.333820	0.667111	-0.352436
11	1	0	3.769544	-1.738936	-0.368845
12	6	0	-0.805777	-0.592383	0.242876
13	6	0	-1.267072	0.851186	0.621339
14	8	0	-1.174975	-1.557955	1.208917
15	1	0	-0.621232	-1.411971	1.984842
16	6	0	-2.576976	1.099423	-0.145124
17	1	0	-3.360432	1.545856	0.476740
18	1	0	-2.362586	1.800412	-0.962277
19	6	0	-1.616877	-0.909246	-1.012127
20	1	0	-1.143556	-0.419143	-1.874723
21	1	0	-1.647404	-1.988232	-1.197303
22	6	0	-2.968319	-0.267034	-0.718506
23	1	0	-3.619701	-0.189990	-1.595439
24	1	0	-3.493395	-0.863709	0.037963
25	1	0	-1.416485	0.900263	1.713316
26	1	0	-0.045547	2.600358	0.652215

Zero-point correction= 0.221023 (Hartree/Particle)
Thermal correction to Energy= 0.231339
Thermal correction to Enthalpy= 0.232283
Thermal correction to Gibbs Free Energy= 0.185510
Sum of electronic and zero-point Energies= -556.377193
Sum of electronic and thermal Energies= -556.366877
Sum of electronic and thermal Enthalpies= -556.365933
Sum of electronic and thermal Free Energies= -556.412706
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -556.73313235

5'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.610702	-0.023654	-0.007893

2	6	0	-0.406862	0.695368	0.030823
3	6	0	-0.493492	2.080229	0.139561
4	6	0	-1.719351	2.733484	0.223038
5	6	0	-2.896491	1.997140	0.200340
6	6	0	-2.845282	0.614364	0.081893
7	1	0	0.423643	2.664924	0.155771
8	1	0	-1.752682	3.816658	0.304707
9	1	0	-3.860551	2.494465	0.269787
10	1	0	-3.764883	0.032189	0.053920
11	7	0	-1.488499	-1.436991	-0.165450
12	7	0	-2.516154	-2.113240	-0.136846
13	7	0	-3.397342	-2.835230	-0.127754
14	6	0	0.917796	-0.028211	-0.076084
15	6	0	2.219275	0.757817	0.198618
16	6	0	1.319374	-0.983980	1.075352
17	6	0	2.772208	-0.469935	0.972644
18	1	0	1.996553	1.536948	0.941529
19	1	0	0.834165	-0.710288	2.020043
20	1	0	1.151467	-2.050762	0.881999
21	1	0	3.232658	-0.210926	1.935112
22	8	0	1.033775	-0.653646	-1.341598
23	1	0	0.364749	-1.351111	-1.365614
24	6	0	3.701268	-1.379828	0.194286
25	1	0	4.650385	-0.879983	-0.035937
26	1	0	3.932923	-2.281362	0.774693
27	1	0	3.245033	-1.693525	-0.750765
28	6	0	2.973705	1.348510	-0.968988
29	1	0	2.406981	2.163570	-1.436235
30	1	0	3.940383	1.753649	-0.646076
31	1	0	3.154253	0.595130	-1.741340

Zero-point correction= 0.255303 (Hartree/Particle)
Thermal correction to Energy= 0.270241
Thermal correction to Enthalpy= 0.271186
Thermal correction to Gibbs Free Energy= 0.213672
Sum of electronic and zero-point Energies= -704.984563
Sum of electronic and thermal Energies= -704.969625
Sum of electronic and thermal Enthalpies= -704.968680
Sum of electronic and thermal Free Energies= -705.026194
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -705.40198236

INT1-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.940144	1.920099	0.608543
2	6	0	-2.968702	1.200670	-0.015747
3	6	0	-3.729153	1.915761	-0.949851
4	6	0	-3.519400	3.259339	-1.224146
5	6	0	-2.511944	3.951792	-0.562044
6	6	0	-1.713888	3.271385	0.341872
7	1	0	-4.522881	1.398815	-1.485495
8	1	0	-4.146417	3.764904	-1.954548
9	1	0	-2.332488	5.004856	-0.762642
10	1	0	-0.881289	3.775039	0.830523
11	7	0	-0.992366	1.234493	1.449609
12	7	0	-0.553140	1.853923	2.429646
13	7	0	-0.083358	2.311891	3.356766
14	45	0	0.704965	0.191213	0.352936
15	45	0	2.509078	-0.847053	-0.858161
16	8	0	-0.118261	-1.697433	0.573711
17	6	0	0.473810	-2.702295	0.056304
18	8	0	1.556457	-2.668441	-0.585326
19	8	0	3.326183	1.038945	-1.055114
20	6	0	2.720262	2.034673	-0.567794
21	8	0	1.625254	2.011058	0.077948
22	8	0	3.474552	-1.069800	0.956973
23	6	0	2.929664	-0.624997	2.006478
24	8	0	1.791116	-0.064735	2.086380
25	8	0	1.418913	-0.557827	-2.592418
26	6	0	0.269952	-0.037025	-2.506691
27	8	0	-0.290045	0.388212	-1.449424
28	6	0	-3.283656	-0.269369	0.218110
29	6	0	-4.784868	-0.689206	0.244912

30	6	0	-3.111744	-1.215156	-1.000389
31	6	0	-4.429164	-1.927176	-0.624310
32	1	0	-5.370978	0.003217	-0.372185
33	1	0	-3.181018	-0.668597	-1.948557
34	1	0	-2.186691	-1.807997	-1.000538
35	1	0	-5.116506	-2.083231	-1.466639
36	8	0	-2.692980	-0.794868	1.376010
37	6	0	3.333478	3.385041	-0.796493
38	1	0	4.414154	3.293428	-0.921408
39	1	0	2.916401	3.807763	-1.716962
40	1	0	3.092532	4.059632	0.027686
41	6	0	3.704451	-0.740712	3.286042
42	1	0	3.030076	-0.955084	4.118191
43	1	0	4.472879	-1.510766	3.198363
44	1	0	4.190481	0.219542	3.489443
45	6	0	-0.532628	0.064122	-3.770880
46	1	0	0.125570	0.223439	-4.627601
47	1	0	-1.062914	-0.883014	-3.922525
48	1	0	-1.271460	0.864938	-3.689631
49	6	0	-0.184328	-4.033737	0.262781
50	1	0	0.195138	-4.764443	-0.453280
51	1	0	0.037870	-4.383121	1.276780
52	1	0	-1.271638	-3.935041	0.180245
53	1	0	-1.799997	-1.116026	1.170866
54	6	0	-5.454661	-0.844710	1.589021
55	1	0	-6.464507	-1.258319	1.475593
56	1	0	-4.880926	-1.503344	2.246312
57	1	0	-5.544791	0.126419	2.091218
58	6	0	-4.239451	-3.236404	0.116538
59	1	0	-3.859832	-4.010455	-0.563737
60	1	0	-3.524658	-3.122263	0.939853
61	1	0	-5.182818	-3.603098	0.540206

Zero-point correction= 0.470471 (Hartree/Particle)
Thermal correction to Energy= 0.507111
Thermal correction to Enthalpy= 0.508055
Thermal correction to Gibbs Free Energy= 0.402923
Sum of electronic and zero-point Energies= -1837.363034
Sum of electronic and thermal Energies= -1837.326394
Sum of electronic and thermal Enthalpies= -1837.325450
Sum of electronic and thermal Free Energies= -1837.430582
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1840.38490919

TS1-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.823015	1.748219	0.659379
2	6	0	-3.061641	1.294199	0.135187
3	6	0	-3.785287	2.211155	-0.633907
4	6	0	-3.354829	3.514850	-0.834288
5	6	0	-2.141016	3.949126	-0.300801
6	6	0	-1.370109	3.056822	0.415084
7	1	0	-4.729900	1.904128	-1.074533
8	1	0	-3.971041	4.198198	-1.414427
9	1	0	-1.797406	4.967527	-0.463016
10	1	0	-0.391733	3.334695	0.802749
11	7	0	-1.005464	0.823416	1.307950
12	7	0	-0.560865	1.403637	2.816653
13	7	0	0.094980	1.162573	3.690007
14	45	0	0.724696	0.208017	0.350536
15	45	0	2.535819	-0.813065	-0.902714
16	8	0	-0.068212	-1.696821	0.552846
17	6	0	0.523599	-2.682544	0.005992
18	8	0	1.597770	-2.639832	-0.653466
19	8	0	3.338355	1.089352	-1.077697
20	6	0	2.742332	2.070676	-0.558739
21	8	0	1.654702	2.034754	0.104410
22	8	0	3.505257	-1.055145	0.915992
23	6	0	2.957503	-0.646558	1.973992
24	8	0	1.817081	-0.082868	2.060374
25	8	0	1.438044	-0.513980	-2.629164
26	6	0	0.295983	0.013946	-2.527275
27	8	0	-0.249099	0.442484	-1.462546

28	6	0	-3.511886	-0.151734	0.251113
29	6	0	-4.977422	-0.551450	-0.065617
30	6	0	-3.082061	-1.069284	-0.929286
31	6	0	-4.444214	-1.787836	-0.843956
32	1	0	-5.395915	0.139454	-0.808421
33	1	0	-2.965391	-0.497465	-1.858575
34	1	0	-2.167426	-1.648050	-0.746179
35	1	0	-4.938837	-1.939960	-1.812958
36	8	0	-3.201231	-0.720420	1.497285
37	6	0	3.353553	3.430521	-0.737127
38	1	0	2.699931	4.037111	-1.372111
39	1	0	3.427062	3.933380	0.231195
40	1	0	4.338597	3.350209	-1.199258
41	6	0	3.717817	-0.822796	3.255031
42	1	0	3.101007	-0.560421	4.116269
43	1	0	4.064249	-1.856923	3.332923
44	1	0	4.606121	-0.183600	3.231547
45	6	0	-0.527746	0.125153	-3.777233
46	1	0	0.112222	0.336759	-4.636745
47	1	0	-1.020648	-0.837743	-3.953547
48	1	0	-1.295467	0.893992	-3.661454
49	6	0	-0.134458	-4.018887	0.191659
50	1	0	0.263888	-4.745349	-0.518591
51	1	0	0.058850	-4.371612	1.210180
52	1	0	-1.218976	-3.919399	0.080705
53	1	0	-2.237769	-0.656901	1.607006
54	6	0	-5.939939	-0.702061	1.088391
55	1	0	-6.901658	-1.103398	0.745923
56	1	0	-5.536550	-1.369069	1.855476
57	1	0	-6.129582	0.268745	1.563265
58	6	0	-4.412596	-3.099583	-0.084026
59	1	0	-5.424439	-3.472922	0.119264
60	1	0	-3.889309	-3.867054	-0.669954
61	1	0	-3.892383	-2.986321	0.873279

Zero-point correction= 0.465740 (Hartree/Particle)
Thermal correction to Energy= 0.502737
Thermal correction to Enthalpy= 0.503681
Thermal correction to Gibbs Free Energy= 0.398368
Sum of electronic and zero-point Energies= -1837.319910
Sum of electronic and thermal Energies= -1837.282913
Sum of electronic and thermal Enthalpies= -1837.281969
Sum of electronic and thermal Free Energies= -1837.387282
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1840.33744842

[1]INT2-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.001783	1.217950	-0.283014
2	6	0	3.444546	1.032290	-0.351634
3	6	0	4.245707	2.150107	-0.177603
4	6	0	3.692955	3.418765	-0.002294
5	6	0	2.309413	3.622965	0.024895
6	6	0	1.472482	2.540871	-0.103064
7	1	0	5.327850	2.054382	-0.194581
8	1	0	4.360982	4.271273	0.105691
9	1	0	1.906878	4.624372	0.151158
10	1	0	0.393552	2.649973	-0.086284
11	7	0	1.244257	0.134095	-0.367560
12	45	0	-0.681194	0.005900	-0.089816
13	45	0	-3.085712	-0.363557	0.208064
14	8	0	-0.390237	-1.535013	1.263186
15	6	0	-1.398224	-2.120224	1.772985
16	8	0	-2.610827	-1.858120	1.556031
17	8	0	-3.395745	1.153942	-1.171635
18	6	0	-2.405900	1.749611	-1.665349
19	8	0	-1.176158	1.523583	-1.409152
20	8	0	-2.986307	-1.726399	-1.347085
21	6	0	-1.877954	-1.926579	-1.912883
22	8	0	-0.768021	-1.370786	-1.633520
23	8	0	-2.998142	1.028335	1.747278
24	6	0	-1.897165	1.551564	2.053163
25	8	0	-0.773009	1.349291	1.484095

26	6	0	4.007397	-0.369161	-0.500189
27	6	0	4.132451	-1.021707	0.914978
28	6	0	5.552828	-0.469045	-0.613482
29	6	0	5.624777	-0.652195	0.927418
30	1	0	6.061338	0.421232	-1.009056
31	1	0	5.754845	0.330111	1.405221
32	6	0	-2.663743	2.830713	-2.675627
33	1	0	-2.082878	3.722362	-2.424178
34	1	0	-2.323968	2.487529	-3.658067
35	1	0	-3.727687	3.068041	-2.719757
36	6	0	-1.834366	-2.940417	-3.020363
37	1	0	-1.149753	-2.610717	-3.805220
38	1	0	-1.451092	-3.884999	-2.620127
39	1	0	-2.835374	-3.108126	-3.421849
40	6	0	-1.877335	2.488415	3.227250
41	1	0	-1.611652	1.918409	4.124049
42	1	0	-1.122909	3.265925	3.088221
43	1	0	-2.866043	2.926201	3.377545
44	6	0	-1.083243	-3.241608	2.721311
45	1	0	-0.582101	-4.045060	2.172491
46	1	0	-0.387994	-2.890436	3.488870
47	1	0	-1.996904	-3.622703	3.180049
48	8	0	3.350972	-1.103222	-1.481885
49	1	0	3.485638	-0.649912	1.717639
50	1	0	3.978054	-2.102461	0.801974
51	1	0	2.405065	-1.085515	-1.238364
52	6	0	5.998618	-1.670872	-1.423072
53	1	0	5.740920	-1.537696	-2.477828
54	1	0	7.083928	-1.804604	-1.341820
55	1	0	5.511285	-2.594919	-1.094457
56	6	0	6.607707	-1.634262	1.523382
57	1	0	7.646182	-1.321320	1.357598
58	1	0	6.458234	-1.727704	2.605554
59	1	0	6.487979	-2.633706	1.087910

Zero-point correction= 0.458630 (Hartree/Particle)
Thermal correction to Energy= 0.493631
Thermal correction to Enthalpy= 0.494576
Thermal correction to Gibbs Free Energy= 0.392313
Sum of electronic and zero-point Energies= -1727.907682
Sum of electronic and thermal Energies= -1727.872681
Sum of electronic and thermal Enthalpies= -1727.871737
Sum of electronic and thermal Free Energies= -1727.973999
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1730.89416043

^{3}INT2-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.172547	1.509312	-0.201979
2	6	0	3.569056	1.162648	-0.313756
3	6	0	4.491312	2.178664	-0.155929
4	6	0	4.095511	3.499493	0.092504
5	6	0	2.741314	3.833289	0.190224
6	6	0	1.777810	2.858621	0.046031
7	1	0	5.553373	1.955260	-0.224096
8	1	0	4.853324	4.270812	0.208028
9	1	0	2.446886	4.862325	0.381596
10	1	0	0.713646	3.066520	0.116845
11	7	0	1.267828	0.563076	-0.329398
12	45	0	-0.666199	0.045103	-0.104003
13	45	0	-3.022542	-0.417958	0.211863
14	8	0	-0.259898	-1.598691	1.078985
15	6	0	-1.233034	-2.266535	1.550181
16	8	0	-2.460796	-2.028830	1.377672
17	8	0	-3.438019	1.226839	-0.966293
18	6	0	-2.477173	1.891014	-1.442398
19	8	0	-1.238453	1.665837	-1.264512
20	8	0	-2.922592	-1.600841	-1.480869
21	6	0	-1.822519	-1.725064	-2.085772
22	8	0	-0.718274	-1.182108	-1.762854
23	8	0	-2.976725	0.799353	1.879513
24	6	0	-1.886380	1.347361	2.198693
25	8	0	-0.777404	1.242044	1.585971

26	6	0	3.881385	-0.300936	-0.573387
27	6	0	5.377711	-0.692851	-0.493129
28	6	0	3.640581	-1.146755	0.703694
29	6	0	5.149024	-1.049969	1.001080
30	1	0	6.097757	0.115329	-0.678975
31	1	0	2.924035	-0.774086	1.444569
32	1	0	3.349788	-2.165090	0.413315
33	1	0	5.339894	-0.156695	1.613893
34	8	0	3.264612	-0.738494	-1.756610
35	6	0	-2.816682	3.050235	-2.333869
36	1	0	-2.075807	3.845113	-2.224168
37	1	0	-2.793275	2.710805	-3.374892
38	1	0	-3.820211	3.418036	-2.111871
39	6	0	-1.790589	-2.589242	-3.312084
40	1	0	-1.020224	-3.357235	-3.197257
41	1	0	-2.763636	-3.052574	-3.481512
42	1	0	-1.512061	-1.978905	-4.176591
43	6	0	-1.879189	2.187950	3.442475
44	1	0	-1.137382	2.985074	3.360869
45	1	0	-2.874405	2.597426	3.626698
46	1	0	-1.604699	1.554507	4.292730
47	6	0	-0.877378	-3.474367	2.367242
48	1	0	0.108010	-3.354193	2.821668
49	1	0	-1.640213	-3.649863	3.128788
50	1	0	-0.849141	-4.348361	1.707736
51	1	0	2.310038	-0.791059	-1.600229
52	6	0	5.731788	-1.866584	-1.385002
53	1	0	5.690701	-1.574414	-2.438704
54	1	0	6.744375	-2.224489	-1.163304
55	1	0	5.036913	-2.704501	-1.261791
56	6	0	5.849535	-2.242813	1.609171
57	1	0	6.936855	-2.100103	1.645462
58	1	0	5.503679	-2.417195	2.634964
59	1	0	5.652929	-3.157199	1.036341

Zero-point correction= 0.456316 (Hartree/Particle)
Thermal correction to Energy= 0.491940
Thermal correction to Enthalpy= 0.492885
Thermal correction to Gibbs Free Energy= 0.387568
Sum of electronic and zero-point Energies= -1727.914110
Sum of electronic and thermal Energies= -1727.878485
Sum of electronic and thermal Enthalpies= -1727.877541
Sum of electronic and thermal Free Energies= -1727.982858
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1730.89880919

^{3}TS2-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.170840	1.337188	0.225180
2	6	0	3.584188	1.125502	0.408744
3	6	0	4.448417	2.187633	0.232050
4	6	0	3.968994	3.450951	-0.129956
5	6	0	2.599898	3.658529	-0.334965
6	6	0	1.703340	2.625500	-0.167947
7	1	0	5.517707	2.044772	0.378212
8	1	0	4.668167	4.274706	-0.251702
9	1	0	2.239050	4.644614	-0.616893
10	1	0	0.633439	2.753140	-0.303105
11	7	0	1.329304	0.330424	0.432968
12	45	0	-0.685307	0.017868	0.142841
13	45	0	-3.053579	-0.344488	-0.241023
14	8	0	-0.330088	-1.759252	-0.843870
15	6	0	-1.318302	-2.413046	-1.304072
16	8	0	-2.536110	-2.096967	-1.212494
17	8	0	-3.414600	1.426157	0.760933
18	6	0	-2.436641	2.084988	1.208222
19	8	0	-1.205672	1.785408	1.098421
20	8	0	-3.088052	-1.369486	1.553637
21	6	0	-2.020950	-1.494958	2.215491
22	8	0	-0.880246	-1.028314	1.905048
23	8	0	-2.860085	0.702081	-2.015005
24	6	0	-1.725182	1.150953	-2.333431
25	8	0	-0.650229	1.042638	-1.663425

26	6	0	3.996548	-0.310211	0.638510
27	6	0	4.487831	-0.978985	-0.701942
28	6	0	5.427628	-0.520031	1.215246
29	6	0	5.948685	-0.791293	-0.207907
30	1	0	5.851098	0.302745	1.801856
31	1	0	6.361806	0.131078	-0.640029
32	6	0	-2.740642	3.344801	1.966997
33	1	0	-3.780646	3.639966	1.818955
34	1	0	-2.064303	4.143945	1.652778
35	1	0	-2.564207	3.167079	3.032869
36	6	0	-2.080420	-2.284949	3.490056
37	1	0	-3.116494	-2.463982	3.782002
38	1	0	-1.541511	-1.756282	4.280448
39	1	0	-1.576651	-3.244817	3.336423
40	6	0	-1.610027	1.863035	-3.650978
41	1	0	-2.588095	2.217578	-3.980975
42	1	0	-1.221292	1.160990	-4.396345
43	1	0	-0.901133	2.690662	-3.573530
44	6	0	-0.977573	-3.679087	-2.035617
45	1	0	-0.319960	-4.295545	-1.416226
46	1	0	-0.424803	-3.428131	-2.946510
47	1	0	-1.882794	-4.230008	-2.295279
48	8	0	3.048904	-0.981932	1.358665
49	1	0	4.241369	-0.402261	-1.604113
50	1	0	1.910848	-0.550030	0.886130
51	6	0	6.940751	-1.919206	-0.384843
52	1	0	7.889350	-1.689868	0.115157
53	1	0	7.158907	-2.101244	-1.444231
54	1	0	6.561471	-2.855742	0.042026
55	1	0	5.427183	-1.428986	1.827969
56	6	0	3.999903	-2.402517	-0.846287
57	1	0	4.501802	-2.907854	-1.680301
58	1	0	4.170068	-2.986747	0.065761
59	1	0	2.920062	-2.416280	-1.034522

Zero-point correction= 0.451044 (Hartree/Particle)
Thermal correction to Energy= 0.485910
Thermal correction to Enthalpy= 0.486854
Thermal correction to Gibbs Free Energy= 0.383197
Sum of electronic and zero-point Energies= -1727.897122
Sum of electronic and thermal Energies= -1727.862256
Sum of electronic and thermal Enthalpies= -1727.861312
Sum of electronic and thermal Free Energies= -1727.964969
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1730.87449361

^{1}TS4-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.070714	1.302258	-0.597598
2	6	0	-3.505677	1.025940	-0.780164
3	6	0	-4.436642	2.060230	-0.510146
4	6	0	-4.002627	3.264215	-0.026919
5	6	0	-2.624535	3.520186	0.245305
6	6	0	-1.687026	2.574811	-0.021358
7	1	0	-5.493510	1.902662	-0.713993
8	1	0	-4.727136	4.058517	0.142083
9	1	0	-2.335359	4.488929	0.644446
10	1	0	-0.624914	2.744526	0.134145
11	7	0	-1.229388	0.371801	-0.952799
12	45	0	0.671569	0.123236	-0.318154
13	45	0	2.882817	-0.448478	0.558324
14	8	0	0.120550	-1.839841	0.065758
15	6	0	0.959031	-2.620665	0.618753
16	8	0	2.142515	-2.345020	0.948812
17	8	0	3.452350	1.496357	0.109524
18	6	0	2.606368	2.294645	-0.369241
19	8	0	1.384629	2.044459	-0.633187
20	8	0	3.387238	-1.035414	-1.361557
21	6	0	2.541302	-0.900726	-2.286982
22	8	0	1.362221	-0.436998	-2.182289
23	8	0	2.198955	0.194150	2.412971
24	6	0	1.005692	0.573966	2.536567
25	8	0	0.125607	0.639186	1.618574

26	6	0	-3.880984	-0.322760	-1.134360
27	6	0	-4.122357	-0.659136	0.677804
28	6	0	-5.338761	-0.754100	-1.226458
29	6	0	-5.598994	-0.799515	0.285994
30	1	0	-5.990436	-0.103212	-1.821428
31	1	0	-6.137230	0.100948	0.611308
32	6	0	3.066545	3.688840	-0.690751
33	1	0	4.053950	3.874128	-0.264781
34	1	0	2.343879	4.418122	-0.314577
35	1	0	3.112694	3.806077	-1.778323
36	6	0	2.945097	-1.336582	-3.667287
37	1	0	2.740873	-0.533727	-4.381134
38	1	0	2.336787	-2.196791	-3.964151
39	1	0	4.001750	-1.607749	-3.690846
40	6	0	0.546621	0.971387	3.912298
41	1	0	-0.155478	1.806507	3.851840
42	1	0	1.402907	1.229230	4.538169
43	1	0	0.022337	0.125434	4.369647
44	6	0	0.466776	-4.016456	0.880494
45	1	0	0.379581	-4.547963	-0.072678
46	1	0	-0.531816	-3.980590	1.326247
47	1	0	1.159206	-4.552886	1.531328
48	8	0	-2.997013	-1.106196	-1.709624
49	1	0	-3.896308	0.149697	1.379522
50	1	0	-2.011198	-0.603985	-1.482397
51	6	0	-6.323450	-2.025369	0.807351
52	1	0	-7.343527	-2.067509	0.408295
53	1	0	-6.391311	-2.019653	1.901563
54	1	0	-5.812629	-2.947953	0.506430
55	1	0	-5.349191	-1.753932	-1.674668
56	6	0	-3.275040	-1.863010	0.930496
57	1	0	-3.447017	-2.219286	1.956431
58	1	0	-3.481693	-2.674558	0.225942
59	1	0	-2.207001	-1.616128	0.838884

Zero-point correction= 0.452905 (Hartree/Particle)
Thermal correction to Energy= 0.488107
Thermal correction to Enthalpy= 0.489051
Thermal correction to Gibbs Free Energy= 0.385317
Sum of electronic and zero-point Energies= -1727.903998
Sum of electronic and thermal Energies= -1727.868796
Sum of electronic and thermal Enthalpies= -1727.867852
Sum of electronic and thermal Free Energies= -1727.971586
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1730.88499525

^{3}INT3-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.187557	1.303790	-0.292974
2	6	0	-3.612671	1.147952	-0.453794
3	6	0	-4.429310	2.239134	-0.230516
4	6	0	-3.903221	3.482353	0.139273
5	6	0	-2.524704	3.640756	0.304623
6	6	0	-1.675222	2.574980	0.099980
7	1	0	-5.507462	2.139779	-0.338649
8	1	0	-4.574320	4.322878	0.298362
9	1	0	-2.119285	4.607797	0.591396
10	1	0	-0.599059	2.669082	0.212386
11	7	0	-1.333844	0.296862	-0.487931
12	45	0	0.705017	0.050273	-0.135739
13	45	0	3.057011	-0.393743	0.270700
14	8	0	0.282113	-1.736453	0.816486
15	6	0	1.245956	-2.426193	1.277526
16	8	0	2.472172	-2.140698	1.218677
17	8	0	3.474318	1.378092	-0.712590
18	6	0	2.522517	2.075070	-1.155850
19	8	0	1.281194	1.813267	-1.062061
20	8	0	3.079627	-1.404436	-1.535168
21	6	0	2.018158	-1.482775	-2.212986
22	8	0	0.886063	-0.993280	-1.907979
23	8	0	2.859278	0.648709	2.050116
24	6	0	1.733801	1.126770	2.359623
25	8	0	0.663316	1.054428	1.678479

26	6	0	-4.109798	-0.251960	-0.738322
27	6	0	-4.355085	-1.082358	0.578152
28	6	0	-5.675738	-0.383059	-1.002052
29	6	0	-5.869389	-0.764417	0.469974
30	1	0	-6.150418	0.507982	-1.423656
31	1	0	-6.090807	0.135842	1.059457
32	6	0	2.873339	3.336206	-1.892983
33	1	0	3.916558	3.604435	-1.717888
34	1	0	2.209243	4.148230	-1.585934
35	1	0	2.718953	3.174173	-2.964839
36	6	0	2.102080	-2.199587	-3.530149
37	1	0	2.819339	-3.020618	-3.463543
38	1	0	2.463787	-1.497286	-4.288839
39	1	0	1.119241	-2.563040	-3.836004
40	6	0	1.646943	1.842473	3.678400
41	1	0	2.457419	2.572730	3.752584
42	1	0	1.789910	1.116087	4.484749
43	1	0	0.679024	2.332013	3.797496
44	6	0	0.859629	-3.712369	1.951275
45	1	0	0.120565	-3.509580	2.731837
46	1	0	1.735900	-4.202273	2.378436
47	1	0	0.385702	-4.374090	1.219427
48	8	0	-3.466992	-0.843067	-1.752452
49	1	0	-3.864853	-0.637440	1.455073
50	6	0	-6.883620	-1.841985	0.779305
51	1	0	-7.900434	-1.503662	0.547957
52	1	0	-6.859570	-2.119831	1.839782
53	1	0	-6.695054	-2.749129	0.192495
54	1	0	-5.840165	-1.231393	-1.674163
55	6	0	-3.961635	-2.534657	0.435962
56	1	0	-4.332748	-3.123596	1.282932
57	1	0	-4.347632	-2.977900	-0.489320
58	1	0	-2.870107	-2.634329	0.406545
59	1	0	-1.753634	-0.561985	-0.860655

Zero-point correction= 0.455320 (Hartree/Particle)
Thermal correction to Energy= 0.491017
Thermal correction to Enthalpy= 0.491962
Thermal correction to Gibbs Free Energy= 0.385547
Sum of electronic and zero-point Energies= -1727.902008
Sum of electronic and thermal Energies= -1727.866311
Sum of electronic and thermal Enthalpies= -1727.865367
Sum of electronic and thermal Free Energies= -1727.971782
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1730.88516075

[1]INT5-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.490268	0.875379	0.518496
2	6	0	3.910177	0.334688	0.445946
3	6	0	4.929268	1.418176	0.649975
4	6	0	4.644837	2.709145	0.432668
5	6	0	3.297407	3.115900	0.075901
6	6	0	2.268933	2.243960	0.087600
7	1	0	5.940794	1.097831	0.900121
8	1	0	5.419712	3.466655	0.519785
9	1	0	3.114833	4.160771	-0.166118
10	1	0	1.239776	2.545918	-0.097642
11	7	0	1.486056	0.179112	0.925130
12	45	0	-0.586098	0.143837	0.335010
13	45	0	-2.837610	-0.243714	-0.486900
14	8	0	-0.398570	-1.900090	0.577783
15	6	0	-1.363811	-2.648465	0.218497
16	8	0	-2.474762	-2.272080	-0.240805
17	8	0	-3.037695	1.804983	-0.680031
18	6	0	-2.060982	2.546530	-0.386475
19	8	0	-0.923247	2.171517	0.040766
20	8	0	-2.032021	-0.363328	-2.397358
21	6	0	-0.786494	-0.243302	-2.543363
22	8	0	0.068868	-0.031955	-1.626235
23	8	0	-3.474028	-0.107001	1.473799
24	6	0	-2.627506	0.121497	2.383469
25	8	0	-1.377540	0.289165	2.235088

26	6	0	4.225396	-0.359092	-0.936259
27	6	0	4.128718	-0.816102	1.457926
28	6	0	4.066085	-1.882511	-0.721425
29	6	0	4.533551	-2.073844	0.720911
30	1	0	4.757225	-2.382455	-1.415454
31	1	0	5.632553	-2.126498	0.772934
32	6	0	-2.238893	4.025908	-0.581341
33	1	0	-1.745619	4.573892	0.225103
34	1	0	-1.765941	4.319708	-1.524589
35	1	0	-3.299427	4.279195	-0.627710
36	6	0	-0.227820	-0.365330	-3.933758
37	1	0	0.348228	0.533090	-4.176875
38	1	0	0.463999	-1.213781	-3.971275
39	1	0	-1.026526	-0.508208	-4.663130
40	6	0	-3.134595	0.183342	3.796158
41	1	0	-2.846971	-0.736090	4.316790
42	1	0	-2.666217	1.018161	4.323563
43	1	0	-4.221622	0.277719	3.810815
44	6	0	-1.134567	-4.124346	0.379444
45	1	0	-0.151636	-4.387987	-0.022653
46	1	0	-1.130331	-4.373824	1.445465
47	1	0	-1.918962	-4.693281	-0.121981
48	1	0	1.717060	-0.732059	1.320137
49	6	0	2.673654	-2.447059	-0.974948
50	1	0	2.344945	-2.245939	-2.001014
51	1	0	2.684267	-3.535180	-0.836085
52	1	0	1.901396	-2.039193	-0.313621
53	1	0	5.307812	-0.199744	-1.077515
54	6	0	3.515150	0.207433	-2.148820
55	1	0	2.424247	0.149487	-2.047584
56	1	0	3.789981	1.255814	-2.310089
57	1	0	4.146933	-2.962842	1.231651
58	8	0	3.992153	-0.700751	2.650479
59	1	0	3.806010	-0.355609	-3.045411

Zero-point correction= 0.460182 (Hartree/Particle)
Thermal correction to Energy= 0.495046
Thermal correction to Enthalpy= 0.495991
Thermal correction to Gibbs Free Energy= 0.394620
Sum of electronic and zero-point Energies= -1727.986842
Sum of electronic and thermal Energies= -1727.951977
Sum of electronic and thermal Enthalpies= -1727.951033
Sum of electronic and thermal Free Energies= -1728.052404
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1730.97703818

^{1}TS5-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.530901	0.946894	-0.742340
2	6	0	3.930765	0.613714	-0.601549
3	6	0	4.843312	1.663584	-0.313251
4	6	0	4.434367	2.956788	-0.125292
5	6	0	3.070962	3.277237	-0.323162
6	6	0	2.153802	2.314648	-0.644395
7	1	0	5.901075	1.408542	-0.235189
8	1	0	5.150646	3.733870	0.126080
9	1	0	2.745414	4.310438	-0.221300
10	1	0	1.098517	2.542708	-0.764923
11	7	0	1.562520	-0.000444	-0.664242
12	45	0	-0.509404	0.027862	-0.209468
13	45	0	-2.875326	-0.207709	0.309793
14	8	0	-0.640415	-1.704997	-1.334639
15	6	0	-1.767904	-2.288755	-1.408812
16	8	0	-2.839054	-1.935784	-0.847422
17	8	0	-2.718381	1.531866	1.419079
18	6	0	-1.595660	2.100017	1.513607
19	8	0	-0.505718	1.733514	0.973536
20	8	0	-2.302933	-1.301919	1.979390
21	6	0	-1.080267	-1.521107	2.186223
22	8	0	-0.103017	-1.140868	1.466201
23	8	0	-3.255647	0.907472	-1.394637
24	6	0	-2.288571	1.350728	-2.071780
25	8	0	-1.050993	1.176518	-1.840874

26	6	0	2.794433	0.048345	1.168798
27	6	0	4.515037	-0.758902	-0.896159
28	6	0	3.218400	-1.388648	1.137840
29	6	0	4.560995	-1.540861	0.433108
30	1	0	2.420129	-2.000787	0.706788
31	1	0	3.287778	-1.658413	2.200044
32	6	0	-1.521088	3.348398	2.348681
33	1	0	-2.483830	3.557475	2.817601
34	1	0	-1.225961	4.191365	1.716028
35	1	0	-0.746148	3.229546	3.111651
36	6	0	-0.715768	-2.312341	3.413165
37	1	0	-0.079781	-1.700720	4.061095
38	1	0	-0.136158	-3.194419	3.123248
39	1	0	-1.611101	-2.618182	3.956500
40	6	0	-2.615414	2.158543	-3.297190
41	1	0	-2.353698	1.578351	-4.188063
42	1	0	-2.010061	3.069020	-3.312837
43	1	0	-3.677884	2.405602	-3.324008
44	6	0	-1.830667	-3.509628	-2.284377
45	1	0	-2.548812	-4.225986	-1.879089
46	1	0	-0.843920	-3.965463	-2.389238
47	1	0	-2.180380	-3.209942	-3.278240
48	8	0	2.474851	0.851994	1.949783
49	1	0	1.809627	-0.902352	-1.056980
50	1	0	5.302073	-1.020423	1.061960
51	6	0	4.973828	-2.995925	0.305493
52	1	0	5.932260	-3.082688	-0.219463
53	1	0	5.090329	-3.462230	1.290302
54	1	0	4.231044	-3.580205	-0.251177
55	6	0	3.894291	-1.535362	-2.060497
56	1	0	4.620253	-2.249861	-2.463422
57	1	0	3.009801	-2.124951	-1.789864
58	1	0	3.606742	-0.861481	-2.874141
59	1	0	5.563188	-0.579134	-1.180291

Zero-point correction= 0.457766 (Hartree/Particle)
Thermal correction to Energy= 0.492588
Thermal correction to Enthalpy= 0.493532
Thermal correction to Gibbs Free Energy= 0.392800
Sum of electronic and zero-point Energies= -1727.937558
Sum of electronic and thermal Energies= -1727.902736
Sum of electronic and thermal Enthalpies= -1727.901792
Sum of electronic and thermal Free Energies= -1728.002524
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1730.92811111

6'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.079867	0.524279	0.467563
2	6	0	-0.667616	-0.719205	-0.038542
3	6	0	-1.647659	-1.545035	-0.589391
4	6	0	-2.979726	-1.147355	-0.654419
5	6	0	-3.360061	0.096992	-0.167547
6	6	0	-2.402533	0.935020	0.392453
7	1	0	-1.357368	-2.520049	-0.980637
8	1	0	-3.719690	-1.812078	-1.093821
9	1	0	-4.397525	0.416386	-0.225149
10	1	0	-2.655682	1.918925	0.777959
11	7	0	-0.088179	1.405487	1.028178
12	6	0	0.831858	1.796043	0.025954
13	6	0	0.770515	-1.219032	0.046053
14	6	0	2.129919	1.040635	0.074050
15	6	0	1.859158	-0.322733	-0.605340
16	1	0	2.494707	0.889094	1.100612
17	1	0	2.899635	1.576764	-0.491758
18	8	0	0.510249	2.507918	-0.894577
19	1	0	0.390637	0.943237	1.795171
20	6	0	1.111628	-1.674101	1.468905
21	1	0	0.335684	-2.350096	1.843602
22	1	0	2.065261	-2.212596	1.500043
23	1	0	1.188193	-0.845319	2.183560
24	6	0	3.175769	-1.077851	-0.741520
25	1	0	3.029020	-2.064862	-1.196764

26	1	0	3.878287	-0.519831	-1.370165
27	1	0	3.658500	-1.225589	0.233121
28	1	0	0.784649	-2.133770	-0.568366
29	1	0	1.492637	-0.087904	-1.617349

Zero-point correction= 0.247989 (Hartree/Particle)
Thermal correction to Energy= 0.260272
Thermal correction to Enthalpy= 0.261216
Thermal correction to Gibbs Free Energy= 0.210224
Sum of electronic and zero-point Energies= -595.632822
Sum of electronic and thermal Energies= -595.620539
Sum of electronic and thermal Enthalpies= -595.619595
Sum of electronic and thermal Free Energies= -595.670587
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -596.02496550

[1]INT2'-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.574286	0.127932	-0.341428
2	45	0	2.783796	-0.488246	0.544851
3	8	0	1.466295	1.817022	-1.146537
4	6	0	2.722537	1.986392	-0.991221
5	8	0	3.509166	1.227408	-0.373839
6	8	0	1.072668	-0.909007	-2.055492
7	6	0	2.186490	-1.523588	-2.102980
8	8	0	3.077820	-1.542726	-1.213105
9	8	0	-0.088933	-1.650542	0.527751
10	6	0	0.706089	-2.371954	1.208425
11	8	0	1.930530	-2.158989	1.413453
12	8	0	0.261602	1.136304	1.441125
13	6	0	1.187002	1.166102	2.317664
14	8	0	2.316278	0.618632	2.239605
15	7	0	-1.311901	0.363709	-0.758305
16	6	0	-2.016844	1.461988	-0.502027
17	6	0	-3.414169	1.320636	-0.143890
18	6	0	-1.451364	2.774211	-0.596773
19	6	0	-4.143729	2.477320	0.092737
20	6	0	-2.227204	3.894826	-0.411402
21	1	0	-0.400438	2.841891	-0.866746
22	6	0	-3.570672	3.739065	-0.055276
23	1	0	-5.174045	2.384970	0.423286
24	1	0	-1.800903	4.888670	-0.521037
25	1	0	-4.182758	4.620885	0.125017
26	6	0	-4.045952	-0.027907	0.086294
27	6	0	-3.894036	-1.137121	-1.008515
28	6	0	-3.341467	-0.981086	1.082207
29	6	0	-3.521773	-2.158206	0.101384
30	1	0	-3.001320	-0.918546	-1.600083
31	1	0	-2.291961	-0.721779	1.251845
32	1	0	-3.877953	-1.054620	2.036261
33	1	0	-2.580319	-2.680982	-0.111994
34	8	0	-5.390288	0.106416	0.508315
35	1	0	-5.930400	0.291094	-0.269461
36	6	0	-5.078860	-1.390486	-1.912745
37	1	0	-4.868609	-2.223671	-2.593274
38	1	0	-5.986668	-1.651642	-1.355615
39	1	0	-5.298303	-0.514859	-2.540005
40	6	0	-4.599711	-3.141849	0.508477
41	1	0	-4.844105	-3.842301	-0.300239
42	1	0	-4.271165	-3.734563	1.371849
43	1	0	-5.520536	-2.621462	0.800898
44	6	0	3.287253	3.228256	-1.620079
45	1	0	2.839370	4.109677	-1.150406
46	1	0	4.371050	3.258453	-1.499857
47	1	0	3.023226	3.254484	-2.681251
48	6	0	2.434327	-2.314630	-3.355808
49	1	0	3.478271	-2.627865	-3.409198
50	1	0	1.790208	-3.199992	-3.350747
51	1	0	2.164180	-1.719409	-4.231934
52	6	0	0.099165	-3.612260	1.801369
53	1	0	-0.900642	-3.388456	2.185355
54	1	0	-0.010952	-4.365207	1.013542
55	1	0	0.738505	-4.013770	2.589528

56	6	0	0.860855	1.920115	3.575589
57	1	0	1.773226	2.151090	4.128168
58	1	0	0.309908	2.833004	3.336282
59	1	0	0.214038	1.297963	4.203133

Zero-point correction= 0.457806 (Hartree/Particle)
Thermal correction to Energy= 0.493223
Thermal correction to Enthalpy= 0.494167
Thermal correction to Gibbs Free Energy= 0.389751
Sum of electronic and zero-point Energies= -1727.904407
Sum of electronic and thermal Energies= -1727.868990
Sum of electronic and thermal Enthalpies= -1727.868046
Sum of electronic and thermal Free Energies= -1727.972462
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1730.88794747

^{3}INT2'-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.548174	0.109384	-0.158538
2	45	0	2.895497	-0.335810	0.248769
3	8	0	1.150597	1.512056	-1.563955
4	6	0	2.394529	1.689188	-1.760089
5	8	0	3.340236	1.095635	-1.173739
6	8	0	0.587834	-1.381345	-1.588825
7	6	0	1.684430	-1.984357	-1.809315
8	8	0	2.789385	-1.769363	-1.237400
9	8	0	0.120687	-1.314210	1.279297
10	6	0	1.078116	-1.920361	1.854856
11	8	0	2.310159	-1.745705	1.645706
12	8	0	0.665492	1.559714	1.317944
13	6	0	1.769404	1.737866	1.922965
14	8	0	2.852373	1.128038	1.707982
15	7	0	-1.403442	0.606469	-0.445783
16	6	0	-2.324115	1.538122	-0.283326
17	6	0	-3.682471	1.186296	0.036566
18	6	0	-1.954845	2.909515	-0.433845
19	6	0	-4.586841	2.219826	0.214720
20	6	0	-2.897617	3.899032	-0.261749
21	1	0	-0.918251	3.123827	-0.681463
22	6	0	-4.214044	3.558848	0.066264
23	1	0	-5.605052	1.968882	0.500568
24	1	0	-2.614846	4.942838	-0.374638
25	1	0	-4.955809	4.340369	0.213929
26	6	0	-4.075124	-0.260308	0.201530
27	6	0	-3.652364	-1.269845	-0.915941
28	6	0	-3.276486	-1.116797	1.211128
29	6	0	-3.187785	-2.264517	0.181886
30	1	0	-2.767013	-0.882813	-1.436309
31	1	0	-2.299689	-0.695733	1.468893
32	1	0	-3.844228	-1.323853	2.126331
33	1	0	-2.162826	-2.622228	0.015515
34	8	0	-5.446342	-0.383201	0.523913
35	1	0	-5.954323	-0.194549	-0.274640
36	6	0	-4.697270	-1.672594	-1.930604
37	1	0	-4.297030	-2.418632	-2.626845
38	1	0	-5.584536	-2.111011	-1.458894
39	1	0	-5.016690	-0.810528	-2.533206
40	6	0	-4.113016	-3.428963	0.471791
41	1	0	-4.179212	-4.120196	-0.378181
42	1	0	-3.751470	-3.999678	1.336329
43	1	0	-5.125960	-3.080963	0.709391
44	6	0	2.753338	2.705934	-2.805373
45	1	0	2.265108	3.657474	-2.576056
46	1	0	3.834895	2.839325	-2.857236
47	1	0	2.373742	2.371541	-3.775792
48	6	0	1.643260	-3.082303	-2.832354
49	1	0	1.369043	-4.017327	-2.332051
50	1	0	0.888261	-2.869233	-3.591871
51	1	0	2.627722	-3.213011	-3.286046
52	6	0	0.686124	-2.920799	2.903287
53	1	0	-0.284900	-3.360702	2.662707
54	1	0	1.452859	-3.692376	2.997289
55	1	0	0.596569	-2.406342	3.866089

56	6	0	1.758972	2.777445	3.006680
57	1	0	2.760980	2.918769	3.414625
58	1	0	1.373966	3.720539	2.608503
59	1	0	1.077029	2.459145	3.801313

Zero-point correction= 0.456895 (Hartree/Particle)
Thermal correction to Energy= 0.492369
Thermal correction to Enthalpy= 0.493313
Thermal correction to Gibbs Free Energy= 0.388628
Sum of electronic and zero-point Energies= -1727.915934
Sum of electronic and thermal Energies= -1727.880460
Sum of electronic and thermal Enthalpies= -1727.879516
Sum of electronic and thermal Free Energies= -1727.984201
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1730.89973352

^{3}TS6-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	2.757752	-0.260060	-0.794251
2	6	0	3.022241	-0.568101	2.080923
3	6	0	3.763433	-0.791699	3.370047
4	8	0	3.694215	-0.624604	1.012786
5	8	0	0.367113	-2.029930	0.263939
6	6	0	0.885122	-4.174356	-0.551446
7	6	0	1.205880	-2.712771	-0.415860
8	8	0	2.258782	-2.285141	-0.949159
9	8	0	1.782124	-0.321675	2.194404
10	8	0	1.651921	0.143899	-2.517540
11	8	0	1.125030	2.035697	0.578292
12	8	0	3.075749	1.768919	-0.545151
13	6	0	2.495821	3.919379	0.240489
14	6	0	2.210090	2.453580	0.066400
15	8	0	-0.281742	0.307432	-1.350417
16	6	0	0.411687	0.329030	-2.418353
17	6	0	-0.360413	0.605592	-3.679899
18	45	0	0.678149	0.016658	0.476289
19	1	0	1.510724	-4.637784	-1.315901
20	1	0	1.064269	-4.668333	0.409329
21	1	0	4.733951	-1.253883	3.181068
22	1	0	3.163621	-1.409692	4.042828
23	1	0	-1.118986	-0.171779	-3.820842
24	1	0	0.304497	0.630694	-4.544568
25	1	0	3.198023	4.264262	-0.520926
26	1	0	1.567036	4.493331	0.202297
27	7	0	-1.159101	0.173151	1.458910
28	6	0	-2.005450	1.033206	0.915447
29	6	0	-3.021501	0.567995	-0.053506
30	6	0	-2.029221	2.406634	1.280486
31	6	0	-3.601475	1.594831	-0.905774
32	6	0	-2.807636	3.315540	0.607954
33	1	0	-1.351376	2.710419	2.073677
34	6	0	-3.543432	2.905716	-0.536837
35	1	0	-4.108084	1.298579	-1.820900
36	1	0	-2.791674	4.364090	0.893091
37	1	0	-4.026200	3.656531	-1.158677
38	6	0	-3.162930	-0.812635	-0.417085
39	6	0	-4.452467	-1.261210	-1.051783
40	6	0	-4.511709	-0.119780	0.989048
41	6	0	-5.463214	-0.556793	-0.132515
42	1	0	-4.695482	0.883571	1.389174
43	1	0	-5.845843	0.345674	-0.622653
44	8	0	-2.359766	-1.785009	-0.105487
45	1	0	-1.487311	-1.517710	0.277206
46	1	0	-0.175147	-4.299556	-0.790436
47	1	0	3.918234	0.175031	3.860827
48	1	0	2.947089	4.075130	1.226368
49	1	0	-0.886584	1.560212	-3.579741
50	1	0	-4.523477	-1.010845	-2.117654
51	6	0	-6.637283	-1.408321	0.311118
52	1	0	-7.255409	-1.693251	-0.547818
53	1	0	-7.276923	-0.864220	1.015877
54	1	0	-6.304641	-2.330856	0.802070
55	1	0	-4.505055	-2.352684	-0.964724

56	6	0	-4.188657	-1.090503	2.086588
57	1	0	-4.978916	-1.059246	2.847911
58	1	0	-4.092388	-2.123894	1.736098
59	1	0	-3.246465	-0.811443	2.576994

Zero-point correction= 0.454675 (Hartree/Particle)
Thermal correction to Energy= 0.489939
Thermal correction to Enthalpy= 0.490883
Thermal correction to Gibbs Free Energy= 0.386819
Sum of electronic and zero-point Energies= -1727.860669
Sum of electronic and thermal Energies= -1727.825405
Sum of electronic and thermal Enthalpies= -1727.824461
Sum of electronic and thermal Free Energies= -1727.928525
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1730.84292581

^{1}TS7-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.095472	1.092241	-0.690061
2	6	0	-3.568755	0.780465	-0.832077
3	6	0	-4.516797	1.872906	-0.641482
4	6	0	-4.113404	3.035615	-0.078984
5	6	0	-2.750274	3.258680	0.309840
6	6	0	-1.800817	2.341591	0.010138
7	1	0	-5.539692	1.761693	-0.994621
8	1	0	-4.835430	3.841573	0.039795
9	1	0	-2.482796	4.198934	0.785742
10	1	0	-0.749895	2.525750	0.212269
11	7	0	-1.231674	0.223805	-1.072250
12	45	0	0.659986	0.093779	-0.336965
13	45	0	2.904050	-0.338061	0.600837
14	8	0	1.465945	-0.321347	-2.197329
15	6	0	2.685520	-0.665239	-2.278557
16	8	0	3.516796	-0.769979	-1.336288
17	8	0	2.073505	0.129888	2.458196
18	6	0	0.851923	0.409990	2.549502
19	8	0	-0.000091	0.466989	1.604720
20	8	0	2.317646	-2.314972	0.864592
21	6	0	1.164428	-2.665101	0.501745
22	8	0	0.269084	-1.937033	-0.030215
23	8	0	3.315078	1.670916	0.265586
24	6	0	2.425333	2.410980	-0.225583
25	8	0	1.239965	2.076823	-0.551329
26	6	0	-4.049308	-0.435544	-1.385049
27	6	0	0.311943	0.726079	3.920103
28	1	0	-0.046299	1.760428	3.937889
29	1	0	-0.546317	0.081984	4.135556
30	1	0	1.083012	0.590180	4.680156
31	6	0	0.797602	-4.114570	0.688896
32	1	0	-0.240630	-4.201007	1.022279
33	1	0	0.881363	-4.629770	-0.274010
34	1	0	1.471645	-4.591103	1.403120
35	6	0	2.788922	3.847043	-0.490774
36	1	0	2.977528	3.971356	-1.562448
37	1	0	1.956720	4.504206	-0.225454
38	1	0	3.689062	4.122173	0.061882
39	6	0	3.171365	-0.988510	-3.666543
40	1	0	2.953032	-0.150923	-4.335325
41	1	0	4.241968	-1.200019	-3.661758
42	1	0	2.623601	-1.856894	-4.045929
43	6	0	-3.908505	-0.467370	0.628666
44	6	0	-5.418940	-0.690194	0.471834
45	6	0	-5.446251	-0.906433	-1.049608
46	1	0	-6.234016	-0.379130	-1.601151
47	1	0	-5.932084	0.245503	0.719267
48	1	0	-3.611001	0.323559	1.326740
49	8	0	-3.264235	-1.190094	-2.110715
50	1	0	-3.648114	-2.068555	-2.245354
51	6	0	-6.010094	-1.809097	1.306846
52	1	0	-7.084318	-1.909926	1.115368
53	1	0	-5.880518	-1.610149	2.376689
54	1	0	-5.539413	-2.775268	1.088998
55	6	0	-3.005163	-1.657669	0.754781

56	1	0	-2.879282	-1.904746	1.815900
57	1	0	-2.002412	-1.446473	0.351814
58	1	0	-3.393372	-2.549097	0.246136
59	1	0	-5.541321	-1.972954	-1.301585

Zero-point correction= 0.455924 (Hartree/Particle)
Thermal correction to Energy= 0.491393
Thermal correction to Enthalpy= 0.492337
Thermal correction to Gibbs Free Energy= 0.387829
Sum of electronic and zero-point Energies= -1727.856104
Sum of electronic and thermal Energies= -1727.820635
Sum of electronic and thermal Enthalpies= -1727.819691
Sum of electronic and thermal Free Energies= -1727.924198
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1730.84820639

^{3}TS8-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.532506	-0.114546	-0.134597
2	45	0	-2.888999	0.335510	0.251857
3	8	0	-1.117984	-1.797403	-1.199513
4	6	0	-2.360640	-2.045357	-1.315824
5	8	0	-3.310949	-1.372268	-0.834956
6	8	0	-0.657811	1.057281	-1.835447
7	6	0	-1.779528	1.573674	-2.132491
8	8	0	-2.862064	1.444477	-1.496833
9	8	0	-0.104806	1.590246	0.955223
10	6	0	-1.069636	2.268733	1.431854
11	8	0	-2.298365	2.016939	1.311333
12	8	0	-0.550962	-1.245509	1.599382
13	6	0	-1.633491	-1.337995	2.259970
14	8	0	-2.741383	-0.809308	1.971400
15	7	0	1.486452	-0.422356	-0.387800
16	6	0	2.341035	-1.435304	-0.243230
17	6	0	3.746545	-1.185236	-0.076860
18	6	0	1.869343	-2.780214	-0.269531
19	6	0	4.609377	-2.260536	0.035106
20	6	0	2.762878	-3.824131	-0.154971
21	1	0	0.802040	-2.936573	-0.406827
22	6	0	4.132306	-3.573230	-0.005311
23	1	0	5.670679	-2.060758	0.168021
24	1	0	2.400775	-4.849138	-0.183508
25	1	0	4.829699	-4.402671	0.085864
26	6	0	4.224324	0.235613	0.031281
27	6	0	3.318583	1.301199	-0.607102
28	6	0	3.991321	0.957842	1.383734
29	6	0	3.400039	2.180190	0.641339
30	1	0	2.201579	0.656492	-0.515781
31	1	0	3.259154	0.437106	2.010354
32	1	0	4.915858	1.124237	1.947661
33	1	0	2.422900	2.511801	1.018787
34	8	0	5.588210	0.367686	-0.320690
35	1	0	5.684100	0.071778	-1.234529
36	6	0	3.471399	1.751992	-2.022813
37	1	0	2.716545	2.500608	-2.289062
38	1	0	4.461415	2.202120	-2.192273
39	1	0	3.360692	0.906317	-2.715768
40	6	0	4.352867	3.358114	0.519814
41	1	0	3.973204	4.112177	-0.180754
42	1	0	4.490955	3.844752	1.492921
43	1	0	5.337375	3.027505	0.166759
44	6	0	-2.713761	-3.257822	-2.129687
45	1	0	-2.093430	-4.105948	-1.827682
46	1	0	-3.772023	-3.499222	-2.018273
47	1	0	-2.497764	-3.053527	-3.183445
48	6	0	-1.818381	2.441454	-3.358456
49	1	0	-1.952096	3.483601	-3.050654
50	1	0	-0.895646	2.348250	-3.933442
51	1	0	-2.681986	2.170363	-3.971569
52	6	0	-0.678077	3.488665	2.216930
53	1	0	-0.060311	4.141724	1.592567
54	1	0	-1.562242	4.027069	2.561400
55	1	0	-0.067830	3.186736	3.074037

56	6	0	-1.560209	-2.155525	3.518432
57	1	0	-2.552442	-2.282557	3.954039
58	1	0	-1.111512	-3.128793	3.300787
59	1	0	-0.905994	-1.650202	4.235953

Zero-point correction= 0.450561 (Hartree/Particle)
Thermal correction to Energy= 0.486057
Thermal correction to Enthalpy= 0.487002
Thermal correction to Gibbs Free Energy= 0.381749
Sum of electronic and zero-point Energies= -1727.900538
Sum of electronic and thermal Energies= -1727.865042
Sum of electronic and thermal Enthalpies= -1727.864098
Sum of electronic and thermal Free Energies= -1727.969350
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1730.87832192

[1]TS9-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.462591	0.067877	-0.300365
2	45	0	2.715774	-0.317817	0.570340
3	8	0	1.316104	1.612544	-1.402152
4	6	0	2.576902	1.786523	-1.389624
5	8	0	3.417230	1.140104	-0.710684
6	8	0	0.897667	-1.271755	-1.822262
7	6	0	2.023334	-1.864009	-1.797389
8	8	0	2.937978	-1.719081	-0.940565
9	8	0	-0.158025	-1.488873	0.892527
10	6	0	0.667728	-2.035094	1.696457
11	8	0	1.888326	-1.762030	1.811817
12	8	0	0.158412	1.347311	1.296317
13	6	0	1.134791	1.602025	2.073583
14	8	0	2.296569	1.118268	2.010079
15	7	0	-1.342736	0.377033	-1.129980
16	6	0	-2.120572	1.400083	-0.641286
17	6	0	-3.434986	1.204965	-0.152619
18	6	0	-1.613561	2.716350	-0.725938
19	6	0	-4.210255	2.301245	0.196069
20	6	0	-2.422955	3.790579	-0.395815
21	1	0	-0.601114	2.857506	-1.092665
22	6	0	-3.721553	3.598022	0.069376
23	1	0	-5.208354	2.118954	0.590472
24	1	0	-2.021488	4.797269	-0.491443
25	1	0	-4.339213	4.446841	0.350683
26	6	0	-3.921470	-0.204205	0.028766
27	6	0	-3.181361	-1.246818	-0.815172
28	6	0	-3.483309	-1.000666	1.279555
29	6	0	-3.148270	-2.213687	0.377313
30	1	0	-2.070491	-0.771385	-0.942520
31	1	0	-2.588973	-0.564544	1.740272
32	1	0	-4.272002	-1.134186	2.028483
33	1	0	-2.173155	-2.673889	0.563378
34	8	0	-5.327924	-0.297003	-0.090801
35	1	0	-5.579549	0.135212	-0.916816
36	6	0	-3.594415	-1.579730	-2.212585
37	1	0	-2.971954	-2.370566	-2.644684
38	1	0	-4.638234	-1.923071	-2.224576
39	1	0	-3.516307	-0.694612	-2.857178
40	6	0	-4.239998	-3.271667	0.322711
41	1	0	-4.058189	-3.998890	-0.478139
42	1	0	-4.274720	-3.821347	1.271240
43	1	0	-5.223323	-2.815344	0.161718
44	6	0	3.088700	2.886528	-2.274935
45	1	0	2.744101	3.850323	-1.886476
46	1	0	4.179111	2.876432	-2.307035
47	1	0	2.674529	2.773058	-3.280548
48	6	0	2.284666	-2.815261	-2.931030
49	1	0	3.104413	-3.491086	-2.681488
50	1	0	1.378088	-3.375589	-3.172209
51	1	0	2.561380	-2.236245	-3.818562
52	6	0	0.097562	-3.118783	2.565940
53	1	0	-0.859487	-2.793217	2.985073
54	1	0	-0.095578	-4.005482	1.952279
55	1	0	0.797548	-3.379434	3.361241

56	6	0	0.842370	2.564039	3.189637
57	1	0	1.770065	2.988298	3.578112
58	1	0	0.167148	3.349568	2.841652
59	1	0	0.337660	2.024967	3.998445

Zero-point correction= 0.452415 (Hartree/Particle)
Thermal correction to Energy= 0.487291
Thermal correction to Enthalpy= 0.488236
Thermal correction to Gibbs Free Energy= 0.386884
Sum of electronic and zero-point Energies= -1727.888737
Sum of electronic and thermal Energies= -1727.853860
Sum of electronic and thermal Enthalpies= -1727.852916
Sum of electronic and thermal Free Energies= -1727.954268
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1730.86702639

^{3}INT7-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.593644	0.109878	-0.152047
2	45	0	2.929685	-0.399226	0.280435
3	8	0	1.238239	1.796874	-1.172381
4	6	0	2.488081	2.023948	-1.249225
5	8	0	3.411872	1.324266	-0.755255
6	8	0	0.737990	-1.036675	-1.870600
7	6	0	1.858095	-1.565409	-2.154326
8	8	0	2.928922	-1.464230	-1.495353
9	8	0	0.095209	-1.608960	0.887524
10	6	0	1.034679	-2.320591	1.368546
11	8	0	2.270635	-2.093823	1.281559
12	8	0	0.591199	1.204867	1.603128
13	6	0	1.655967	1.252902	2.296608
14	8	0	2.759264	0.706246	2.024393
15	7	0	-1.456592	0.376735	-0.407418
16	6	0	-2.291787	1.410005	-0.268924
17	6	0	-3.711359	1.248861	-0.072775
18	6	0	-1.745325	2.727309	-0.321490
19	6	0	-4.489056	2.388459	0.048730
20	6	0	-2.558635	3.832387	-0.207587
21	1	0	-0.673352	2.814360	-0.482164
22	6	0	-3.935461	3.669630	-0.021369
23	1	0	-5.554795	2.264935	0.222184
24	1	0	-2.129206	4.829723	-0.263151
25	1	0	-4.580480	4.539716	0.076735
26	6	0	-4.343828	-0.115376	0.078900
27	6	0	-3.811647	-1.287583	-0.712390
28	6	0	-4.013248	-0.930606	1.358410
29	6	0	-3.740752	-2.188724	0.490842
30	1	0	-1.927629	-0.533335	-0.440897
31	1	0	-3.124638	-0.561247	1.881803
32	1	0	-4.858138	-0.991102	2.052781
33	1	0	-2.752732	-2.645390	0.667776
34	8	0	-5.764891	-0.039850	-0.029731
35	1	0	-5.971212	0.213358	-0.938323
36	6	0	-3.911064	-1.558659	-2.161482
37	1	0	-3.216105	-2.347331	-2.475210
38	1	0	-4.923511	-1.894494	-2.448360
39	1	0	-3.685963	-0.657519	-2.749594
40	6	0	-4.826584	-3.256133	0.535413
41	1	0	-4.677257	-4.007818	-0.249814
42	1	0	-4.834639	-3.774918	1.501453
43	1	0	-5.811235	-2.795834	0.384873
44	6	0	2.886862	3.243419	-2.030884
45	1	0	2.262195	4.093834	-1.745166
46	1	0	3.941769	3.472275	-1.870931
47	1	0	2.716076	3.053966	-3.095667
48	6	0	1.893312	-2.420732	-3.389271
49	1	0	1.599037	-3.440920	-3.119747
50	1	0	1.185310	-2.047919	-4.132505
51	1	0	2.905429	-2.453937	-3.797426
52	6	0	0.599909	-3.548105	2.118792
53	1	0	-0.046559	-4.158961	1.481307
54	1	0	1.464865	-4.128770	2.442703
55	1	0	0.007676	-3.248160	2.989143

56	6	0	1.564242	2.032098	3.578048
57	1	0	2.552027	2.156850	4.024449
58	1	0	1.103325	3.005341	3.388652
59	1	0	0.914154	1.494513	4.275885

Zero-point correction= 0.455216 (Hartree/Particle)
Thermal correction to Energy= 0.491505
Thermal correction to Enthalpy= 0.492450
Thermal correction to Gibbs Free Energy= 0.384866
Sum of electronic and zero-point Energies= -1727.912291
Sum of electronic and thermal Energies= -1727.876001
Sum of electronic and thermal Enthalpies= -1727.875057
Sum of electronic and thermal Free Energies= -1727.982641
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -1730.89654986

^{1}INT8-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.075536	1.530092	-0.260997
2	6	0	1.139994	0.856316	-0.174205
3	6	0	0.937030	-0.519819	-0.004960
4	6	0	2.428740	1.373870	-0.254971
5	6	0	2.005476	-1.389718	0.101886
6	6	0	3.500602	0.487187	-0.151024
7	1	0	2.596767	2.441201	-0.385181
8	6	0	3.303790	-0.879787	0.028784
9	1	0	1.825023	-2.453780	0.247862
10	1	0	4.514234	0.879033	-0.205365
11	1	0	4.158823	-1.545545	0.111707
12	6	0	-0.536186	-0.764675	0.049385
13	6	0	-1.164747	0.663265	0.221740
14	6	0	-1.312579	-0.894040	-1.279124
15	6	0	-2.183502	0.327605	-0.898113
16	1	0	-0.092543	2.495057	0.045178
17	1	0	-0.672348	-0.731764	-2.151318
18	1	0	-1.843886	-1.846662	-1.386708
19	1	0	-2.240953	1.110834	-1.664424
20	8	0	-0.957381	-1.755473	0.948686
21	1	0	-0.479119	-1.614106	1.775358
22	6	0	-1.638703	1.067167	1.595819
23	1	0	-2.105619	2.060848	1.583934
24	1	0	-2.370075	0.357082	1.995005
25	1	0	-0.784892	1.103061	2.286800
26	6	0	-3.568284	-0.062042	-0.420303
27	1	0	-4.095160	0.778910	0.047672
28	1	0	-4.177908	-0.412633	-1.261350
29	1	0	-3.514341	-0.880373	0.308828

Zero-point correction= 0.247374 (Hartree/Particle)
Thermal correction to Energy= 0.259397
Thermal correction to Enthalpy= 0.260342
Thermal correction to Gibbs Free Energy= 0.210691
Sum of electronic and zero-point Energies= -595.614598
Sum of electronic and thermal Energies= -595.602574
Sum of electronic and thermal Enthalpies= -595.601630
Sum of electronic and thermal Free Energies= -595.651280
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -596.00294995

^{1}TS4`

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.082032	0.164402	0.078213
2	45	0	-0.675591	-2.166841	-0.329370
3	8	0	1.275894	-0.507395	1.471371
4	6	0	1.395321	-1.752614	1.689350
5	8	0	0.764091	-2.674381	1.104369
6	8	0	-1.505098	0.173564	1.582294
7	6	0	-2.199967	-0.873616	1.781395
8	8	0	-2.082175	-1.973516	1.176571
9	8	0	-1.509853	0.682078	-1.337476
10	6	0	-2.189364	-0.239829	-1.891951

11	8	0	-2.068522	-1.479305	-1.692728
12	8	0	1.271102	0.006044	-1.472071
13	6	0	1.390095	-1.094349	-2.093869
14	8	0	0.763917	-2.160671	-1.848148
15	6	0	2.418700	-2.159724	2.750702
16	6	0	2.409661	-1.120045	-3.233564
17	6	0	3.032636	-0.934581	3.416732
18	1	0	3.768224	-1.255896	4.166450
19	1	0	2.265017	-0.337033	3.919719
20	6	0	3.020872	0.258857	-3.452161
21	1	0	2.249018	0.992871	-3.707686
22	1	0	3.742684	0.212364	-4.278722
23	6	0	3.506367	-2.150372	-2.871021
24	1	0	4.260944	-2.112521	-3.670796
25	1	0	3.054069	-3.150106	-2.898870
26	6	0	1.703091	-1.584890	-4.507728
27	1	0	1.222266	-2.556803	-4.359499
28	1	0	2.429302	-1.672852	-5.326061
29	1	0	0.935357	-0.864846	-4.817383
30	6	0	1.712747	-3.024271	3.796520
31	1	0	2.437753	-3.375653	4.541857
32	1	0	1.237155	-3.894059	3.332489
33	1	0	0.939567	-2.451611	4.323819
34	6	0	3.511221	-3.011445	2.059638
35	1	0	3.053748	-3.958477	1.745414
36	1	0	4.265884	-3.251878	2.823313
37	6	0	-3.254935	-0.767410	2.884336
38	6	0	-3.222162	0.225447	-2.920447
39	6	0	-4.131618	0.485735	2.643730
40	1	0	-4.844038	0.541128	3.480554
41	6	0	-4.116284	1.325076	-2.298980
42	1	0	-4.821716	1.643546	-3.081261
43	1	0	-3.482310	2.189571	-2.063388
44	6	0	-4.868614	0.897299	-1.068903
45	6	0	-6.178214	0.417854	-1.140321
46	6	0	-4.244445	0.947286	0.178631
47	6	0	-6.834295	-0.012243	0.008300
48	1	0	-6.687641	0.390070	-2.103830
49	6	0	-4.874321	0.488366	1.336084
50	1	0	-3.234941	1.349458	0.250285
51	6	0	-6.184099	0.013670	1.237444
52	1	0	-7.859029	-0.372388	-0.055443
53	1	0	-6.698336	-0.330892	2.134862
54	6	0	-2.507436	-0.592618	4.209889
55	1	0	-1.866090	-1.459737	4.412594
56	1	0	-3.226760	-0.507627	5.034491
57	1	0	-1.882120	0.306315	4.196882
58	6	0	-4.110850	-2.026038	2.937907
59	1	0	-4.861381	-1.924548	3.733431
60	1	0	-3.499618	-2.908922	3.150223
61	1	0	-4.630939	-2.200493	1.990757
62	6	0	-2.446052	0.831142	-4.094454
63	1	0	-3.146041	1.178533	-4.865184
64	1	0	-1.786047	0.083660	-4.552946
65	1	0	-1.834619	1.679691	-3.769558
66	6	0	-4.063749	-0.945326	-3.410665
67	1	0	-3.437110	-1.710152	-3.880091
68	1	0	-4.790297	-0.587932	-4.152857
69	1	0	-4.610325	-1.420387	-2.589985
70	1	0	-3.487698	1.372165	2.707319
71	1	0	3.532209	-0.283778	2.690480
72	1	0	3.538098	0.621940	-2.557001
73	6	0	4.155224	-1.935773	-1.532126
74	6	0	3.599983	-2.524837	-0.394684
75	6	0	5.309765	-1.162975	-1.385479
76	6	0	4.160495	-2.357203	0.872688
77	1	0	2.704354	-3.138081	-0.497797
78	6	0	5.885971	-0.989165	-0.130459
79	1	0	5.770465	-0.715048	-2.265947
80	6	0	5.314959	-1.580130	0.993098
81	1	0	6.800403	-0.406486	-0.030540
82	1	0	5.778604	-1.456710	1.971951
83	6	0	1.668774	2.541802	0.541571
84	6	0	1.842723	3.977675	0.849838
85	6	0	3.145898	4.457260	1.151221

86	6	0	4.223362	3.622431	1.052961
87	6	0	4.094788	2.262729	0.633420
88	6	0	2.869949	1.734010	0.390908
89	1	0	3.281730	5.481998	1.488916
90	1	0	5.209249	3.999263	1.318518
91	1	0	4.980888	1.638308	0.537778
92	1	0	2.753701	0.694615	0.102256
93	7	0	0.449449	2.093029	0.446809
94	6	0	0.657091	4.809543	0.825744
95	6	0	1.203183	5.269422	-0.857372
96	6	0	1.421547	6.650323	-0.264793
97	6	0	0.758011	6.312977	1.078495
98	1	0	-0.262383	6.696507	1.157734
99	1	0	1.308330	6.596873	1.982798
100	1	0	0.943281	7.457502	-0.828895
101	1	0	2.484496	6.894665	-0.174224
102	1	0	2.014104	4.776048	-1.396296
103	1	0	0.236781	5.097447	-1.338882
104	8	0	-0.523835	4.259875	0.882308
105	1	0	-0.301664	3.121864	0.680986

Zero-point correction= 0.858415 (Hartree/Particle)
Thermal correction to Energy= 0.910150
Thermal correction to Enthalpy= 0.911095
Thermal correction to Gibbs Free Energy= 0.777671
Sum of electronic and zero-point Energies= -2579.701020
Sum of electronic and thermal Energies= -2579.649285
Sum of electronic and thermal Enthalpies= -2579.648341
Sum of electronic and thermal Free Energies= -2579.781764
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -2583.28470087

^{3}TS2'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.104581	0.136291	-0.208806
2	45	0	-0.730155	-1.979477	0.788802
3	8	0	1.177298	-0.927862	-1.426320
4	6	0	1.261028	-2.188549	-1.316490
5	8	0	0.625986	-2.907113	-0.493240
6	8	0	-1.567288	-0.173324	-1.630082
7	6	0	-2.279951	-1.225335	-1.554525
8	8	0	-2.174568	-2.128328	-0.678423
9	8	0	-1.452653	1.060404	1.057030
10	6	0	-2.125122	0.338081	1.860830
11	8	0	-2.040183	-0.915253	1.977555
12	8	0	1.304530	0.305633	1.291274
13	6	0	1.415416	-0.600796	2.171467
14	8	0	0.743910	-1.670575	2.224267
15	6	0	2.232015	-2.891527	-2.264738
16	6	0	2.474165	-0.382421	3.251802
17	6	0	2.867409	-1.898856	-3.230941
18	1	0	3.559150	-2.430859	-3.897627
19	1	0	2.106505	-1.407050	-3.846017
20	6	0	3.143369	0.977750	3.094021
21	1	0	2.411434	1.787246	3.187414
22	1	0	3.900259	1.105957	3.879274
23	6	0	3.516297	-1.522634	3.143884
24	1	0	4.293840	-1.320213	3.895502
25	1	0	3.023617	-2.459902	3.433552
26	6	0	1.794615	-0.472828	4.619430
27	1	0	1.292628	-1.436656	4.749571
28	1	0	2.543047	-0.356854	5.413578
29	1	0	1.049974	0.323116	4.742256
30	6	0	1.460061	-3.956747	-3.045436
31	1	0	2.148071	-4.510181	-3.696997
32	1	0	0.970277	-4.665844	-2.370744
33	1	0	0.692591	-3.499010	-3.681620
34	6	0	3.312806	-3.592777	-1.407202
35	1	0	2.829076	-4.409656	-0.856097
36	1	0	4.029646	-4.050395	-2.105296
37	6	0	-3.339731	-1.390686	-2.641989
38	6	0	-3.103001	1.078885	2.772712
39	6	0	-4.244206	-0.134016	-2.656915

40	1	0	-4.995012	-0.289473	-3.446069
41	6	0	-4.056182	1.935935	1.905070
42	1	0	-4.747447	2.441351	2.595993
43	1	0	-3.463494	2.717287	1.412383
44	6	0	-4.829724	1.161504	0.873981
45	6	0	-6.101894	0.651813	1.142477
46	6	0	-4.265985	0.920497	-0.379861
47	6	0	-6.782960	-0.085751	0.180007
48	1	0	-6.564178	0.845527	2.110563
49	6	0	-4.922718	0.159128	-1.347572
50	1	0	-3.283574	1.333370	-0.607082
51	6	0	-6.195592	-0.335752	-1.055555
52	1	0	-7.779360	-0.466917	0.393399
53	1	0	-6.731265	-0.913935	-1.808536
54	6	0	-2.613403	-1.489246	-3.986757
55	1	0	-1.960294	-2.370580	-4.013872
56	1	0	-3.346953	-1.592493	-4.796333
57	1	0	-2.004014	-0.600177	-4.178194
58	6	0	-4.162395	-2.651349	-2.408475
59	1	0	-4.911000	-2.750711	-3.205701
60	1	0	-3.526843	-3.542764	-2.419127
61	1	0	-4.681580	-2.624609	-1.445377
62	6	0	-2.282784	2.010292	3.670030
63	1	0	-2.953675	2.580943	4.324488
64	1	0	-1.600997	1.435903	4.309997
65	1	0	-1.690635	2.714983	3.077134
66	6	0	-3.887417	0.096488	3.632767
67	1	0	-3.216359	-0.501572	4.257526
68	1	0	-4.569721	0.652362	4.289584
69	1	0	-4.476055	-0.595378	3.022516
70	1	0	-3.631489	0.725470	-2.957605
71	1	0	3.422772	-1.114169	-2.705574
72	1	0	3.630181	1.084570	2.118366
73	6	0	4.132488	-1.685864	1.782878
74	6	0	3.518132	-2.522163	0.849175
75	6	0	5.302098	-1.018643	1.411662
76	6	0	4.028604	-2.693552	-0.438496
77	1	0	2.613802	-3.059358	1.135831
78	6	0	5.833433	-1.187863	0.136333
79	1	0	5.806630	-0.377055	2.134001
80	6	0	5.199243	-2.014770	-0.786214
81	1	0	6.758575	-0.682419	-0.136077
82	1	0	5.625390	-2.152998	-1.779831
83	6	0	1.878212	2.364614	-1.057572
84	6	0	2.098743	3.751905	-1.381147
85	6	0	3.394461	4.208118	-1.532863
86	6	0	4.486353	3.352065	-1.357237
87	6	0	4.284560	2.010931	-1.012854
88	6	0	3.009646	1.513032	-0.860170
89	1	0	3.575167	5.249066	-1.794624
90	1	0	5.494967	3.736266	-1.489883
91	1	0	5.130920	1.341914	-0.868531
92	1	0	2.836883	0.471706	-0.603245
93	7	0	0.631968	1.908942	-0.955335
94	6	0	0.868987	4.637200	-1.392356
95	6	0	1.036235	5.978939	-2.176819
96	6	0	0.756701	5.484007	-0.083407
97	6	0	1.315827	6.697883	-0.845638
98	1	0	-0.305291	5.594753	0.160835
99	1	0	1.303786	5.132626	0.798082
100	1	0	0.807692	7.654465	-0.693231
101	1	0	2.385796	6.847381	-0.663547
102	8	0	-0.242098	3.942088	-1.774158
103	1	0	1.791928	5.995684	-2.969229
104	1	0	0.065800	6.253624	-2.600436
105	1	0	-0.088299	2.729376	-1.264797

Zero-point correction= 0.857387 (Hartree/Particle)
Thermal correction to Energy= 0.908781
Thermal correction to Enthalpy= 0.909726
Thermal correction to Gibbs Free Energy= 0.776580
Sum of electronic and zero-point Energies= -2579.699365
Sum of electronic and thermal Energies= -2579.647972
Sum of electronic and thermal Enthalpies= -2579.647027
Sum of electronic and thermal Free Energies= -2579.780173

M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -2583.27976058

^{3}TS8`

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.052508	0.016069	-0.429030
2	45	0	-0.595090	-1.554275	1.340791
3	8	0	1.236792	-1.419607	-1.174393
4	6	0	1.341547	-2.540369	-0.587859
5	8	0	0.752830	-2.879598	0.477386
6	8	0	-1.548387	-0.844737	-1.570580
7	6	0	-2.209204	-1.808225	-1.068075
8	8	0	-2.045240	-2.305739	0.079665
9	8	0	-1.393497	1.345123	0.454271
10	6	0	-2.015967	0.974938	1.503061
11	8	0	-1.917032	-0.147953	2.067132
12	8	0	1.383121	0.785400	0.825510
13	6	0	1.541089	0.309608	1.989210
14	8	0	0.901175	-0.656557	2.492080
15	6	0	2.283033	-3.567560	-1.215625
16	6	0	2.627571	0.966168	2.839424
17	6	0	2.817417	-3.082206	-2.557636
18	1	0	3.466375	-3.854796	-2.990917
19	1	0	1.999861	-2.886333	-3.259750
20	6	0	3.212149	2.182819	2.127585
21	1	0	2.438915	2.938067	1.942757
22	1	0	3.989153	2.635864	2.757860
23	6	0	3.722875	-0.094623	3.109437
24	1	0	4.528362	0.408021	3.665430
25	1	0	3.298270	-0.857563	3.774838
26	6	0	2.019375	1.390428	4.176664
27	1	0	1.563513	0.540376	4.693607
28	1	0	2.799444	1.815704	4.820967
29	1	0	1.249359	2.158563	4.033287
30	6	0	1.515739	-4.876559	-1.412101
31	1	0	2.189350	-5.642987	-1.816207
32	1	0	1.099030	-5.239110	-0.467513
33	1	0	0.691692	-4.746346	-2.124458
34	6	0	3.443096	-3.819633	-0.220479
35	1	0	3.034123	-4.358155	0.644214
36	1	0	4.154418	-4.496237	-0.717243
37	6	0	-3.298146	-2.407504	-1.956300
38	6	0	-2.964416	2.000946	2.124614
39	6	0	-4.289894	-1.281423	-2.338517
40	1	0	-5.069406	-1.738917	-2.966183
41	6	0	-4.064434	2.364332	1.096629
42	1	0	-4.768639	3.036874	1.608771
43	1	0	-3.605380	2.946908	0.287701
44	6	0	-4.799379	1.191917	0.510623
45	6	0	-5.991830	0.724604	1.065881
46	6	0	-4.282516	0.538968	-0.609902
47	6	0	-6.642974	-0.373271	0.513434
48	1	0	-6.417740	1.235395	1.929572
49	6	0	-4.912636	-0.574987	-1.166426
50	1	0	-3.356732	0.904896	-1.056579
51	6	0	-6.106217	-1.020707	-0.593619
52	1	0	-7.577895	-0.723507	0.945670
53	1	0	-6.619433	-1.878763	-1.027541
54	6	0	-2.634489	-2.931940	-3.232101
55	1	0	-1.909977	-3.722650	-2.998988
56	1	0	-3.394961	-3.360286	-3.897381
57	1	0	-2.111475	-2.132468	-3.766537
58	6	0	-4.014238	-3.546009	-1.241818
59	1	0	-4.794675	-3.954844	-1.897392
60	1	0	-3.315872	-4.351537	-0.992025
61	1	0	-4.479606	-3.210457	-0.310116
62	6	0	-2.160507	3.262944	2.447794
63	1	0	-2.821567	4.021850	2.885248
64	1	0	-1.369357	3.048498	3.176992
65	1	0	-1.694533	3.683343	1.549560
66	6	0	-3.592811	1.448975	3.398340
67	1	0	-2.826463	1.189006	4.135940
68	1	0	-4.252588	2.208917	3.837641

69	1	0	-4.181839	0.547956	3.200258
70	1	0	-3.753329	-0.555942	-2.963474
71	1	0	3.399346	-2.159727	-2.461577
72	1	0	3.652766	1.922816	1.158533
73	6	0	4.275053	-0.761185	1.880842
74	6	0	3.680461	-1.929799	1.402570
75	6	0	5.373855	-0.243655	1.191629
76	6	0	4.143522	-2.578350	0.256934
77	1	0	2.827098	-2.350519	1.935873
78	6	0	5.857199	-0.883737	0.054424
79	1	0	5.862320	0.658396	1.560444
80	6	0	5.244922	-2.042020	-0.414622
81	1	0	6.730177	-0.486089	-0.460927
82	1	0	5.634341	-2.548944	-1.297533
83	7	0	0.576824	1.461801	-1.789838
84	6	0	1.799480	2.008596	-1.874550
85	6	0	1.958567	3.418554	-2.086939
86	6	0	2.961932	1.195855	-1.738151
87	6	0	3.232079	3.950478	-2.175868
88	6	0	4.216906	1.759870	-1.837311
89	1	0	2.821749	0.130902	-1.569560
90	6	0	4.360148	3.133932	-2.059834
91	1	0	3.335708	5.023717	-2.322056
92	1	0	5.093443	1.124119	-1.729333
93	1	0	5.352468	3.572787	-2.135213
94	6	0	0.728277	4.275955	-2.110878
95	6	0	-0.564557	3.581701	-2.546060
96	6	0	0.032471	4.534001	-0.744086
97	6	0	-1.326772	4.173777	-1.378231
98	1	0	-0.239521	2.340568	-2.190421
99	1	0	-0.908194	3.549646	-3.584885
100	1	0	0.341768	3.808633	0.019036
101	1	0	0.171088	5.553420	-0.372901
102	1	0	-1.956506	3.477342	-0.813004
103	1	0	-1.917326	5.054464	-1.661079
104	8	0	0.935752	5.523318	-2.737228
105	1	0	1.172224	5.355024	-3.657175

Zero-point correction= 0.857287 (Hartree/Particle)
Thermal correction to Energy= 0.908661
Thermal correction to Enthalpy= 0.909605
Thermal correction to Gibbs Free Energy= 0.778233
Sum of electronic and zero-point Energies= -2579.697327
Sum of electronic and thermal Energies= -2579.645953
Sum of electronic and thermal Enthalpies= -2579.645009
Sum of electronic and thermal Free Energies= -2579.776380
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -2583.27777650

^{3}TS17'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.012318	-0.086848	-0.417767
2	45	0	-0.336501	-1.746699	1.329493
3	8	0	1.373120	-1.374217	-1.250531
4	6	0	1.596118	-2.499267	-0.707738
5	8	0	1.067483	-2.930756	0.354877
6	8	0	-1.483420	-1.042764	-1.517909
7	6	0	-2.060936	-2.050812	-1.000487
8	8	0	-1.801770	-2.559741	0.124211
9	8	0	-1.430691	1.097893	0.553126
10	6	0	-1.975919	0.642284	1.610602
11	8	0	-1.730872	-0.468749	2.151916
12	8	0	1.399729	0.766958	0.807574
13	6	0	1.662728	0.270309	1.943062
14	8	0	1.150404	-0.775833	2.432748
15	6	0	2.614614	-3.409854	-1.392631
16	6	0	2.710795	1.012088	2.772905
17	6	0	3.077670	-2.825368	-2.721039
18	1	0	3.796485	-3.511059	-3.189165
19	1	0	2.234912	-2.690575	-3.407208
20	6	0	3.153779	2.290967	2.068864
21	1	0	2.303335	2.958239	1.887708
22	1	0	3.882565	2.820019	2.697416

23	6	0	3.913990	0.061774	2.989793
24	1	0	4.685224	0.634650	3.525823
25	1	0	3.590045	-0.747992	3.656592
26	6	0	2.104420	1.352551	4.134861
27	1	0	1.741765	0.455156	4.645725
28	1	0	2.860742	1.834510	4.767472
29	1	0	1.266332	2.051666	4.026227
30	6	0	1.961351	-4.773033	-1.628191
31	1	0	2.690195	-5.462974	-2.072178
32	1	0	1.595516	-5.203822	-0.691035
33	1	0	1.114899	-4.687218	-2.321191
34	6	0	3.811098	-3.594214	-0.425411
35	1	0	3.463338	-4.182188	0.433777
36	1	0	4.561001	-4.201814	-0.953664
37	6	0	-3.154916	-2.701673	-1.845882
38	6	0	-3.008239	1.545422	2.288007
39	6	0	-4.185926	-1.621864	-2.256392
40	1	0	-4.938736	-2.120839	-2.884983
41	6	0	-4.082758	1.966289	1.257066
42	1	0	-4.802696	2.604367	1.791077
43	1	0	-3.603015	2.597825	0.497569
44	6	0	-4.803121	0.820520	0.600576
45	6	0	-6.017550	0.347055	1.101965
46	6	0	-4.249371	0.183352	-0.511474
47	6	0	-6.648199	-0.742707	0.511648
48	1	0	-6.473883	0.842973	1.958894
49	6	0	-4.855784	-0.926388	-1.103071
50	1	0	-3.309185	0.551509	-0.921483
51	6	0	-6.068375	-1.380324	-0.579693
52	1	0	-7.598187	-1.098077	0.905205
53	1	0	-6.563063	-2.236374	-1.038784
54	6	0	-2.488803	-3.251752	-3.110742
55	1	0	-1.733776	-4.006842	-2.856474
56	1	0	-3.241159	-3.731565	-3.749466
57	1	0	-2.000889	-2.454322	-3.680879
58	6	0	-3.830497	-3.833937	-1.083583
59	1	0	-4.616276	-4.276721	-1.710057
60	1	0	-3.111017	-4.617645	-0.825890
61	1	0	-4.285306	-3.479102	-0.153425
62	6	0	-2.277059	2.798560	2.777240
63	1	0	-2.994740	3.498997	3.223477
64	1	0	-1.537350	2.544197	3.546151
65	1	0	-1.760204	3.306875	1.955426
66	6	0	-3.653574	0.834301	3.470915
67	1	0	-2.902600	0.544854	4.212448
68	1	0	-4.374673	1.508684	3.951802
69	1	0	-4.180426	-0.072494	3.157458
70	1	0	-3.673993	-0.884454	-2.888018
71	1	0	3.561742	-1.851788	-2.594787
72	1	0	3.612890	2.085088	1.095904
73	6	0	4.481471	-0.530015	1.730321
74	6	0	3.961467	-1.730838	1.244522
75	6	0	5.510793	0.087408	1.016994
76	6	0	4.427828	-2.314093	0.065908
77	1	0	3.165805	-2.224617	1.803155
78	6	0	5.999108	-0.486957	-0.153180
79	1	0	5.940153	1.017507	1.390366
80	6	0	5.460173	-1.678511	-0.628546
81	1	0	6.818134	-0.010455	-0.689599
82	1	0	5.855261	-2.133415	-1.536751
83	7	0	0.418600	1.446410	-1.747911
84	6	0	1.561627	2.150912	-1.784654
85	6	0	1.526463	3.577990	-1.894949
86	6	0	2.818313	1.488929	-1.690994
87	6	0	2.717782	4.280991	-1.915777
88	6	0	3.987323	2.220925	-1.728836
89	1	0	2.817043	0.405300	-1.595879
90	6	0	3.944232	3.615274	-1.840448
91	1	0	2.677095	5.366272	-1.982742
92	1	0	4.941559	1.702913	-1.652529
93	1	0	4.868816	4.187734	-1.859898
94	6	0	0.188539	4.275814	-1.880932
95	6	0	-0.921169	3.442258	-2.507962
96	8	0	0.263831	5.564472	-2.476838
97	1	0	0.504178	5.445091	-3.403114

98	6	0	-2.219528	3.723456	-1.778434
99	1	0	-3.011689	4.076639	-2.448683
100	1	0	-2.591170	2.796585	-1.311783
101	6	0	-0.356878	4.493735	-0.463009
102	1	0	-0.216902	3.564637	0.111623
103	1	0	0.179135	5.307071	0.039200
104	6	0	-1.842941	4.748896	-0.696593
105	1	0	-2.445581	4.647879	0.213954
106	1	0	-1.981790	5.766790	-1.078894
107	1	0	-0.925742	3.389610	-3.602214
108	1	0	-0.490785	2.256648	-2.146965

Zero-point correction= 0.886828 (Hartree/Particle)
Thermal correction to Energy= 0.939156
Thermal correction to Enthalpy= 0.940100
Thermal correction to Gibbs Free Energy= 0.807457
Sum of electronic and zero-point Energies= -2618.983830
Sum of electronic and thermal Energies= -2618.931502
Sum of electronic and thermal Enthalpies= -2618.930558
Sum of electronic and thermal Free Energies= -2619.063201
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -2622.60301863

^{1}TS13`

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.277430	0.151259	-0.390014
2	45	0	-1.000664	-1.552187	1.175420
3	8	0	-1.606783	1.446381	0.546536
4	6	0	-2.302104	1.023884	1.526957
5	8	0	-2.277249	-0.139715	2.004253
6	8	0	1.142628	0.706358	1.036675
7	6	0	1.213651	0.057958	2.131707
8	8	0	0.489344	-0.917991	2.459377
9	8	0	0.977010	-1.245332	-1.225923
10	6	0	0.990692	-2.427876	-0.756301
11	8	0	0.311582	-2.844570	0.220679
12	8	0	-1.752880	-0.523593	-1.669857
13	6	0	-2.519338	-1.468295	-1.292882
14	8	0	-2.459679	-2.073035	-0.188567
15	7	0	0.701838	1.454204	-1.652533
16	6	0	0.973073	2.734092	-1.532865
17	6	0	2.251062	3.256920	-2.008948
18	6	0	0.024817	3.626852	-0.914008
19	6	0	2.453977	4.649727	-1.922947
20	6	0	0.276974	4.961047	-0.863445
21	1	0	-0.889247	3.186105	-0.521945
22	6	0	1.496603	5.475205	-1.388818
23	1	0	3.393676	5.072984	-2.271954
24	1	0	-0.447634	5.643829	-0.426867
25	1	0	1.675547	6.547828	-1.355223
26	6	0	3.331935	2.291814	-2.308728
27	6	0	4.605815	2.769746	-3.067477
28	6	0	5.817206	2.531752	-2.146781
29	1	0	6.656416	2.062064	-2.670018
30	1	0	6.181749	3.492436	-1.755015
31	6	0	3.935453	2.301820	-0.707669
32	6	0	5.288864	1.690079	-0.989899
33	1	0	5.931020	1.720675	-0.099118
34	1	0	5.156684	0.642937	-1.286323
35	1	0	4.644370	2.146152	-3.964617
36	1	0	4.540686	3.812007	-3.399748
37	1	0	4.032938	3.318812	-0.307712
38	1	0	3.222041	1.718576	-0.116974
39	6	0	2.276964	0.519634	3.129933
40	6	0	1.932326	-3.395829	-1.470524
41	6	0	-3.596147	-1.894658	-2.291111
42	1	0	1.488709	0.970586	-2.162903
43	8	0	3.023934	1.050621	-2.588971
44	6	0	2.060445	2.007381	3.415095
45	1	0	2.839085	2.371435	4.097503
46	1	0	2.098392	2.599469	2.493265
47	1	0	1.088806	2.179494	3.894707
48	6	0	3.683358	0.337697	2.506197

49	1	0	4.409900	0.562291	3.301475
50	1	0	3.823386	1.103462	1.732902
51	6	0	2.172182	-0.280207	4.423404
52	1	0	1.183080	-0.169185	4.879767
53	1	0	2.338381	-1.347955	4.249386
54	1	0	2.925411	0.080587	5.136310
55	6	0	3.374680	-2.837267	-1.363081
56	1	0	4.037869	-3.571363	-1.844818
57	1	0	3.428158	-1.909830	-1.949805
58	6	0	1.543087	-3.439558	-2.950578
59	1	0	2.219911	-4.115166	-3.488980
60	1	0	0.521447	-3.818201	-3.079513
61	1	0	1.605422	-2.446855	-3.407500
62	6	0	1.832043	-4.790932	-0.868096
63	1	0	2.516035	-5.467078	-1.398078
64	1	0	2.088398	-4.796783	0.195720
65	1	0	0.815005	-5.185914	-0.964530
66	6	0	3.961426	-1.020780	1.925707
67	6	0	3.606077	-1.308121	0.605910
68	6	0	4.574840	-2.020334	2.683728
69	6	0	3.828615	-2.565758	0.042931
70	1	0	3.142815	-0.540070	-0.015850
71	6	0	4.821157	-3.272915	2.132210
72	1	0	4.874184	-1.806260	3.709833
73	6	0	4.449584	-3.545773	0.820469
74	1	0	5.312433	-4.039996	2.727038
75	1	0	4.649169	-4.526044	0.387728
76	6	0	-2.894162	-2.396369	-3.555689
77	1	0	-3.643024	-2.677799	-4.306916
78	1	0	-2.241366	-1.628530	-3.983273
79	1	0	-2.288265	-3.284769	-3.338928
80	6	0	-4.460377	-3.005441	-1.707277
81	1	0	-4.968365	-2.685307	-0.792332
82	1	0	-5.218898	-3.302242	-2.443807
83	1	0	-3.856222	-3.884397	-1.460434
84	6	0	-4.145414	2.659274	1.081429
85	6	0	-4.459891	-0.664193	-2.660635
86	1	0	-5.226349	-1.015119	-3.367698
87	1	0	-3.825854	0.049538	-3.202129
88	6	0	-5.110365	0.023958	-1.492869
89	6	0	-4.414508	1.014125	-0.798165
90	6	0	-6.397811	-0.309469	-1.067046
91	6	0	-4.956972	1.647047	0.321481
92	1	0	-3.417206	1.293960	-1.136995
93	6	0	-6.964417	0.328405	0.031233
94	1	0	-6.961960	-1.067522	-1.610223
95	6	0	-6.247493	1.297622	0.724527
96	1	0	-7.973191	0.070888	0.346803
97	1	0	-6.694836	1.797339	1.583873
98	6	0	-3.226369	2.055970	2.171611
99	6	0	-2.344816	3.168691	2.746290
100	1	0	-2.973519	3.960126	3.173763
101	1	0	-1.702041	2.782764	3.547239
102	1	0	-1.702160	3.609427	1.974724
103	6	0	-4.050273	1.423694	3.285711
104	1	0	-3.403146	1.005246	4.063226
105	1	0	-4.694102	2.186378	3.743789
106	1	0	-4.682975	0.613426	2.909862
107	1	0	-3.521248	3.233850	0.383553
108	1	0	-4.810122	3.377359	1.584475

Zero-point correction= 0.891850 (Hartree/Particle)
Thermal correction to Energy= 0.944045
Thermal correction to Enthalpy= 0.944989
Thermal correction to Gibbs Free Energy= 0.811852
Sum of electronic and zero-point Energies= -2618.971040
Sum of electronic and thermal Energies= -2618.918845
Sum of electronic and thermal Enthalpies= -2618.917901
Sum of electronic and thermal Free Energies= -2619.051037
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d,p)-LANL2DZ energy= -2622.59688135