Supporting Information

Computational Insights into the Zeolite-Supported Gold Nanocluster-Catalyzed Ethanol Dehydrogenation to Acetaldehyde

Yi Zhang,[a] Kangjian Tang,[a,b] and Xiaoguang Bao*[a,b]*

[a] *Innovation Center for Chemical Sciences, College of Chemistry, Chemical Engineering and Materials Science, Soochow University, 199 Ren-Ai Road, Suzhou Industrial Park, Suzhou, Jiangsu 215123, China.*

[b] *Jiangsu Key Laboratory of Advanced Negative Carbon Technologies, Soochow University, Suzhou, Jiangsu 215123, China.*

E-mail: kjtang@suda.edu.cn; xgbao@suda.edu.cn

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1. Zeolite model

The 34T cluster model shown in Fig. 1 was chosen because it exhibits intersecting straight and sinusoidal channels, which well represents the microstructure of zeolites. The initial structure was constructed from the periodic framework of Silicalite-1 zeolite (using X-ray crystal structure) and then trimmed to obtain an appropriate cluster size. The dangling Si bonds resulting from cutting the cluster were saturated with H atoms, with a bond length of 1.42 Å (corresponding to the Si-H distance in silane) oriented towards the crystal Si-O bonds. This model provides a reasonable-sized cluster to capture the spatial environment provided by the 10-ring windows in Silicalite-1, which has been used in previous studies as well.

2. Energy calculation

(a) Adsorption energy is calculated by the following equation:

$$E_{ads} = E_{sub+cat} - E_{sub} - E_{cat} \qquad (\text{eq. } 1)$$

where $E_{sub+cat}$ is the total energy of substrate adsorbed on the catalyst, E_{sub} is the energy of substrate, and E_{cat} is the energy of the catalyst.

(b) Binding energy (BE) is calculated by the following equation:

$$BE = E[Au_3\text{-}S1] - E[S1] - E[Au_3] \qquad (\text{eq. } 2)$$

where $E[Au_3\text{-}S1]$ is the total energy of the Au_3 cluster anchored at the channel of S1 zeolite, E[S1] is the energy of the S1 zeolite, and $E[Au_3]$ is the energy of the Au_3 cluster.

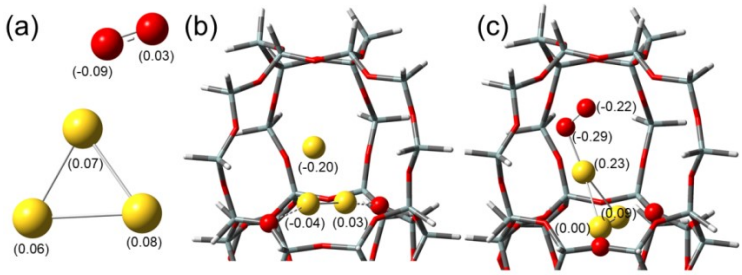

Fig. S1 (a) Optimized structures and NBO charge analysis for O_2 adsorption on the Au_3 cluster; (b) structure of the Au_3-S1 model; (c) structure of O_2 adsorption on the Au_3-S1 model.

Substantial charge transfer is found when O_2 is adsorbed on the gold cluster moiety of the Au_3-S1 model. Thus, it is reasonable to propose that the Au_3 cluster moiety of Au_3-S1 model might undergo single electron oxidation in the presence of O_2 to form the Au_3^+-S1 model.

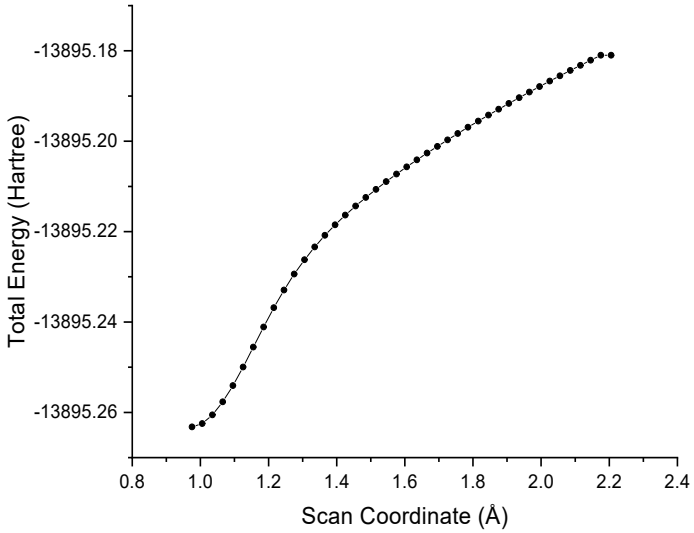

Fig. S2 The energy profile for the lengthening of the H-O bond of the ethanol adsorbed at the Au_3^+-S1 catalyst model, indicating the absence of a transition state for O–H bond breaking of ethanol and H-shift toward to the nearest O atom of the framework of S1. Nevertheless, this route can be excluded due to the significantly endergonic feature of O–H bond breaking of ethanol.

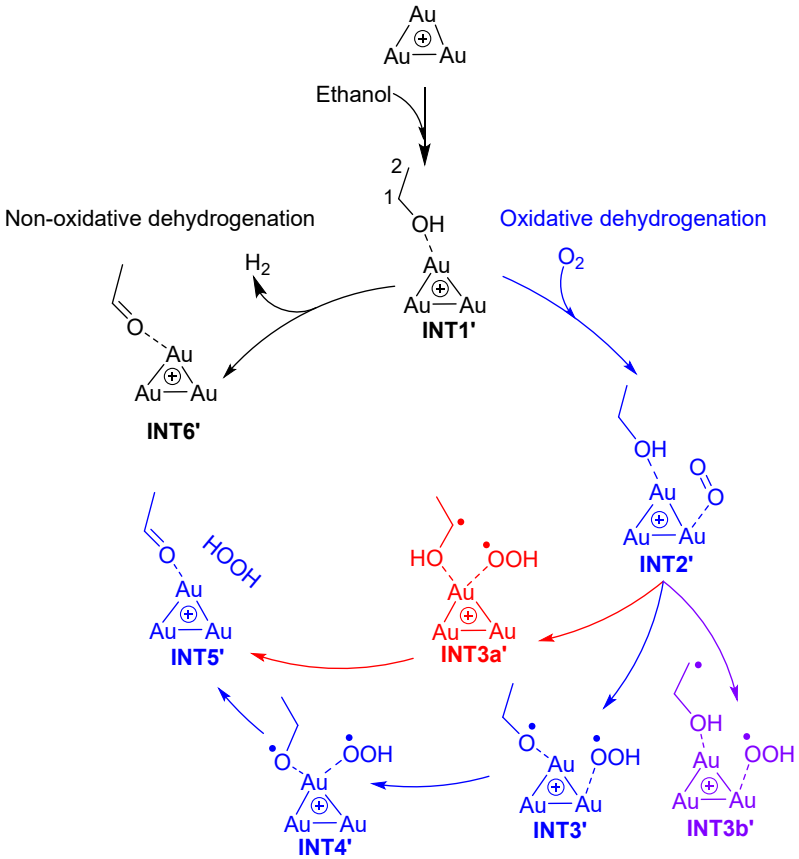

Fig. S3 Dehydrogenation pathways of ethanol under aerobic and anaerobic conditions catalyzed by Au_3 cluster cation.

4. Cartesian Coordinates and Energies

Fig. 1 (a)

Charge: 0 multiplicity: 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.352983	-4.937574	1.335054
2	14	0	-6.554976	-2.979526	2.355149
3	14	0	-4.433520	-4.634368	-1.774582
4	14	0	-6.576236	-2.547187	-2.410161
5	8	0	-5.190672	-3.639054	1.791522
6	8	0	-6.763432	-1.653045	1.425734
7	8	0	-4.457787	-5.252849	-0.262689
8	8	0	-5.194233	-3.210160	-1.864287
9	8	0	-6.436539	-0.964271	-2.040565
10	14	0	1.743342	-1.788289	3.668497
11	14	0	4.815037	-1.661151	3.650688
12	14	0	5.721682	-3.206971	-1.824068
13	14	0	3.394854	-5.047050	-2.793286
14	14	0	-1.441192	-4.813173	-2.674191
15	14	0	1.716100	-0.818621	-3.886555
16	14	0	4.835425	-1.041604	-3.839348
17	14	0	5.708934	-3.514227	1.323369
18	14	0	3.445481	-5.472455	1.978991
19	14	0	-1.354704	-5.123645	2.077009
20	14	0	1.214015	-3.539440	1.112457
21	8	0	3.281227	-1.691656	4.211791
22	8	0	4.845191	-4.506568	-2.268154
23	8	0	-0.384497	-3.666455	-2.202694
24	8	0	2.202310	-3.974564	-2.512127
25	8	0	5.096933	-1.829158	-2.437694
26	8	0	1.208993	-1.533843	-2.523251
27	8	0	-2.927651	-4.310655	-2.264161
28	8	0	5.705446	-3.014633	-0.215559
29	8	0	1.253460	-2.780342	-0.304335
30	8	0	3.313142	-0.448953	-3.869717
31	8	0	4.926144	-4.938581	1.512337
32	8	0	-0.277153	-4.091828	1.413555
33	8	0	2.239963	-4.803170	1.088281
34	8	0	4.937291	-2.359601	2.184890
35	8	0	1.725665	-2.472771	2.207001
36	8	0	-2.840796	-4.548123	1.769411
37	14	0	-7.271698	-0.118155	1.537989
38	14	0	-7.279360	0.314438	-1.500225
39	8	0	-7.139803	0.599421	0.093081
40	14	0	-0.979793	3.283478	4.138705
41	14	0	1.104791	1.061373	4.427724
42	14	0	5.857973	1.100311	4.475922
43	14	0	-4.262442	4.238114	-4.101135
44	14	0	3.553810	3.087829	4.003915
45	14	0	-6.685313	2.263817	-3.715517
46	14	0	2.860228	5.542080	-1.180452
47	14	0	-0.200314	5.570349	-1.114643
48	14	0	-1.267072	4.080706	-3.574116
49	14	0	1.011399	2.125323	-4.321609
50	14	0	5.949823	1.774494	-4.374523
51	14	0	-4.012775	3.414774	4.734541
52	14	0	3.635237	3.680953	-3.499495

53	14	0	-6.387066	1.640482	3.926958
54	14	0	2.888874	5.147979	1.978634
55	14	0	-0.194037	5.253149	1.996525
56	8	0	-0.193010	1.885851	3.931815
57	8	0	1.086282	-0.308316	3.552687
58	8	0	5.316818	-0.115930	3.515783
59	8	0	5.012281	2.480645	4.324014
60	8	0	-5.258949	2.961636	-4.006245
61	8	0	2.462580	1.896335	4.125162
62	8	0	1.318269	5.625932	-1.729820
63	8	0	-1.034423	4.060305	2.707692
64	8	0	3.541345	3.746604	2.509109
65	8	0	-6.686598	1.644741	-2.204136
66	8	0	-2.813134	3.645089	-3.674443
67	8	0	2.896181	5.037123	0.361256
68	8	0	-0.181643	4.976735	0.397717
69	8	0	-0.406393	2.749819	-3.873355
70	8	0	0.878434	0.557024	-3.956872
71	8	0	5.901939	0.184800	-3.968025
72	8	0	4.881877	2.639009	-3.487313
73	8	0	-5.050790	2.558514	3.822907
74	8	0	2.219755	2.872330	-3.519274
75	8	0	1.352265	5.302585	2.553156
76	8	0	-1.089481	4.590206	-2.038577
77	8	0	3.740559	4.545411	-2.116956
78	8	0	-6.369218	0.701271	2.600181
79	8	0	-2.491127	2.879091	4.537868
80	1	0	-7.673765	-3.873147	2.118214
81	1	0	-7.674984	-3.224426	-1.719075
82	1	0	-8.639298	-0.171478	1.992051
83	1	0	-8.671378	0.052712	-1.837519
84	1	0	-7.597689	2.441465	4.077600
85	1	0	-7.668628	3.311144	-3.679883
86	1	0	-4.626610	5.398035	-3.205477
87	1	0	-4.247434	4.781653	4.353861
88	1	0	-0.879624	6.481875	2.338733
89	1	0	-0.806344	6.890694	-1.109628
90	1	0	-4.885267	-6.109386	2.008142
91	1	0	-5.093075	-5.609691	-2.625319
92	1	0	-1.299340	-6.462071	1.476858
93	1	0	-1.208258	-6.105092	-2.036529
94	1	0	3.372687	-6.855939	1.595229
95	1	0	3.145719	-6.290831	-2.096255
96	1	0	7.078899	-3.750444	1.738171
97	1	0	7.061516	-3.480177	-2.301007
98	1	0	7.127477	1.529499	4.013936
99	1	0	7.274876	2.260820	-4.069323
100	1	0	3.637014	6.313198	2.466628
101	1	0	3.406387	6.869437	-1.220109
102	1	0	-6.361490	0.822691	5.108796
103	1	0	-6.429956	-2.721638	3.804447
104	1	0	-4.202311	3.283335	6.152130
105	1	0	-0.341718	4.122289	5.179732
106	1	0	3.359011	4.122405	4.983403
107	1	0	1.027713	0.817320	5.865763
108	1	0	5.876436	0.680589	5.875643
109	1	0	5.596321	-2.417790	4.608432
110	1	0	-1.163775	-5.145011	3.526584
111	1	0	3.259939	-5.221815	3.436717
112	1	0	0.996170	-2.591096	4.596006

113	1	0	3.438715	-5.227408	-4.235663
114	1	0	-1.396181	-4.989702	-4.113833
115	1	0	5.022796	-1.955694	-4.957515
116	1	0	1.407113	-1.660270	-5.030880
117	1	0	-6.766887	-2.698474	-3.866899
118	1	0	5.667302	1.934785	-5.807111
119	1	0	3.727597	4.574888	-4.664434
120	1	0	-0.883151	5.108029	-4.556386
121	1	0	-4.170046	4.511778	-5.530537
122	1	0	-6.942906	1.246017	-4.749004
123	1	0	1.210035	2.220277	-5.754077
124	14	0	1.059351	-3.009138	-1.889955

Zero-point correction= 0.308019 (Hartree/Particle)
Thermal correction to Energy= 0.379304
Thermal correction to Enthalpy= 0.380249
Thermal correction to Gibbs Free Energy= 0.219642
Sum of electronic and zero-point Energies= -13333.718995
Sum of electronic and thermal Energies= -13333.647710
Sum of electronic and thermal Enthalpies= -13333.646766
Sum of electronic and thermal Free Energies= -13333.807372

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -13335.706188

Fig. 1 (b)

Charge: 0 multiplicity: 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.122343	5.037056	1.419625
2	14	0	6.348859	3.060065	2.346234
3	14	0	4.161857	4.828792	-1.695018
4	14	0	6.304782	2.772863	-2.427241
5	8	0	4.976302	3.733240	1.821688
6	8	0	6.560693	1.771621	1.365932
7	8	0	4.197221	5.411352	-0.169063
8	8	0	4.929164	3.414792	-1.840865
9	8	0	6.179926	1.178424	-2.109434
10	14	0	-1.922294	1.788564	3.737457
11	14	0	-4.991156	1.643488	3.763972
12	14	0	-5.990374	3.356355	-1.640476
13	14	0	-3.691562	5.227625	-2.595969
14	14	0	1.162548	5.025621	-2.550921
15	14	0	-1.999002	1.046060	-3.843894
16	14	0	-5.125134	1.259539	-3.733850
17	14	0	-5.929560	3.563610	1.512266
18	14	0	-3.671070	5.512140	2.192372
19	14	0	1.135398	5.183349	2.208426
20	14	0	-1.443507	3.622303	1.233188
21	8	0	-3.451292	1.667815	4.307307
22	8	0	-5.132832	4.679295	-2.056954
23	8	0	0.087694	3.877796	-2.113227
24	8	0	-2.519042	4.101807	-2.411847
25	8	0	-5.366732	2.001594	-2.306415
26	8	0	-1.427711	1.692582	-2.444139
27	8	0	2.649231	4.507410	-2.177541
28	8	0	-5.945876	3.110217	-0.041902
29	8	0	-1.530980	2.921991	-0.217201

30	8	0	-3.591346	0.688455	-3.786939
31	8	0	-5.158638	4.989962	1.731478
32	8	0	0.046287	4.179495	1.516021
33	8	0	-2.480354	4.878936	1.257917
34	8	0	-5.135360	2.387869	2.322025
35	8	0	-1.937518	2.519143	2.297526
36	8	0	2.619211	4.628018	1.867377
37	14	0	7.068112	0.234409	1.429025
38	14	0	7.033751	-0.111301	-1.614601
39	8	0	6.926010	-0.450442	-0.030038
40	14	0	0.831107	-3.278099	4.021861
41	14	0	-1.260079	-1.074832	4.404668
42	14	0	-6.010555	-1.145969	4.516208
43	14	0	4.004134	-3.964333	-4.294086
44	14	0	-3.702133	-3.108949	3.949596
45	14	0	6.419780	-1.989818	-3.880516
46	14	0	-3.072008	-5.397463	-1.316990
47	14	0	-0.015368	-5.415649	-1.304994
48	14	0	1.018838	-3.841192	-3.719560
49	14	0	-1.285928	-1.886492	-4.375425
50	14	0	-6.226637	-1.552007	-4.346701
51	14	0	3.886763	-3.416886	4.561978
52	14	0	-3.893884	-3.471972	-3.561577
53	14	0	6.230182	-1.598884	3.775025
54	14	0	-3.064785	-5.101573	1.853925
55	14	0	0.006626	-5.198195	1.826358
56	8	0	0.055472	-1.868895	3.899640
57	8	0	-1.266514	0.314743	3.569169
58	8	0	-5.489211	0.100587	3.584134
59	8	0	-5.154969	-2.513938	4.313751
60	8	0	4.994463	-2.686306	-4.182195
61	8	0	-2.600366	-1.929939	4.083918
62	8	0	-1.541336	-5.455714	-1.902925
63	8	0	0.824644	-3.964575	2.526141
64	8	0	-3.716378	-3.721429	2.433979
65	8	0	6.439869	-1.425366	-2.349353
66	8	0	2.557487	-3.389818	-3.831247
67	8	0	-3.079398	-4.945197	0.241553
68	8	0	-0.023191	-4.892860	0.236283
69	8	0	0.140604	-2.509970	-3.969788
70	8	0	-1.157277	-0.318928	-3.979554
71	8	0	-6.177203	0.025922	-3.891514
72	8	0	-5.145325	-2.436822	-3.498219
73	8	0	4.899795	-2.527854	3.660186
74	8	0	-2.487021	-2.647428	-3.579140
75	8	0	-1.521895	-5.280553	2.417014
76	8	0	0.866713	-4.406005	-2.199635
77	8	0	-3.977094	-4.377951	-2.204771
78	8	0	6.185529	-0.616286	2.484249
79	8	0	2.353037	-2.907469	4.388446
80	1	0	7.459788	3.968291	2.123425
81	1	0	7.409485	3.437973	-1.731749
82	1	0	8.442003	0.277574	1.869595
83	1	0	8.420547	0.171438	-1.965151
84	1	0	7.443377	-2.403908	3.888081
85	1	0	7.407947	-3.034200	-3.892758
86	1	0	4.383523	-5.151256	-3.440036
87	1	0	4.109195	-4.769731	4.139326
88	1	0	0.721709	-6.425535	2.120313
89	1	0	0.600934	-6.728281	-1.337575

90	1	0	4.658860	6.191582	2.121722
91	1	0	4.802880	5.835869	-2.527325
92	1	0	1.063928	6.540853	1.652193
93	1	0	0.924571	6.291642	-1.869032
94	1	0	-3.607850	6.905455	1.848591
95	1	0	-3.430795	6.455342	-1.861324
96	1	0	-7.295992	3.776838	1.948018
97	1	0	-7.334924	3.631029	-2.097417
98	1	0	-7.285570	-1.570779	4.060373
99	1	0	-7.544714	-2.053968	-4.038711
100	1	0	-3.793969	-6.285532	2.317326
101	1	0	-3.612478	-6.726818	-1.387616
102	1	0	6.213919	-0.824385	4.986042
103	1	0	6.245967	2.758698	3.790742
104	1	0	4.082223	-3.327706	5.983382
105	1	0	0.212402	-4.157358	5.040128
106	1	0	-3.490689	-4.171727	4.896182
107	1	0	-1.163677	-0.882543	5.846992
108	1	0	-6.012375	-0.772717	5.929537
109	1	0	-5.765965	2.364671	4.754653
110	1	0	0.964255	5.160708	3.662052
111	1	0	-3.460623	5.216098	3.637057
112	1	0	-1.167380	2.563327	4.682596
113	1	0	-3.748855	5.456781	-4.028252
114	1	0	1.088364	5.241703	-3.982110
115	1	0	-5.326770	2.200202	-4.828212
116	1	0	-1.710776	1.926563	-4.961435
117	1	0	6.473354	2.973260	-3.881632
118	1	0	-5.963726	-1.665844	-5.788116
119	1	0	-3.994752	-4.329250	-4.754942
120	1	0	0.619776	-4.840283	-4.728429
121	1	0	3.889382	-4.196431	-5.729985
122	1	0	6.656680	-0.941166	-4.887344
123	1	0	-1.504825	-1.928538	-5.806790
124	14	0	-1.332170	3.191044	-1.791519
125	79	0	-0.313568	-0.035851	-0.927190
126	79	0	0.603180	-1.816500	0.715369
127	79	0	2.237165	0.492575	0.277000

Zero-point correction= 0.308999 (Hartree/Particle)
Thermal correction to Energy= 0.387925
Thermal correction to Enthalpy= 0.388869
Thermal correction to Gibbs Free Energy= 0.201663
Sum of electronic and zero-point Energies= -13739.989811
Sum of electronic and thermal Energies= -13739.910884
Sum of electronic and thermal Enthalpies= -13739.909940
Sum of electronic and thermal Free Energies= -13740.097146

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -13743.2401912

Fig. 1 (c)

Charge: 0 multiplicity: 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.385928	-4.127716	1.065141
2	14	0	6.498277	-2.154361	-0.138825
3	14	0	3.884606	-3.061390	3.946289

4	14	0	5.634255	-0.575860	4.294452
5	8	0	5.154315	-2.845576	0.450484
6	8	0	6.358063	-0.615616	0.413420
7	8	0	4.238598	-4.043189	2.689484
8	8	0	4.459697	-1.560758	3.741819
9	8	0	5.380897	0.827284	3.498975
10	14	0	-1.514438	-2.615261	-2.864941
11	14	0	-4.540821	-2.955376	-3.318717
12	14	0	-6.211463	-3.246970	2.185931
13	14	0	-3.899607	-4.411548	3.925791
14	14	0	0.823455	-3.468984	4.429017
15	14	0	-2.929474	0.164915	4.082375
16	14	0	-5.944824	-0.544832	3.657226
17	14	0	-5.611876	-4.310627	-0.732468
18	14	0	-3.070645	-5.993184	-0.520125
19	14	0	1.610808	-4.940796	-0.033149
20	14	0	-1.255479	-3.583142	0.114954
21	8	0	-2.935631	-2.841236	-3.634764
22	8	0	-5.289243	-4.250372	3.078980
23	8	0	-0.259568	-2.650796	3.527454
24	8	0	-2.809152	-3.266748	3.536369
25	8	0	-5.861755	-1.681045	2.491507
26	8	0	-2.116089	-0.772203	3.039472
27	8	0	2.291086	-2.849202	4.119220
28	8	0	-5.929391	-3.451754	0.601820
29	8	0	-1.629084	-2.506696	1.248480
30	8	0	-4.531009	0.270616	3.743762
31	8	0	-4.665441	-5.610802	-0.431211
32	8	0	0.306780	-3.981543	0.188684
33	8	0	-2.147023	-4.929920	0.320920
34	8	0	-4.824068	-3.300206	-1.753139
35	8	0	-1.678104	-2.897111	-1.288250
36	8	0	2.941220	-4.087817	0.339321
37	14	0	6.732873	0.907003	-0.020774
38	14	0	6.158191	2.054387	2.769916
39	8	0	6.272818	1.918021	1.155817
40	14	0	0.655190	2.560899	-4.283258
41	14	0	-1.103745	0.036069	-4.276259
42	14	0	-5.731897	-0.680087	-4.986964
43	14	0	2.310121	5.978871	3.781430
44	14	0	-3.797434	1.689737	-4.742368
45	14	0	4.968868	4.368877	4.279330
46	14	0	-4.291890	5.413469	-0.348350
47	14	0	-1.291040	5.898219	0.012347
48	14	0	-0.507400	5.236268	2.901298
49	14	0	-2.646755	3.196241	3.812598
50	14	0	-7.446830	2.107575	3.263550
51	14	0	3.707101	2.992868	-4.460510
52	14	0	-5.245607	4.076995	2.247396
53	14	0	6.085957	1.863748	-2.892964
54	14	0	-3.717827	4.261815	-3.261427
55	14	0	-0.714815	4.837423	-2.871029
56	8	0	-0.046689	1.169341	-3.821390
57	8	0	-1.031911	-1.046274	-3.035145
58	8	0	-5.238163	-1.522881	-3.666710
59	8	0	-5.106565	0.819421	-5.095069
60	8	0	3.444176	4.887898	4.175316
61	8	0	-2.599435	0.644738	-4.390841
62	8	0	-2.891009	5.867467	0.372295
63	8	0	0.373261	3.655923	-3.112136

64	8	0	-4.096000	2.684010	-3.482806
65	8	0	5.301100	3.406482	3.001655
66	8	0	1.036186	5.079981	3.329316
67	8	0	-3.997736	4.546948	-1.690611
68	8	0	-0.981477	4.955024	-1.275490
69	8	0	-1.251114	3.901996	3.419281
70	8	0	-2.274127	1.626664	3.901441
71	8	0	-7.153004	0.492486	3.303238
72	8	0	-6.343519	2.881852	2.336110
73	8	0	4.661626	2.575212	-3.215351
74	8	0	-3.771543	3.527909	2.676970
75	8	0	-2.131944	4.504897	-3.639052
76	8	0	-0.469292	5.321085	1.275578
77	8	0	-5.207087	4.549964	0.682546
78	8	0	5.949262	1.310143	-1.370289
79	8	0	2.241402	2.288901	-4.345290
80	1	0	7.654161	-2.777399	0.483943
81	1	0	6.908853	-1.219774	3.971628
82	1	0	8.157686	0.946476	-0.243894
83	1	0	7.491920	2.100541	3.353576
84	1	0	7.209372	2.778267	-3.073588
85	1	0	5.819577	5.514792	4.104142
86	1	0	2.691773	6.927076	2.670148
87	1	0	3.716718	4.433789	-4.429173
88	1	0	-0.122698	6.033042	-3.431683
89	1	0	-0.845502	7.254578	-0.261652
90	1	0	5.160658	-5.322248	0.791817
91	1	0	4.494576	-3.681108	5.107467
92	1	0	1.600397	-6.084213	0.888984
93	1	0	0.854624	-4.899185	4.132307
94	1	0	-2.903440	-7.211900	0.225024
95	1	0	-3.392936	-5.735023	3.627549
96	1	0	-6.854163	-4.846139	-1.256737
97	1	0	-7.576266	-3.599065	2.526340
98	1	0	-7.099539	-0.353998	-4.837210
99	1	0	-8.744360	2.295837	2.657361
100	1	0	-4.498352	5.142641	-4.142756
101	1	0	-4.982436	6.610421	-0.741888
102	1	0	6.364357	0.785880	-3.800445
103	1	0	6.603324	-2.278564	-1.604913
104	1	0	4.157475	2.553544	-5.752475
105	1	0	0.116443	2.997634	-5.589778
106	1	0	-3.537228	2.473985	-5.921959
107	1	0	-0.728610	-0.545497	-5.558162
108	1	0	-5.453453	-1.427748	-6.211686
109	1	0	-5.051407	-4.041629	-4.140335
110	1	0	1.678429	-5.344370	-1.435013
111	1	0	-2.654934	-6.079333	-1.949755
112	1	0	-0.535244	-3.493769	-3.436886
113	1	0	-4.175042	-4.240126	5.344341
114	1	0	0.547869	-3.295400	5.843560
115	1	0	-6.220849	-1.176382	4.941070
116	1	0	-2.731073	-0.317107	5.440008
117	1	0	5.584503	-0.332413	5.752948
118	1	0	-7.440163	2.656073	4.627082
119	1	0	-5.641291	5.204487	3.107887
120	1	0	-1.173424	6.400795	3.510278
121	1	0	1.937625	6.575406	5.059163
122	1	0	5.155832	3.686437	5.570773
123	1	0	-3.104042	3.605000	5.126213

124	14	0	-1.689162	-2.315618	2.850898
125	79	0	3.258917	-1.806386	-2.774412
126	79	0	3.174544	-0.600866	-0.136060
127	79	0	1.013493	-0.553878	-1.576750

Zero-point correction= 0.308947 (Hartree/Particle)
Thermal correction to Energy= 0.387777
Thermal correction to Enthalpy= 0.388721
Thermal correction to Gibbs Free Energy= 0.201706
Sum of electronic and zero-point Energies= -13739.989177
Sum of electronic and thermal Energies= -13739.910347
Sum of electronic and thermal Enthalpies= -13739.909403
Sum of electronic and thermal Free Energies= -13740.096418

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -13743.239318

Fig. 1 (d)

Charge: 0 multiplicity: 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.385928	-4.127716	1.065141
2	14	0	6.498277	-2.154361	-0.138825
3	14	0	3.884606	-3.061390	3.946289
4	14	0	5.634255	-0.575860	4.294452
5	8	0	5.154315	-2.845576	0.450484
6	8	0	6.358063	-0.615616	0.413420
7	8	0	4.238598	-4.043189	2.689484
8	8	0	4.459697	-1.560758	3.741819
9	8	0	5.380897	0.827284	3.498975
10	14	0	-1.514438	-2.615261	-2.864941
11	14	0	-4.540821	-2.955376	-3.318717
12	14	0	-6.211463	-3.246970	2.185931
13	14	0	-3.899607	-4.411548	3.925791
14	14	0	0.823455	-3.468984	4.429017
15	14	0	-2.929474	0.164915	4.082375
16	14	0	-5.944824	-0.544832	3.657226
17	14	0	-5.611876	-4.310627	-0.732468
18	14	0	-3.070645	-5.993184	-0.520125
19	14	0	1.610808	-4.940796	-0.033149
20	14	0	-1.255479	-3.583142	0.114954
21	8	0	-2.935631	-2.841236	-3.634764
22	8	0	-5.289243	-4.250372	3.078980
23	8	0	-0.259568	-2.650796	3.527454
24	8	0	-2.809152	-3.266748	3.536369
25	8	0	-5.861755	-1.681045	2.491507
26	8	0	-2.116089	-0.772203	3.039472
27	8	0	2.291086	-2.849202	4.119220
28	8	0	-5.929391	-3.451754	0.601820
29	8	0	-1.629084	-2.506696	1.248480
30	8	0	-4.531009	0.270616	3.743762
31	8	0	-4.665441	-5.610802	-0.431211
32	8	0	0.306780	-3.981543	0.188684
33	8	0	-2.147023	-4.929920	0.320920
34	8	0	-4.824068	-3.300206	-1.753139
35	8	0	-1.678104	-2.897111	-1.288250
36	8	0	2.941220	-4.087817	0.339321
37	14	0	6.732873	0.907003	-0.020774

38	14	0	6.158191	2.054387	2.769916
39	8	0	6.272818	1.918021	1.155817
40	14	0	0.655190	2.560899	-4.283258
41	14	0	-1.103745	0.036069	-4.276259
42	14	0	-5.731897	-0.680087	-4.986964
43	14	0	2.310121	5.978871	3.781430
44	14	0	-3.797434	1.689737	-4.742368
45	14	0	4.968868	4.368877	4.279330
46	14	0	-4.291890	5.413469	-0.348350
47	14	0	-1.291040	5.898219	0.012347
48	14	0	-0.507400	5.236268	2.901298
49	14	0	-2.646755	3.196241	3.812598
50	14	0	-7.446830	2.107575	3.263550
51	14	0	3.707101	2.992868	-4.460510
52	14	0	-5.245607	4.076995	2.247396
53	14	0	6.085957	1.863748	-2.892964
54	14	0	-3.717827	4.261815	-3.261427
55	14	0	-0.714815	4.837423	-2.871029
56	8	0	-0.046689	1.169341	-3.821390
57	8	0	-1.031911	-1.046274	-3.035145
58	8	0	-5.238163	-1.522881	-3.666710
59	8	0	-5.106565	0.819421	-5.095069
60	8	0	3.444176	4.887898	4.175316
61	8	0	-2.599435	0.644738	-4.390841
62	8	0	-2.891009	5.867467	0.372295
63	8	0	0.373261	3.655923	-3.112136
64	8	0	-4.096000	2.684010	-3.482806
65	8	0	5.301100	3.406482	3.001655
66	8	0	1.036186	5.079981	3.329316
67	8	0	-3.997736	4.546948	-1.690611
68	8	0	-0.981477	4.955024	-1.275490
69	8	0	-1.251114	3.901996	3.419281
70	8	0	-2.274127	1.626664	3.901441
71	8	0	-7.153004	0.492486	3.303238
72	8	0	-6.343519	2.881852	2.336110
73	8	0	4.661626	2.575212	-3.215351
74	8	0	-3.771543	3.527909	2.676970
75	8	0	-2.131944	4.504897	-3.639052
76	8	0	-0.469292	5.321085	1.275578
77	8	0	-5.207087	4.549964	0.682546
78	8	0	5.949262	1.310143	-1.370289
79	8	0	2.241402	2.288901	-4.345290
80	1	0	7.654161	-2.777399	0.483943
81	1	0	6.908853	-1.219774	3.971628
82	1	0	8.157686	0.946476	-0.243894
83	1	0	7.491920	2.100541	3.353576
84	1	0	7.209372	2.778267	-3.073588
85	1	0	5.819577	5.514792	4.104142
86	1	0	2.691773	6.927076	2.670148
87	1	0	3.716718	4.433789	-4.429173
88	1	0	-0.122698	6.033042	-3.431683
89	1	0	-0.845502	7.254578	-0.261652
90	1	0	5.160658	-5.322248	0.791817
91	1	0	4.494576	-3.681108	5.107467
92	1	0	1.600397	-6.084213	0.888984
93	1	0	0.854624	-4.899185	4.132307
94	1	0	-2.903440	-7.211900	0.225024
95	1	0	-3.392936	-5.735023	3.627549
96	1	0	-6.854163	-4.846139	-1.256737
97	1	0	-7.576266	-3.599065	2.526340

98	1	0	-7.099539	-0.353998	-4.837210
99	1	0	-8.744360	2.295837	2.657361
100	1	0	-4.498352	5.142641	-4.142756
101	1	0	-4.982436	6.610421	-0.741888
102	1	0	6.364357	0.785880	-3.800445
103	1	0	6.603324	-2.278564	-1.604913
104	1	0	4.157475	2.553544	-5.752475
105	1	0	0.116443	2.997634	-5.589778
106	1	0	-3.537228	2.473985	-5.921959
107	1	0	-0.728610	-0.545497	-5.558162
108	1	0	-5.453453	-1.427748	-6.211686
109	1	0	-5.051407	-4.041629	-4.140335
110	1	0	1.678429	-5.344370	-1.435013
111	1	0	-2.654934	-6.079333	-1.949755
112	1	0	-0.535244	-3.493769	-3.436886
113	1	0	-4.175042	-4.240126	5.344341
114	1	0	0.547869	-3.295400	5.843560
115	1	0	-6.220849	-1.176382	4.941070
116	1	0	-2.731073	-0.317107	5.440008
117	1	0	5.584503	-0.332413	5.752948
118	1	0	-7.440163	2.656073	4.627082
119	1	0	-5.641291	5.204487	3.107887
120	1	0	-1.173424	6.400795	3.510278
121	1	0	1.937625	6.575406	5.059163
122	1	0	5.155832	3.686437	5.570773
123	1	0	-3.104042	3.605000	5.126213
124	14	0	-1.689162	-2.315618	2.850898
125	79	0	3.258917	-1.806386	-2.774412
126	79	0	3.174544	-0.600866	-0.136060
127	79	0	1.013493	-0.553878	-1.576750

Zero-point correction=	0.308911 (Hartree/Particle)
Thermal correction to Energy=	0.387923
Thermal correction to Enthalpy=	0.388867
Thermal correction to Gibbs Free Energy=	0.200565
Sum of electronic and zero-point Energies=	-13739.988721
Sum of electronic and thermal Energies=	-13739.909709
Sum of electronic and thermal Enthalpies=	-13739.908765
Sum of electronic and thermal Free Energies=	-13740.097067

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -13743.237167

Fig. 1 (e)

Charge: 0 multiplicity: 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	5.115207	4.745767	1.582308
2	14	0	7.154767	2.580917	2.514993
3	14	0	5.201141	4.587478	-1.534682
4	14	0	7.184098	2.377185	-2.262767
5	8	0	5.848404	3.366056	1.973519
6	8	0	7.275981	1.292960	1.518219
7	8	0	5.254521	5.136189	0.002969
8	8	0	5.850865	3.115258	-1.688859
9	8	0	6.922858	0.793631	-1.971661
10	14	0	-1.217009	1.953156	3.723032
11	14	0	-4.288812	2.057597	3.688162

12	14	0	-5.035050	3.915172	-1.707662
13	14	0	-2.573057	5.638783	-2.578384
14	14	0	2.238828	5.025795	-2.447138
15	14	0	-1.224445	1.334187	-3.887561
16	14	0	-4.309635	1.791786	-3.830831
17	14	0	-5.028155	4.077302	1.447154
18	14	0	-2.632009	5.829493	2.210798
19	14	0	2.134621	5.120069	2.317263
20	14	0	-0.533703	3.788950	1.264407
21	8	0	-2.762210	1.949924	4.258004
22	8	0	-4.049309	5.163072	-2.070821
23	8	0	1.107607	3.897783	-2.085554
24	8	0	-1.429620	4.496019	-2.370222
25	8	0	-4.490695	2.533941	-2.391666
26	8	0	-0.760979	1.958090	-2.441139
27	8	0	3.677316	4.400486	-2.045398
28	8	0	-5.059474	3.643632	-0.112287
29	8	0	-0.618823	3.129347	-0.205160
30	8	0	-2.838718	1.078888	-3.930916
31	8	0	-4.139048	5.430594	1.694731
32	8	0	0.995384	4.207082	1.584302
33	8	0	-1.462726	5.125142	1.296999
34	8	0	-4.346218	2.838108	2.261541
35	8	0	-1.130289	2.709171	2.297196
36	8	0	3.575386	4.449223	1.993266
37	14	0	7.663195	-0.280994	1.563810
38	14	0	7.664378	-0.569626	-1.489466
39	8	0	7.491383	-0.922242	0.087289
40	14	0	1.122429	-3.325052	3.970586
41	14	0	-0.789344	-0.966434	4.352680
42	14	0	-5.546526	-0.652222	4.372373
43	14	0	4.388844	-4.124335	-4.293173
44	14	0	-3.387760	-2.776818	3.833658
45	14	0	6.946839	-2.356922	-3.800639
46	14	0	-2.833478	-5.034148	-1.482981
47	14	0	0.214695	-5.292520	-1.399119
48	14	0	1.411538	-3.768631	-3.773240
49	14	0	-0.706433	-1.618037	-4.436354
50	14	0	-5.612370	-0.899659	-4.498111
51	14	0	4.127825	-3.709487	4.569542
52	14	0	-3.449476	-3.006964	-3.703413
53	14	0	6.630071	-2.079825	3.859945
54	14	0	-2.845518	-4.808499	1.699980
55	14	0	0.213285	-5.123594	1.731853
56	8	0	0.445629	-1.864623	3.836053
57	8	0	-0.666664	0.438512	3.552731
58	8	0	-4.908027	0.563216	3.478651
59	8	0	-4.806904	-2.089312	4.152593
60	8	0	5.476749	-2.930641	-4.138030
61	8	0	-2.207588	-1.694945	4.027347
62	8	0	-1.298922	-5.205746	-2.026918
63	8	0	1.139730	-4.043224	2.507926
64	8	0	-3.402451	-3.360133	2.283717
65	8	0	6.979773	-1.816902	-2.259241
66	8	0	2.986130	-3.442473	-3.846328
67	8	0	-2.854967	-4.629276	0.094142
68	8	0	0.216939	-4.799103	0.147110
69	8	0	0.659878	-2.361780	-4.018981
70	8	0	-0.455736	-0.073076	-4.005947
71	8	0	-5.470529	0.666138	-4.015980

72	8	0	-4.616978	-1.877796	-3.649424
73	8	0	5.232475	-2.892775	3.700778
74	8	0	-1.978532	-2.307915	-3.690247
75	8	0	-1.340187	-5.085118	2.293118
76	8	0	1.187239	-4.342888	-2.267230
77	8	0	-3.634500	-3.928963	-2.364808
78	8	0	6.691175	-1.073748	2.584089
79	8	0	2.653052	-3.049140	4.401521
80	1	0	8.337625	3.402075	2.329277
81	1	0	8.323934	2.940105	-1.534919
82	1	0	9.027265	-0.350846	2.028473
83	1	0	9.075741	-0.392625	-1.807251
84	1	0	7.776914	-2.976152	3.979462
85	1	0	7.850253	-3.475127	-3.810634
86	1	0	4.657971	-5.350174	-3.453442
87	1	0	4.260197	-5.071029	4.124895
88	1	0	0.793228	-6.417127	2.012638
89	1	0	0.719672	-6.653296	-1.451728
90	1	0	5.723573	5.842372	2.313783
91	1	0	5.933811	5.551693	-2.337328
92	1	0	2.178363	6.486093	1.782161
93	1	0	2.091444	6.306004	-1.744814
94	1	0	-2.452483	7.220476	1.895920
95	1	0	-2.236081	6.818030	-1.817466
96	1	0	-6.379727	4.396190	1.869247
97	1	0	-6.347506	4.319669	-2.178137
98	1	0	-6.839067	-0.968677	3.885788
99	1	0	-6.970408	-1.297955	-4.224059
100	1	0	-3.699319	-5.919011	2.125917
101	1	0	-3.479037	-6.313224	-1.582712
102	1	0	6.655208	-1.321254	5.081757
103	1	0	6.997396	2.266689	3.951358
104	1	0	4.310690	-3.661616	5.993513
105	1	0	0.407077	-4.163232	4.962080
106	1	0	-3.281645	-3.878431	4.747313
107	1	0	-0.719527	-0.802248	5.800816
108	1	0	-5.544723	-0.305652	5.792805
109	1	0	-5.024834	2.820574	4.678898
110	1	0	1.927864	5.085851	3.764833
111	1	0	-2.477057	5.495941	3.656461
112	1	0	-0.424565	2.651362	4.698109
113	1	0	-2.588655	5.883273	-4.007384
114	1	0	2.214141	5.280818	-3.872864
115	1	0	-4.404487	2.777015	-4.895194
116	1	0	-0.820129	2.217171	-4.964552
117	1	0	7.397963	2.586967	-3.710297
118	1	0	-5.328136	-1.009394	-5.935839
119	1	0	-3.599336	-3.838405	-4.912916
120	1	0	0.958095	-4.717790	-4.807562
121	1	0	4.288446	-4.321749	-5.735017
122	1	0	7.288825	-1.312757	-4.781913
123	1	0	-0.904907	-1.628076	-5.874215
124	14	0	-0.398022	3.404521	-1.778140
125	79	0	-1.893035	0.431689	-0.713743
126	79	0	-2.855603	-1.477160	0.706927
127	79	0	0.049973	-1.392619	0.175580

Zero-point correction= 0.309152 (Hartree/Particle)
Thermal correction to Energy= 0.387861
Thermal correction to Enthalpy= 0.388806

Thermal correction to Gibbs Free Energy= 0.204096
Sum of electronic and zero-point Energies= -13739.988696
Sum of electronic and thermal Energies= -13739.909986
Sum of electronic and thermal Enthalpies= -13739.909042
Sum of electronic and thermal Free Energies= -13740.093751

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -13743.239158

Fig. 1 (f)

Charge: 0 multiplicity: 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.061853	5.345950	1.327701
2	14	0	6.346832	3.488713	2.343933
3	14	0	4.153204	5.041804	-1.782842
4	14	0	6.378498	3.049861	-2.424995
5	8	0	4.944504	4.078773	1.785367
6	8	0	6.602154	2.172727	1.407363
7	8	0	4.140127	5.661277	-0.272490
8	8	0	4.962909	3.646245	-1.875520
9	8	0	6.297423	1.461255	-2.052442
10	14	0	-1.885764	1.943374	3.666922
11	14	0	-4.960466	1.685824	3.658508
12	14	0	-5.950843	3.190601	-1.799233
13	14	0	-3.726032	5.128592	-2.793764
14	14	0	1.166599	5.111735	-2.685197
15	14	0	-1.850524	0.966316	-3.885721
16	14	0	-4.985448	1.067607	-3.816212
17	14	0	-5.937113	3.503412	1.340790
18	14	0	-3.771892	5.553273	1.990850
19	14	0	1.064341	5.413059	2.074687
20	14	0	-1.441521	3.715379	1.115369
21	8	0	-3.410660	1.746925	4.199506
22	8	0	-5.140071	4.533210	-2.246192
23	8	0	0.121130	3.931855	-2.229467
24	8	0	-2.512250	4.046059	-2.545335
25	8	0	-5.254095	1.843956	-2.413705
26	8	0	-1.301078	1.690714	-2.496080
27	8	0	2.651949	4.636665	-2.258795
28	8	0	-5.897271	2.989169	-0.194082
29	8	0	-1.449380	2.953324	-0.318226
30	8	0	-3.421167	0.554999	-3.818546
31	8	0	-5.229516	4.966793	1.522110
32	8	0	0.017101	4.340673	1.401518
33	8	0	-2.556302	4.891078	1.095085
34	8	0	-5.087182	2.395530	2.199461
35	8	0	-1.853248	2.572414	2.181597
36	8	0	2.561569	4.881475	1.755335
37	14	0	7.182896	0.663882	1.523416
38	14	0	7.202412	0.224994	-1.509851
39	8	0	7.067660	-0.069010	0.083156
40	14	0	1.066689	-3.015300	4.147326
41	14	0	-1.137806	-0.887456	4.449224
42	14	0	-5.888835	-1.106890	4.494351
43	14	0	4.376000	-3.832284	-4.103306
44	14	0	-3.501858	-3.018445	4.014480
45	14	0	6.694164	-1.745416	-3.720984

46	14	0	-2.724016	-5.434353	-1.168306
47	14	0	0.324422	-5.350785	-1.108049
48	14	0	1.358461	-3.790597	-3.586897
49	14	0	-1.013327	-1.951924	-4.317661
50	14	0	-5.964387	-1.803463	-4.361245
51	14	0	4.107324	-3.004171	4.733691
52	14	0	-3.565900	-3.609160	-3.489131
53	14	0	6.386743	-1.123692	3.915411
54	14	0	-2.755877	-5.039973	1.989911
55	14	0	0.328525	-5.024269	2.017633
56	8	0	0.227048	-1.615515	3.886372
57	8	0	-1.137211	0.481903	3.559524
58	8	0	-5.397421	0.122224	3.519214
59	8	0	-4.958094	-2.434791	4.342080
60	8	0	5.282588	-2.497432	-4.001870
61	8	0	-2.414129	-1.807510	4.112302
62	8	0	-1.173567	-5.465970	-1.734078
63	8	0	1.110651	-3.770466	2.701851
64	8	0	-3.462672	-3.663435	2.513482
65	8	0	6.654874	-1.131947	-2.208210
66	8	0	2.890990	-3.334831	-3.621987
67	8	0	-2.735808	-4.922441	0.371373
68	8	0	0.322854	-4.756748	0.406484
69	8	0	0.458592	-2.485836	-3.894083
70	8	0	-0.955499	-0.377891	-3.919476
71	8	0	-5.977384	-0.213451	-3.944893
72	8	0	-4.824683	-2.588726	-3.477939
73	8	0	5.078314	-2.095215	3.807834
74	8	0	-2.153927	-2.772763	-3.496508
75	8	0	-1.209298	-5.119463	2.568360
76	8	0	1.127542	-4.207409	-1.986546
77	8	0	-3.634763	-4.463862	-2.096249
78	8	0	6.307790	-0.190451	2.587136
79	8	0	2.549561	-2.533887	4.527251
80	1	0	7.421989	4.428995	2.101773
81	1	0	7.443133	3.776654	-1.734847
82	1	0	8.545795	0.772206	1.977330
83	1	0	8.579495	0.545342	-1.852070
84	1	0	7.622060	-1.880850	4.067768
85	1	0	7.714167	-2.755303	-3.688955
86	1	0	4.765857	-4.970738	-3.205918
87	1	0	4.376288	-4.362847	4.353580
88	1	0	1.080623	-6.208810	2.347312
89	1	0	1.017772	-6.624197	-1.100486
90	1	0	4.539538	6.542942	1.995368
91	1	0	4.759002	6.047506	-2.638011
92	1	0	0.940632	6.740230	1.471373
93	1	0	0.857693	6.375753	-2.041432
94	1	0	-3.743753	6.932663	1.599339
95	1	0	-3.500408	6.373735	-2.091977
96	1	0	-7.312453	3.670604	1.753373
97	1	0	-7.291898	3.396847	-2.285557
98	1	0	-7.128807	-1.604006	4.034624
99	1	0	-7.261499	-2.349973	-4.047553
100	1	0	-3.439146	-6.234701	2.484890
101	1	0	-3.191755	-6.784474	-1.201705
102	1	0	6.319446	-0.315673	5.099950
103	1	0	6.232453	3.226862	3.791830
104	1	0	4.270437	-2.865863	6.150410
105	1	0	0.447541	-3.871361	5.187098

106	1	0	-3.250137	-4.031173	4.998705
107	1	0	-1.061595	-0.627642	5.872726
108	1	0	-5.911613	-0.699935	5.892788
109	1	0	-5.767858	2.406230	4.621818
110	1	0	0.866211	5.420849	3.522721
111	1	0	-3.556877	5.306972	3.442252
112	1	0	-1.179467	2.777470	4.599418
113	1	0	-3.751724	5.296404	-4.229726
114	1	0	1.089140	5.267238	-4.118030
115	1	0	-5.194971	1.958637	-4.944866
116	1	0	-1.570077	1.819106	-5.025685
117	1	0	6.554042	3.209692	-3.880188
118	1	0	-5.673087	-1.956936	-5.789107
119	1	0	-3.619127	-4.509777	-4.647911
120	1	0	1.010578	-4.843744	-4.549138
121	1	0	4.266684	-4.107565	-5.530908
122	1	0	6.897938	-0.724537	-4.758633
123	1	0	-1.207565	-2.050148	-5.745316
124	14	0	-1.284889	3.233822	-1.902893
125	79	0	-0.290108	0.288135	-0.855755
126	79	0	0.893550	-2.118658	-0.699014
127	79	0	0.323337	-0.736749	1.522142

Zero-point correction= 0.309028 (Hartree/Particle)
Thermal correction to Energy= 0.387205
Thermal correction to Enthalpy= 0.388149
Thermal correction to Gibbs Free Energy= 0.207526
Sum of electronic and zero-point Energies= -13739.827432
Sum of electronic and thermal Energies= -13739.749255
Sum of electronic and thermal Enthalpies= -13739.748311
Sum of electronic and thermal Free Energies= -13739.928934

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -13743.078156

Au_3

Charge: 0 multiplicity: 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	0.000000	0.000000	0.588648
2	79	0	0.000000	-2.487379	-0.294324
3	79	0	0.000000	2.487379	-0.294324

Zero-point correction= 0.000634 (Hartree/Particle)
Thermal correction to Energy= 0.005729
Thermal correction to Enthalpy= 0.006673
Thermal correction to Gibbs Free Energy= -0.036548
Sum of electronic and zero-point Energies= -406.419876
Sum of electronic and thermal Energies= -406.414780
Sum of electronic and thermal Enthalpies= -406.413836
Sum of electronic and thermal Free Energies= -406.457057

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -407.4954317

Au_3^+

Charge: 0 multiplicity: 1

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	79	0	1.352217	-0.780661	0.000000
2	79	0	0.000000	1.561367	0.000000
3	79	0	-1.352217	-0.780706	0.000000

Zero-point correction= 0.000819 (Hartree/Particle)
Thermal correction to Energy= 0.005748
Thermal correction to Enthalpy= 0.006692
Thermal correction to Gibbs Free Energy= -0.034347
Sum of electronic and zero-point Energies= -406.152748
Sum of electronic and thermal Energies= -406.147819
Sum of electronic and thermal Enthalpies= -406.146875
Sum of electronic and thermal Free Energies= -406.187914

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -407.277437

Ethanol

Charge: 0 multiplicity: 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.178597	-0.401223	0.000000
2	1	0	2.122545	0.154822	0.000000
3	1	0	1.152194	-1.042007	0.887000
4	1	0	1.152194	-1.042007	-0.887000
5	6	0	0.000000	0.556692	0.000000
6	1	0	0.037027	1.203759	0.889504
7	1	0	0.037027	1.203759	-0.889504
8	8	0	-1.201119	-0.222578	0.000000
9	1	0	-1.963616	0.369491	0.000000

Zero-point correction= 0.079828 (Hartree/Particle)
Thermal correction to Energy= 0.084142
Thermal correction to Enthalpy= 0.085086
Thermal correction to Gibbs Free Energy= 0.054413
Sum of electronic and zero-point Energies= -154.978148
Sum of electronic and thermal Energies= -154.973835
Sum of electronic and thermal Enthalpies= -154.972891
Sum of electronic and thermal Free Energies= -155.003563

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -155.0748155

O_2

Charge: 0 multiplicity: 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.608011
2	8	0	0.000000	0.000000	-0.608011

Zero-point correction= 0.003779 (Hartree/Particle)
Thermal correction to Energy= 0.006142
Thermal correction to Enthalpy= 0.007087
Thermal correction to Gibbs Free Energy= -0.016199
Sum of electronic and zero-point Energies= -150.316261

Sum of electronic and thermal Energies= -150.313898
Sum of electronic and thermal Enthalpies= -150.312954
Sum of electronic and thermal Free Energies= -150.336240

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -150.369368

H_2

Charge: 0 multiplicity: 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	0.371394
2	1	0	0.000000	0.000000	-0.371394

Zero-point correction= 0.010145 (Hartree/Particle)
Thermal correction to Energy= 0.012505
Thermal correction to Enthalpy= 0.013450
Thermal correction to Gibbs Free Energy= -0.001342
Sum of electronic and zero-point Energies= -1.165337
Sum of electronic and thermal Energies= -1.162977
Sum of electronic and thermal Enthalpies= -1.162033
Sum of electronic and thermal Free Energies= -1.176825

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -1.1717101

Au_3^+-S1

Charge: 1 multiplicity: 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.061853	5.345950	1.327701
2	14	0	6.346832	3.488713	2.343933
3	14	0	4.153204	5.041804	-1.782842
4	14	0	6.378498	3.049861	-2.424995
5	8	0	4.944504	4.078773	1.785367
6	8	0	6.602154	2.172727	1.407363
7	8	0	4.140127	5.661277	-0.272490
8	8	0	4.962909	3.646245	-1.875520
9	8	0	6.297423	1.461255	-2.052442
10	14	0	-1.885764	1.943374	3.666922
11	14	0	-4.960466	1.685824	3.658508
12	14	0	-5.950843	3.190601	-1.799233
13	14	0	-3.726032	5.128592	-2.793764
14	14	0	1.166599	5.111735	-2.685197
15	14	0	-1.850524	0.966316	-3.885721
16	14	0	-4.985448	1.067607	-3.816212
17	14	0	-5.937113	3.503412	1.340790
18	14	0	-3.771892	5.553273	1.990850
19	14	0	1.064341	5.413059	2.074687
20	14	0	-1.441521	3.715379	1.115369
21	8	0	-3.410660	1.746925	4.199506
22	8	0	-5.140071	4.533210	-2.246192
23	8	0	0.121130	3.931855	-2.229467
24	8	0	-2.512250	4.046059	-2.545335
25	8	0	-5.254095	1.843956	-2.413705
26	8	0	-1.301078	1.690714	-2.496080
27	8	0	2.651949	4.636665	-2.258795

28	8	0	-5.897271	2.989169	-0.194082
29	8	0	-1.449380	2.953324	-0.318226
30	8	0	-3.421167	0.554999	-3.818546
31	8	0	-5.229516	4.966793	1.522110
32	8	0	0.017101	4.340673	1.401518
33	8	0	-2.556302	4.891078	1.095085
34	8	0	-5.087182	2.395530	2.199461
35	8	0	-1.853248	2.572414	2.181597
36	8	0	2.561569	4.881475	1.755335
37	14	0	7.182896	0.663882	1.523416
38	14	0	7.202412	0.224994	-1.509851
39	8	0	7.067660	-0.069010	0.083156
40	14	0	1.066689	-3.015300	4.147326
41	14	0	-1.137806	-0.887456	4.449224
42	14	0	-5.888835	-1.106890	4.494351
43	14	0	4.376000	-3.832284	-4.103306
44	14	0	-3.501858	-3.018445	4.014480
45	14	0	6.694164	-1.745416	-3.720984
46	14	0	-2.724016	-5.434353	-1.168306
47	14	0	0.324422	-5.350785	-1.108049
48	14	0	1.358461	-3.790597	-3.586897
49	14	0	-1.013327	-1.951924	-4.317661
50	14	0	-5.964387	-1.803463	-4.361245
51	14	0	4.107324	-3.004171	4.733691
52	14	0	-3.565900	-3.609160	-3.489131
53	14	0	6.386743	-1.123692	3.915411
54	14	0	-2.755877	-5.039973	1.989911
55	14	0	0.328525	-5.024269	2.017633
56	8	0	0.227048	-1.615515	3.886372
57	8	0	-1.137211	0.481903	3.559524
58	8	0	-5.397421	0.122224	3.519214
59	8	0	-4.958094	-2.434791	4.342080
60	8	0	5.282588	-2.497432	-4.001870
61	8	0	-2.414129	-1.807510	4.112302
62	8	0	-1.173567	-5.465970	-1.734078
63	8	0	1.110651	-3.770466	2.701851
64	8	0	-3.462672	-3.663435	2.513482
65	8	0	6.654874	-1.131947	-2.208210
66	8	0	2.890990	-3.334831	-3.621987
67	8	0	-2.735808	-4.922441	0.371373
68	8	0	0.322854	-4.756748	0.406484
69	8	0	0.458592	-2.485836	-3.894083
70	8	0	-0.955499	-0.377891	-3.919476
71	8	0	-5.977384	-0.213451	-3.944893
72	8	0	-4.824683	-2.588726	-3.477939
73	8	0	5.078314	-2.095215	3.807834
74	8	0	-2.153927	-2.772763	-3.496508
75	8	0	-1.209298	-5.119463	2.568360
76	8	0	1.127542	-4.207409	-1.986546
77	8	0	-3.634763	-4.463862	-2.096249
78	8	0	6.307790	-0.190451	2.587136
79	8	0	2.549561	-2.533887	4.527251
80	1	0	7.421989	4.428995	2.101773
81	1	0	7.443133	3.776654	-1.734847
82	1	0	8.545795	0.772206	1.977330
83	1	0	8.579495	0.545342	-1.852070
84	1	0	7.622060	-1.880850	4.067768
85	1	0	7.714167	-2.755303	-3.688955
86	1	0	4.765857	-4.970738	-3.205918
87	1	0	4.376288	-4.362847	4.353580

88	1	0	1.080623	-6.208810	2.347312
89	1	0	1.017772	-6.624197	-1.100486
90	1	0	4.539538	6.542942	1.995368
91	1	0	4.759002	6.047506	-2.638011
92	1	0	0.940632	6.740230	1.471373
93	1	0	0.857693	6.375753	-2.041432
94	1	0	-3.743753	6.932663	1.599339
95	1	0	-3.500408	6.373735	-2.091977
96	1	0	-7.312453	3.670604	1.753373
97	1	0	-7.291898	3.396847	-2.285557
98	1	0	-7.128807	-1.604006	4.034624
99	1	0	-7.261499	-2.349973	-4.047553
100	1	0	-3.439146	-6.234701	2.484890
101	1	0	-3.191755	-6.784474	-1.201705
102	1	0	6.319446	-0.315673	5.099950
103	1	0	6.232453	3.226862	3.791830
104	1	0	4.270437	-2.865863	6.150410
105	1	0	0.447541	-3.871361	5.187098
106	1	0	-3.250137	-4.031173	4.998705
107	1	0	-1.061595	-0.627642	5.872726
108	1	0	-5.911613	-0.699935	5.892788
109	1	0	-5.767858	2.406230	4.621818
110	1	0	0.866211	5.420849	3.522721
111	1	0	-3.556877	5.306972	3.442252
112	1	0	-1.179467	2.777470	4.599418
113	1	0	-3.751724	5.296404	-4.229726
114	1	0	1.089140	5.267238	-4.118030
115	1	0	-5.194971	1.958637	-4.944866
116	1	0	-1.570077	1.819106	-5.025685
117	1	0	6.554042	3.209692	-3.880188
118	1	0	-5.673087	-1.956936	-5.789107
119	1	0	-3.619127	-4.509777	-4.647911
120	1	0	1.010578	-4.843744	-4.549138
121	1	0	4.266684	-4.107565	-5.530908
122	1	0	6.897938	-0.724537	-4.758633
123	1	0	-1.207565	-2.050148	-5.745316
124	14	0	-1.284889	3.233822	-1.902893
125	79	0	-0.290108	0.288135	-0.855755
126	79	0	0.893550	-2.118658	-0.699014
127	79	0	0.323337	-0.736749	1.522142

Zero-point correction= 0.309028 (Hartree/Particle)
Thermal correction to Energy= 0.387205
Thermal correction to Enthalpy= 0.388149
Thermal correction to Gibbs Free Energy= 0.207526
Sum of electronic and zero-point Energies= -13739.827432
Sum of electronic and thermal Energies= -13739.749255
Sum of electronic and thermal Enthalpies= -13739.748311
Sum of electronic and thermal Free Energies= -13739.928934

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -13743.078156

INT1

Charge: 1 multiplicity: 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.248479	5.077511	0.706500

2	14	0	6.497486	3.163091	1.710097
3	14	0	4.152402	4.588313	-2.391285
4	14	0	6.241876	2.447492	-3.020172
5	8	0	5.071063	3.785260	1.229250
6	8	0	6.615526	1.781884	0.848112
7	8	0	4.253168	5.279156	-0.907378
8	8	0	4.891709	3.152607	-2.429093
9	8	0	6.100861	0.895325	-2.534913
10	14	0	-1.725687	2.144074	3.556568
11	14	0	-4.799964	2.052247	3.719999
12	14	0	-6.011870	3.283256	-1.763653
13	14	0	-3.737755	5.035421	-2.988330
14	14	0	1.120098	4.762931	-3.130744
15	14	0	-2.157860	0.727323	-3.926596
16	14	0	-5.272976	1.000610	-3.698069
17	14	0	-5.810080	3.773084	1.345390
18	14	0	-3.503763	5.747729	1.755319
19	14	0	1.290437	5.345818	1.595430
20	14	0	-1.337026	3.739618	0.875109
21	8	0	-3.228630	2.086595	4.182654
22	8	0	-5.143314	4.544322	-2.325437
23	8	0	0.065853	3.658868	-2.536050
24	8	0	-2.559379	3.909165	-2.754657
25	8	0	-5.421524	1.867096	-2.331813
26	8	0	-1.485715	1.486459	-2.615684
27	8	0	2.609950	4.245973	-2.753573
28	8	0	-5.893391	3.168008	-0.154432
29	8	0	-1.476954	2.904079	-0.502800
30	8	0	-3.739928	0.403416	-3.759013
31	8	0	-5.001523	5.195688	1.384157
32	8	0	0.187859	4.278151	1.028810
33	8	0	-2.341821	5.011157	0.844732
34	8	0	-4.978607	2.671929	2.224469
35	8	0	-1.761839	2.720939	2.045912
36	8	0	2.752047	4.681327	1.254035
37	14	0	7.139725	0.251695	1.018138
38	14	0	6.969337	-0.363400	-1.982116
39	8	0	6.905242	-0.551571	-0.364768
40	14	0	0.987832	-2.905578	4.189701
41	14	0	-1.057743	-0.658772	4.450319
42	14	0	-5.818119	-0.635517	4.768334
43	14	0	3.792461	-4.398329	-4.171963
44	14	0	-3.547915	-2.682570	4.287522
45	14	0	6.239074	-2.428131	-4.041197
46	14	0	-3.196661	-5.443003	-0.771392
47	14	0	-0.108783	-5.500791	-0.889471
48	14	0	0.832717	-4.170268	-3.499974
49	14	0	-1.487647	-2.260232	-4.212833
50	14	0	-6.422010	-1.840372	-4.013317
51	14	0	4.059011	-3.052931	4.604116
52	14	0	-4.079151	-3.717899	-3.158795
53	14	0	6.385951	-1.348884	3.557565
54	14	0	-3.046766	-4.864457	2.342943
55	14	0	0.057012	-5.004494	2.201899
56	8	0	0.246104	-1.487206	3.951516
57	8	0	-1.074199	0.654197	3.491624
58	8	0	-5.319511	0.508464	3.698363
59	8	0	-4.961224	-2.014259	4.650653
60	8	0	4.785827	-3.119266	-4.201208
61	8	0	-2.397826	-1.538219	4.238630

62	8	0	-1.666573	-5.562511	-1.362239
63	8	0	0.912895	-3.746501	2.780756
64	8	0	-3.631056	-3.425314	2.832431
65	8	0	6.317300	-1.722548	-2.566452
66	8	0	2.370525	-3.758532	-3.690287
67	8	0	-3.141697	-4.825077	0.726227
68	8	0	0.048365	-4.727035	0.570534
69	8	0	-0.038290	-2.842570	-3.810847
70	8	0	-1.330304	-0.664919	-3.899753
71	8	0	-6.333271	-0.229684	-3.697187
72	8	0	-5.289202	-2.639624	-3.136701
73	8	0	5.024234	-2.242397	3.577149
74	8	0	-2.642197	-2.942798	-3.292564
75	8	0	-1.462468	-5.024630	2.793358
76	8	0	0.720663	-4.575264	-1.917654
77	8	0	-4.106446	-4.495493	-1.723135
78	8	0	6.278748	-0.471676	2.188090
79	8	0	2.529961	-2.512881	4.438435
80	1	0	7.600408	4.030955	1.354125
81	1	0	7.377213	3.156750	-2.431648
82	1	0	8.529197	0.317967	1.394328
83	1	0	8.340466	-0.132425	-2.410738
84	1	0	7.588901	-2.155656	3.687565
85	1	0	7.209378	-3.482843	-3.995827
86	1	0	4.183818	-5.504680	-3.226284
87	1	0	4.242370	-4.438675	4.292200
88	1	0	0.752088	-6.217949	2.575867
89	1	0	0.478438	-6.828879	-0.832215
90	1	0	4.827182	6.287109	1.269138
91	1	0	4.765675	5.512410	-3.330528
92	1	0	1.219431	6.646935	0.921761
93	1	0	0.924895	6.084034	-2.553395
94	1	0	-3.435052	7.098174	1.280966
95	1	0	-3.423948	6.313484	-2.377102
96	1	0	-7.150334	4.047272	1.818509
97	1	0	-7.366088	3.538675	-2.191863
98	1	0	-7.108476	-1.088163	4.404031
99	1	0	-7.723588	-2.294083	-3.599904
100	1	0	-3.748805	-5.992805	2.949492
101	1	0	-3.732967	-6.768322	-0.704635
102	1	0	6.425964	-0.465373	4.688820
103	1	0	6.446444	2.994743	3.173756
104	1	0	4.311503	-2.836334	5.997625
105	1	0	0.395394	-3.688995	5.297232
106	1	0	-3.310391	-3.660354	5.311278
107	1	0	-0.907644	-0.334445	5.861596
108	1	0	-5.746624	-0.144475	6.137958
109	1	0	-5.516090	2.870390	4.674491
110	1	0	1.191424	5.454877	3.050725
111	1	0	-3.229482	5.574594	3.207242
112	1	0	-0.922999	2.992331	4.391182
113	1	0	-3.846736	5.128942	-4.429336
114	1	0	0.985189	4.845922	-4.567822
115	1	0	-5.494275	1.837778	-4.864042
116	1	0	-1.890893	1.498841	-5.124285
117	1	0	6.343670	2.514677	-4.489281
118	1	0	-6.215639	-2.088871	-5.442328
119	1	0	-4.233772	-4.677910	-4.256095
120	1	0	0.371509	-5.254124	-4.377856
121	1	0	3.601693	-4.752400	-5.570423

122	1	0	6.439284	-1.476676	-5.143290
123	1	0	-1.764936	-2.419459	-5.625024
124	14	0	-1.361374	3.050882	-2.104231
125	79	0	-0.316640	-0.142512	-1.235583
126	79	0	0.480500	-2.198437	0.239068
127	79	0	1.237677	0.303450	0.937279
128	6	0	3.331032	2.439538	4.346091
129	1	0	3.988949	2.054004	5.131989
130	1	0	3.799117	3.334855	3.926415
131	1	0	2.378133	2.722584	4.802218
132	6	0	3.126483	1.375120	3.282786
133	1	0	4.068485	1.068510	2.817643
134	1	0	2.644273	0.486694	3.694918
135	8	0	2.217507	1.847815	2.246483
136	1	0	2.613143	2.605097	1.775862

Zero-point correction= 0.391277 (Hartree/Particle)
Thermal correction to Energy= 0.475228
Thermal correction to Enthalpy= 0.476172
Thermal correction to Gibbs Free Energy= 0.282136
Sum of electronic and zero-point Energies= -13894.871921
Sum of electronic and thermal Energies= -13894.787970
Sum of electronic and thermal Enthalpies= -13894.787026
Sum of electronic and thermal Free Energies= -13894.981062

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -13898.190026

INT2

Charge: 1 multiplicity: 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.031948	5.064809	1.491094
2	14	0	-6.203197	3.103831	2.549933
3	14	0	-4.192943	4.790825	-1.631142
4	14	0	-6.357954	2.702848	-2.225428
5	8	0	-4.835611	3.752467	1.965730
6	8	0	-6.426536	1.790481	1.599097
7	8	0	-4.214203	5.361424	-0.109023
8	8	0	-4.898173	3.316757	-1.760217
9	8	0	-6.193952	1.125012	-1.852419
10	14	0	2.126969	1.907982	3.613403
11	14	0	5.209703	1.774696	3.515330
12	14	0	5.964972	3.357096	-1.961661
13	14	0	3.613419	5.217300	-2.860284
14	14	0	-1.217647	4.982891	-2.608823
15	14	0	1.912964	0.989067	-3.939753
16	14	0	5.030810	1.213879	-3.971653
17	14	0	6.038218	3.650300	1.181288
18	14	0	3.805726	5.607368	1.920456
19	14	0	-1.009621	5.259646	2.141218
20	14	0	1.527764	3.682087	1.082316
21	8	0	3.669225	1.758895	4.098866
22	8	0	5.060163	4.652514	-2.360250
23	8	0	-0.173571	3.803902	-2.179099
24	8	0	2.405934	4.153600	-2.562073
25	8	0	5.313696	1.984464	-2.565064
26	8	0	1.417938	1.696656	-2.562364

27	8	0	-2.691703	4.462159	-2.146191
28	8	0	5.982582	3.143305	-0.353540
29	8	0	1.526217	2.926231	-0.337771
30	8	0	3.503029	0.614814	-3.959255
31	8	0	5.264973	5.076566	1.396602
32	8	0	0.047703	4.231725	1.429748
33	8	0	2.577955	4.913492	1.070167
34	8	0	5.262433	2.502255	2.061922
35	8	0	2.008272	2.550535	2.140664
36	8	0	-2.496128	4.674522	1.841135
37	14	0	-6.937505	0.254372	1.729383
38	14	0	-7.031490	-0.166567	-1.306638
39	8	0	-6.831375	-0.459056	0.276776
40	14	0	-0.594744	-3.171860	4.148368
41	14	0	1.522833	-0.963779	4.387763
42	14	0	6.278304	-0.984304	4.300589
43	14	0	-4.096263	-4.066336	-4.025925
44	14	0	3.963455	-2.972129	3.878803
45	14	0	-6.498617	-2.091027	-3.560447
46	14	0	3.142977	-5.384075	-1.308617
47	14	0	0.058819	-5.419339	-1.167524
48	14	0	-1.080194	-3.900985	-3.593599
49	14	0	1.188284	-1.949217	-4.374016
50	14	0	6.126073	-1.594251	-4.563171
51	14	0	-3.611736	-3.303051	4.809083
52	14	0	3.832742	-3.503580	-3.643354
53	14	0	-5.994190	-1.518936	4.078503
54	14	0	3.248804	-5.015242	1.841359
55	14	0	0.140853	-5.122347	1.954169
56	8	0	0.205876	-1.776314	3.923221
57	8	0	1.424091	0.410121	3.463364
58	8	0	5.700914	0.230538	3.354129
59	8	0	5.421363	-2.363443	4.158956
60	8	0	-5.067787	-2.772990	-3.890793
61	8	0	2.873321	-1.766802	4.020624
62	8	0	1.565970	-5.466912	-1.775586
63	8	0	-0.666455	-3.928748	2.699864
64	8	0	3.878574	-3.608274	2.376607
65	8	0	-6.440145	-1.478211	-2.045017
66	8	0	-2.629590	-3.479389	-3.615805
67	8	0	3.214222	-4.869686	0.228713
68	8	0	0.028130	-4.739947	0.345055
69	8	0	-0.234602	-2.559746	-3.892877
70	8	0	1.059087	-0.384145	-3.983524
71	8	0	6.091786	-0.009130	-4.137070
72	8	0	5.057737	-2.443509	-3.650665
73	8	0	-4.655131	-2.433713	3.919795
74	8	0	2.394995	-2.721589	-3.597220
75	8	0	1.706204	-5.185500	2.411745
76	8	0	-0.834117	-4.392077	-2.044275
77	8	0	3.974382	-4.378500	-2.267674
78	8	0	-5.996441	-0.564349	2.758987
79	8	0	-2.090586	-2.756618	4.562639
80	1	0	-7.321043	4.003958	2.344658
81	1	0	-7.426885	3.383146	-1.495805
82	1	0	-8.291244	0.303521	2.217944
83	1	0	-8.427495	0.107164	-1.610839
84	1	0	-7.194470	-2.324734	4.255428
85	1	0	-7.476556	-3.138078	-3.503353
86	1	0	-4.423666	-5.229060	-3.126917

87	1	0	-3.838949	-4.667636	4.423565
88	1	0	-0.527801	-6.354055	2.305386
89	1	0	-0.548438	-6.737861	-1.146556
90	1	0	-4.535592	6.240252	2.175026
91	1	0	-4.869472	5.774304	-2.454528
92	1	0	-0.965284	6.595994	1.549102
93	1	0	-0.969868	6.264514	-1.968002
94	1	0	3.708404	6.987900	1.543356
95	1	0	3.380890	6.449665	-2.144702
96	1	0	7.415753	3.880559	1.562964
97	1	0	7.288484	3.639604	-2.476093
98	1	0	7.523888	-1.415780	3.798232
99	1	0	7.451296	-2.088450	-4.291131
100	1	0	3.990574	-6.187318	2.311690
101	1	0	3.659591	-6.716682	-1.371279
102	1	0	-5.930007	-0.713774	5.264354
103	1	0	-6.032364	2.839945	3.988063
104	1	0	-3.744336	-3.182418	6.230768
105	1	0	0.088025	-4.015188	5.147711
106	1	0	3.782080	-4.014766	4.850920
107	1	0	1.477082	-0.715623	5.820140
108	1	0	6.324263	-0.580117	5.699324
109	1	0	6.011121	2.527383	4.462749
110	1	0	-0.774637	5.264009	3.584682
111	1	0	3.645044	5.340463	3.375310
112	1	0	1.412493	2.701894	4.576256
113	1	0	3.615293	5.401664	-4.298893
114	1	0	-1.214666	5.164280	-4.047425
115	1	0	5.177665	2.134899	-5.087300
116	1	0	1.561312	1.840897	-5.063870
117	1	0	-6.577632	2.872531	-3.671166
118	1	0	5.797210	-1.749440	-5.982194
119	1	0	3.888142	-4.397324	-4.806362
120	1	0	-0.718176	-4.930116	-4.576895
121	1	0	-4.030064	-4.326059	-5.457059
122	1	0	-6.779267	-1.065407	-4.576819
123	1	0	1.342900	-2.034216	-5.810007
124	14	0	1.298504	3.172112	-1.919102
125	79	0	-0.508334	-2.266501	0.010003
126	79	0	0.160213	-0.043958	1.350143
127	79	0	-1.499280	0.121935	-0.769659
128	6	0	-2.571105	0.142794	-4.369978
129	1	0	-2.300226	0.370368	-5.406902
130	1	0	-3.558113	-0.325480	-4.361462
131	1	0	-1.845245	-0.574973	-3.981652
132	6	0	-2.563753	1.420821	-3.558919
133	1	0	-3.302530	2.135907	-3.932033
134	1	0	-1.581034	1.900197	-3.570542
135	8	0	-2.916551	1.123916	-2.178028
136	1	0	-3.466535	1.842164	-1.816916
137	8	0	-3.063168	1.076813	3.088800
138	8	0	-1.975216	1.526966	3.383484

Zero-point correction= 0.395326 (Hartree/Particle)
Thermal correction to Energy= 0.483564
Thermal correction to Enthalpy= 0.484508
Thermal correction to Gibbs Free Energy= 0.276969
Sum of electronic and zero-point Energies= -14045.187496
Sum of electronic and thermal Energies= -14045.099259
Sum of electronic and thermal Enthalpies= -14045.098314

Sum of electronic and thermal Free Energies= -14045.305853

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -14048.564519

INT3

Charge: 1 multiplicity: 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.183297	5.135366	0.874318
2	14	0	6.425853	3.225106	1.906761
3	14	0	4.153945	4.668441	-2.223669
4	14	0	6.267127	2.549387	-2.833214
5	8	0	5.013193	3.844068	1.395141
6	8	0	6.571261	1.848396	1.040308
7	8	0	4.230131	5.352534	-0.737656
8	8	0	4.904445	3.238865	-2.258253
9	8	0	6.135988	0.991044	-2.366667
10	14	0	-1.826468	2.129384	3.582536
11	14	0	-4.900311	2.011501	3.684480
12	14	0	-6.013268	3.288088	-1.811137
13	14	0	-3.730706	5.063408	-2.973431
14	14	0	1.137358	4.829325	-3.023580
15	14	0	-2.098859	0.780099	-3.918090
16	14	0	-5.219501	1.027062	-3.748938
17	14	0	-5.876623	3.747063	1.307259
18	14	0	-3.593680	5.731979	1.779081
19	14	0	1.213035	5.370437	1.711009
20	14	0	-1.390786	3.748819	0.923830
21	8	0	-3.340805	2.069833	4.180275
22	8	0	-5.151647	4.562871	-2.350489
23	8	0	0.067523	3.722516	-2.462052
24	8	0	-2.560434	3.934730	-2.713732
25	8	0	-5.400725	1.880407	-2.379257
26	8	0	-1.451610	1.531535	-2.592357
27	8	0	2.619987	4.320825	-2.616849
28	8	0	-5.920982	3.160201	-0.201573
29	8	0	-1.487991	2.913546	-0.460355
30	8	0	-3.680876	0.440502	-3.784458
31	8	0	-5.084345	5.176374	1.383468
32	8	0	0.118008	4.305278	1.118726
33	8	0	-2.422308	4.999112	0.878245
34	8	0	-5.059794	2.636676	2.189179
35	8	0	-1.828617	2.707953	2.072745
36	8	0	2.686032	4.752970	1.389446
37	14	0	7.102844	0.321960	1.202072
38	14	0	6.995925	-0.265475	-1.806243
39	8	0	6.897339	-0.471845	-0.191121
40	14	0	0.910130	-2.910392	4.222079
41	14	0	-1.167648	-0.681898	4.466714
42	14	0	-5.919693	-0.695428	4.688675
43	14	0	3.897117	-4.305069	-4.094304
44	14	0	-3.636318	-2.721581	4.237506
45	14	0	6.324061	-2.315706	-3.895114
46	14	0	-3.160746	-5.430131	-0.841680
47	14	0	-0.072621	-5.473994	-0.905288
48	14	0	0.918568	-4.103800	-3.481850
49	14	0	-1.401070	-2.203582	-4.219970

50	14	0	-6.341446	-1.819300	-4.114993
51	14	0	3.973626	-3.036445	4.696398
52	14	0	-4.001782	-3.689739	-3.232349
53	14	0	6.311078	-1.307318	3.711307
54	14	0	-3.071229	-4.878553	2.280349
55	14	0	0.037831	-4.997341	2.202614
56	8	0	0.137802	-1.511133	3.967575
57	8	0	-1.191199	0.630788	3.510181
58	8	0	-5.394878	0.458588	3.642775
59	8	0	-5.067507	-2.079312	4.573869
60	8	0	4.878952	-3.019977	-4.087945
61	8	0	-2.504664	-1.560472	4.236266
62	8	0	-1.618064	-5.541245	-1.405923
63	8	0	0.878394	-3.744635	2.806174
64	8	0	-3.671128	-3.447227	2.770465
65	8	0	6.371913	-1.630483	-2.410552
66	8	0	2.459815	-3.686789	-3.619681
67	8	0	-3.130176	-4.824181	0.661264
68	8	0	0.054966	-4.706815	0.566036
69	8	0	0.048437	-2.777167	-3.797285
70	8	0	-1.266485	-0.612859	-3.875478
71	8	0	-6.269904	-0.212237	-3.780313
72	8	0	-5.214745	-2.616172	-3.226096
73	8	0	4.952107	-2.208533	3.695141
74	8	0	-2.560729	-2.914933	-3.327733
75	8	0	-1.493429	-5.032539	2.756947
76	8	0	0.764401	-4.516573	-1.900365
77	8	0	-4.054714	-4.479068	-1.802679
78	8	0	6.219565	-0.423832	2.344377
79	8	0	2.443001	-2.503660	4.503493
80	1	0	7.529131	4.100241	1.581896
81	1	0	7.386952	3.259399	-2.215327
82	1	0	8.484361	0.393832	1.606720
83	1	0	8.373887	-0.022801	-2.205262
84	1	0	7.517423	-2.107550	3.858393
85	1	0	7.299000	-3.366526	-3.842729
86	1	0	4.273908	-5.417138	-3.151472
87	1	0	4.176601	-4.420117	4.376067
88	1	0	0.733878	-6.208629	2.575139
89	1	0	0.532157	-6.790282	-0.843144
90	1	0	4.741521	6.337034	1.462654
91	1	0	4.776272	5.604358	-3.144183
92	1	0	1.138744	6.674033	1.047375
93	1	0	0.916839	6.141097	-2.437887
94	1	0	-3.525118	7.088346	1.318677
95	1	0	-3.436239	6.337562	-2.345448
96	1	0	-7.227609	4.005937	1.755017
97	1	0	-7.360617	3.532800	-2.263290
98	1	0	-7.198700	-1.152703	4.294139
99	1	0	-7.647238	-2.289143	-3.731004
100	1	0	-3.774919	-6.019391	2.861787
101	1	0	-3.681384	-6.760984	-0.798237
102	1	0	6.322547	-0.434999	4.851790
103	1	0	6.347266	3.038997	3.368900
104	1	0	4.200310	-2.833111	6.096998
105	1	0	0.305158	-3.707499	5.311713
106	1	0	-3.400302	-3.705692	5.252829
107	1	0	-1.033490	-0.367778	5.880651
108	1	0	-5.878244	-0.215246	6.063115
109	1	0	-5.641242	2.814565	4.631911

110	1	0	1.077649	5.462221	3.164472
111	1	0	-3.346248	5.548610	3.234726
112	1	0	-1.044482	2.972252	4.440500
113	1	0	-3.809766	5.168925	-4.416217
114	1	0	1.025892	4.922095	-4.461951
115	1	0	-5.424011	1.870076	-4.913262
116	1	0	-1.814046	1.559871	-5.105627
117	1	0	6.398875	2.628894	-4.298712
118	1	0	-6.104883	-2.056097	-5.541346
119	1	0	-4.127665	-4.641587	-4.339733
120	1	0	0.483263	-5.183449	-4.375742
121	1	0	3.732484	-4.647481	-5.499730
122	1	0	6.536835	-1.355462	-4.986917
123	1	0	-1.649109	-2.352878	-5.639103
124	14	0	-1.354114	3.091629	-2.057694
125	79	0	-0.254057	-0.123205	-1.270013
126	79	0	0.375492	-2.271310	0.135377
127	79	0	0.962345	0.166601	1.128016
128	6	0	3.246452	1.864688	4.446751
129	1	0	4.305901	2.052318	4.644553
130	1	0	2.675133	2.752022	4.731867
131	1	0	2.922386	1.023524	5.066232
132	6	0	3.048096	1.542853	2.969310
133	1	0	3.366231	2.404900	2.343982
134	1	0	3.642471	0.684857	2.626822
135	8	0	1.697337	1.382814	2.659723
136	1	0	2.501872	-0.788198	-1.281040
137	8	0	2.235793	0.460690	-2.620324
138	8	0	3.062061	-0.343962	-1.962764

Zero-point correction= 0.392171 (Hartree/Particle)
Thermal correction to Energy= 0.476402
Thermal correction to Enthalpy= 0.477741
Thermal correction to Gibbs Free Energy= 0.274394
Sum of electronic and zero-point Energies= -14045.112893
Sum of electronic and thermal Energies= -14045.020662
Sum of electronic and thermal Enthalpies= -14045.027323
Sum of electronic and thermal Free Energies= -14045.230669

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -14048.494807

INT4

Charge: 1 multiplicity: 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.311353	5.029121	0.842268
2	14	0	6.528912	3.070000	1.818926
3	14	0	4.226481	4.607607	-2.267217
4	14	0	6.310220	2.443710	-2.928017
5	8	0	5.130260	3.720168	1.314002
6	8	0	6.651401	1.707396	0.922466
7	8	0	4.354248	5.252904	-0.778230
8	8	0	4.928597	3.128285	-2.341354
9	8	0	6.126422	0.896474	-2.439795
10	14	0	-1.724180	2.120156	3.586861
11	14	0	-4.797458	2.058789	3.725015
12	14	0	-5.952853	3.405187	-1.743489

13	14	0	-3.649801	5.152576	-2.918888
14	14	0	1.202827	4.822233	-3.029808
15	14	0	-2.118943	0.842666	-3.929311
16	14	0	-5.229680	1.149384	-3.714283
17	14	0	-5.769669	3.834606	1.377003
18	14	0	-3.444777	5.771385	1.839392
19	14	0	1.352465	5.318968	1.708498
20	14	0	-1.290449	3.756536	0.938667
21	8	0	-3.232527	2.088528	4.202666
22	8	0	-5.067339	4.664905	-2.280786
23	8	0	0.133769	3.714760	-2.475600
24	8	0	-2.484832	4.010623	-2.696197
25	8	0	-5.375197	1.991645	-2.333096
26	8	0	-1.455075	1.570663	-2.595627
27	8	0	2.689365	4.276936	-2.656545
28	8	0	-5.844598	3.262675	-0.136773
29	8	0	-1.426459	2.945328	-0.457402
30	8	0	-3.704759	0.531500	-3.779405
31	8	0	-4.950997	5.248941	1.456405
32	8	0	0.228740	4.288137	1.111725
33	8	0	-2.300251	5.025778	0.916221
34	8	0	-4.963862	2.700543	2.237198
35	8	0	-1.734627	2.713942	2.082256
36	8	0	2.810613	4.688788	1.354731
37	14	0	7.141054	0.166250	1.080930
38	14	0	6.987602	-0.396619	-1.922132
39	8	0	6.938135	-0.625111	-0.315822
40	14	0	0.924233	-2.978854	4.143982
41	14	0	-1.106713	-0.715257	4.436803
42	14	0	-5.855105	-0.638533	4.715734
43	14	0	3.776922	-4.349073	-4.221389
44	14	0	-3.616239	-2.706136	4.214914
45	14	0	6.245264	-2.410625	-4.037831
46	14	0	-3.251493	-5.371945	-0.894274
47	14	0	-0.169659	-5.473887	-0.996398
48	14	0	0.814401	-4.096734	-3.567692
49	14	0	-1.476300	-2.146021	-4.262918
50	14	0	-6.406956	-1.670725	-4.091858
51	14	0	3.991132	-3.168000	4.579140
52	14	0	-4.092407	-3.591503	-3.255069
53	14	0	6.349118	-1.471338	3.581126
54	14	0	-3.116611	-4.852880	2.233394
55	14	0	-0.016606	-5.030992	2.119239
56	8	0	0.185781	-1.556159	3.924423
57	8	0	-1.124197	0.610184	3.500814
58	8	0	-5.322116	0.516196	3.674649
59	8	0	-5.027476	-2.034459	4.578474
60	8	0	4.785720	-3.080764	-4.221726
61	8	0	-2.456113	-1.574158	4.207966
62	8	0	-1.721394	-5.506258	-1.485546
63	8	0	0.856724	-3.802919	2.725997
64	8	0	-3.691293	-3.417542	2.742729
65	8	0	6.313886	-1.721243	-2.555057
66	8	0	2.359703	-3.702789	-3.734909
67	8	0	-3.187769	-4.784938	0.615404
68	8	0	-0.027876	-4.731454	0.485708
69	8	0	-0.036374	-2.752857	-3.860653
70	8	0	-1.306613	-0.557513	-3.928609
71	8	0	-6.305248	-0.067349	-3.744659
72	8	0	-5.288199	-2.498144	-3.222824

73	8	0	4.971801	-2.343797	3.577623
74	8	0	-2.643832	-2.834192	-3.363264
75	8	0	-1.539432	-5.040088	2.699357
76	8	0	0.680867	-4.534451	-1.994089
77	8	0	-4.141599	-4.393679	-1.832599
78	8	0	6.261269	-0.565829	2.230238
79	8	0	2.470410	-2.600576	4.405339
80	1	0	7.643013	3.931119	1.488424
81	1	0	7.438475	3.130062	-2.314552
82	1	0	8.527667	0.207219	1.466256
83	1	0	8.362731	-0.170186	-2.347845
84	1	0	7.540801	-2.297167	3.705915
85	1	0	7.204404	-3.476883	-4.003502
86	1	0	4.149450	-5.476451	-3.294285
87	1	0	4.163083	-4.550967	4.242996
88	1	0	0.665281	-6.256494	2.468019
89	1	0	0.410606	-6.800785	-0.952900
90	1	0	4.897280	6.221352	1.424956
91	1	0	4.861805	5.532953	-3.188696
92	1	0	1.296784	6.630554	1.057577
93	1	0	1.022215	6.135824	-2.429559
94	1	0	-3.354679	7.130485	1.390580
95	1	0	-3.324868	6.413792	-2.281302
96	1	0	-7.109641	4.114621	1.843531
97	1	0	-7.300711	3.683159	-2.177123
98	1	0	-7.148033	-1.068060	4.333057
99	1	0	-7.716114	-2.117776	-3.696332
100	1	0	-3.835350	-5.984543	2.812273
101	1	0	-3.800676	-6.692197	-0.855490
102	1	0	6.390238	-0.612017	4.729861
103	1	0	6.463048	2.875131	3.279795
104	1	0	4.238048	-2.981496	5.978481
105	1	0	0.317641	-3.774274	5.233258
106	1	0	-3.387556	-3.701726	5.220333
107	1	0	-0.950075	-0.415497	5.850407
108	1	0	-5.788453	-0.173019	6.094343
109	1	0	-5.511246	2.865530	4.689118
110	1	0	1.238456	5.399581	3.163670
111	1	0	-3.181796	5.569056	3.289572
112	1	0	-0.915004	2.937981	4.442231
113	1	0	-3.745879	5.272634	-4.358365
114	1	0	1.083300	4.934671	-4.466270
115	1	0	-5.428664	2.009927	-4.866576
116	1	0	-1.827778	1.633131	-5.106488
117	1	0	6.413197	2.538656	-4.391415
118	1	0	-6.191819	-1.896388	-5.523360
119	1	0	-4.249702	-4.530428	-4.370933
120	1	0	0.349281	-5.159128	-4.469216
121	1	0	3.594159	-4.673903	-5.628250
122	1	0	6.466790	-1.440722	-5.119035
123	1	0	-1.744039	-2.276536	-5.679127
124	14	0	-1.304490	3.123985	-2.052915
125	79	0	-0.470164	-0.108223	-1.185430
126	79	0	0.170245	-2.294427	0.116363
127	79	0	0.932397	0.104229	1.104119
128	6	0	3.443687	1.965955	4.246182
129	1	0	4.433299	1.711911	4.638795
130	1	0	3.476652	2.989250	3.863303
131	1	0	2.724503	1.920455	5.068995
132	6	0	3.058169	0.999648	3.138751

133	1	0	3.761157	0.999317	2.289436
134	1	0	3.053787	-0.051341	3.485789
135	8	0	1.776243	1.251031	2.643894
136	8	0	3.236550	1.385191	-0.897960
137	8	0	3.792276	0.455646	-0.127361
138	1	0	3.963902	1.747553	-1.461738

Zero-point correction= 0.392674 (Hartree/Particle)
Thermal correction to Energy= 0.480547
Thermal correction to Enthalpy= 0.481491
Thermal correction to Gibbs Free Energy= 0.276833
Sum of electronic and zero-point Energies= -14045.118995
Sum of electronic and thermal Energies= -14045.031122
Sum of electronic and thermal Enthalpies= -14045.030178
Sum of electronic and thermal Free Energies= -14045.234837

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -14048.5003578

INT5

Charge: 1 multiplicity: 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.280866	5.055444	0.844703
2	14	0	6.509593	3.101940	1.822689
3	14	0	4.197551	4.632993	-2.265068
4	14	0	6.290648	2.493546	-2.920681
5	8	0	5.104082	3.749107	1.328196
6	8	0	6.634735	1.740558	0.922728
7	8	0	4.321726	5.278045	-0.771894
8	8	0	4.919850	3.177544	-2.356164
9	8	0	6.091388	0.943575	-2.389329
10	14	0	-1.742469	2.110132	3.586970
11	14	0	-4.814007	2.030468	3.723644
12	14	0	-5.973185	3.379677	-1.745466
13	14	0	-3.679469	5.139920	-2.916993
14	14	0	1.174374	4.836330	-3.025996
15	14	0	-2.122990	0.840069	-3.930681
16	14	0	-5.235759	1.130074	-3.718675
17	14	0	-5.793968	3.802517	1.375797
18	14	0	-3.476927	5.753950	1.841619
19	14	0	1.320430	5.326543	1.713069
20	14	0	-1.312679	3.752123	0.941295
21	8	0	-3.250582	2.078675	4.203178
22	8	0	-5.095265	4.646358	-2.279341
23	8	0	0.108539	3.724440	-2.472865
24	8	0	-2.512305	3.999972	-2.694567
25	8	0	-5.386537	1.970820	-2.337315
26	8	0	-1.462950	1.567904	-2.594513
27	8	0	2.661191	4.302702	-2.651821
28	8	0	-5.866643	3.233306	-0.139144
29	8	0	-1.445972	2.942699	-0.455836
30	8	0	-3.707373	0.520443	-3.782824
31	8	0	-4.977178	5.218132	1.454901
32	8	0	0.207537	4.284465	1.116326
33	8	0	-2.320879	5.022608	0.920572
34	8	0	-4.987159	2.668756	2.234728
35	8	0	-1.756114	2.708960	2.083601

36	8	0	2.783304	4.698771	1.363873
37	14	0	7.135470	0.201604	1.089219
38	14	0	6.990033	-0.354786	-1.914139
39	8	0	6.952002	-0.591122	-0.311558
40	14	0	0.931821	-2.975586	4.138306
41	14	0	-1.116519	-0.722852	4.433306
42	14	0	-5.857998	-0.675289	4.709808
43	14	0	3.796447	-4.322115	-4.226230
44	14	0	-3.613193	-2.726088	4.209471
45	14	0	6.255310	-2.371050	-4.041541
46	14	0	-3.226233	-5.384392	-0.903886
47	14	0	-0.143006	-5.469167	-1.003577
48	14	0	0.833089	-4.084965	-3.573992
49	14	0	-1.466364	-2.144846	-4.268805
50	14	0	-6.398852	-1.695912	-4.100346
51	14	0	3.996617	-3.148746	4.575328
52	14	0	-4.075101	-3.606023	-3.264135
53	14	0	6.347683	-1.443696	3.584962
54	14	0	-3.094806	-4.867769	2.224398
55	14	0	0.007245	-5.029519	2.110660
56	8	0	0.167632	-1.568441	3.910790
57	8	0	-1.144081	0.601082	3.495333
58	8	0	-5.322972	0.482564	3.672943
59	8	0	-5.035523	-2.074530	4.569451
60	8	0	4.799908	-3.048073	-4.222356
61	8	0	-2.472999	-1.575068	4.216226
62	8	0	-1.694516	-5.508922	-1.493366
63	8	0	0.876505	-3.799307	2.717978
64	8	0	-3.672880	-3.434104	2.734671
65	8	0	6.315232	-1.669615	-2.562480
66	8	0	2.376919	-3.681936	-3.740922
67	8	0	-3.168481	-4.798642	0.606238
68	8	0	-0.003064	-4.726738	0.477698
69	8	0	-0.023142	-2.744820	-3.866976
70	8	0	-1.303667	-0.556291	-3.931546
71	8	0	-6.304610	-0.092571	-3.750933
72	8	0	-5.276681	-2.519066	-3.231688
73	8	0	4.980384	-2.328020	3.573133
74	8	0	-2.630419	-2.840626	-3.370835
75	8	0	-1.516537	-5.048176	2.688403
76	8	0	0.702892	-4.525001	-2.001516
77	8	0	-4.120309	-4.410072	-1.842891
78	8	0	6.259595	-0.535561	2.234129
79	8	0	2.472617	-2.589471	4.410184
80	1	0	7.618083	3.971988	1.495857
81	1	0	7.420095	3.174520	-2.308215
82	1	0	8.521971	0.252727	1.469721
83	1	0	8.361473	-0.120845	-2.344939
84	1	0	7.546647	-2.259485	3.705674
85	1	0	7.221403	-3.431472	-4.005405
86	1	0	4.176403	-5.447735	-3.300648
87	1	0	4.180320	-4.531434	4.237771
88	1	0	0.692457	-6.252775	2.458377
89	1	0	0.443014	-6.794362	-0.963330
90	1	0	4.860445	6.247939	1.433384
91	1	0	4.831568	5.565098	-3.181123
92	1	0	1.258145	6.638926	1.064173
93	1	0	0.988407	6.147081	-2.423782
94	1	0	-3.396084	7.114332	1.394689
95	1	0	-3.360163	6.402310	-2.278066

96	1	0	-7.135637	4.078511	1.841465
97	1	0	-7.321830	3.650995	-2.179841
98	1	0	-7.148773	-1.107362	4.324629
99	1	0	-7.706158	-2.150147	-3.706406
100	1	0	-3.809647	-6.004749	2.800031
101	1	0	-3.768898	-6.707689	-0.868576
102	1	0	6.386686	-0.581584	4.730921
103	1	0	6.442228	2.907718	3.285149
104	1	0	4.246004	-2.963722	5.975219
105	1	0	0.330252	-3.775924	5.226459
106	1	0	-3.375262	-3.722570	5.211169
107	1	0	-0.955273	-0.424514	5.846862
108	1	0	-5.795002	-0.207436	6.087904
109	1	0	-5.532650	2.834227	4.686572
110	1	0	1.204815	5.405150	3.168707
111	1	0	-3.216346	5.551526	3.291887
112	1	0	-0.936674	2.930824	4.442829
113	1	0	-3.773870	5.261513	-4.356708
114	1	0	1.057045	4.948787	-4.461934
115	1	0	-5.439356	1.990756	-4.870070
116	1	0	-1.836515	1.633101	-5.108183
117	1	0	6.399250	2.580354	-4.386474
118	1	0	-6.181839	-1.918627	-5.532155
119	1	0	-4.226841	-4.543956	-4.381658
120	1	0	0.375404	-5.148687	-4.477687
121	1	0	3.618475	-4.645207	-5.633990
122	1	0	6.473960	-1.397798	-5.118927
123	1	0	-1.732043	-2.275511	-5.685471
124	14	0	-1.324681	3.122759	-2.051546
125	79	0	-0.461497	-0.105704	-1.185574
126	79	0	0.204315	-2.277094	0.124144
127	79	0	0.929435	0.130989	1.113574
128	6	0	3.334015	1.586294	4.432766
129	1	0	4.402697	1.729945	4.619432
130	1	0	2.792809	2.457794	4.810917
131	1	0	3.003363	0.701463	4.984202
132	6	0	3.091747	1.398301	2.937648
133	1	0	3.414062	2.302543	2.380665
134	1	0	3.653372	0.561430	2.504507
135	8	0	1.728736	1.297459	2.654742
136	8	0	3.482016	1.007743	-0.980555
137	8	0	3.809808	0.126107	-0.040742
138	1	0	4.297822	1.122360	-1.524659

Zero-point correction= 0.393005 (Hartree/Particle)
Thermal correction to Energy= 0.480857
Thermal correction to Enthalpy= 0.481801
Thermal correction to Gibbs Free Energy= 0.277080
Sum of electronic and zero-point Energies= -14045.118987
Sum of electronic and thermal Energies= -14045.031135
Sum of electronic and thermal Enthalpies= -14045.030191
Sum of electronic and thermal Free Energies= -14045.234912

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -14048.5015541

INT6

Charge: 1 multiplicity: 1

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	14	0	3.663484	5.345528	1.047785
2	14	0	5.939559	3.549979	2.189251
3	14	0	3.791617	4.872211	-2.052379
4	14	0	6.032189	2.857821	-2.552677
5	8	0	4.529649	4.098485	1.614967
6	8	0	6.197380	2.176044	1.337013
7	8	0	3.792760	5.547446	-0.564414
8	8	0	4.611562	3.464074	-2.050043
9	8	0	5.901111	1.264349	-2.096855
10	14	0	-2.321366	2.096103	3.487533
11	14	0	-5.384768	1.843699	3.447600
12	14	0	-6.287322	3.029931	-2.108311
13	14	0	-4.028267	4.908580	-3.163694
14	14	0	0.806871	4.874088	-2.987815
15	14	0	-2.173455	0.695122	-3.995894
16	14	0	-5.296574	0.793723	-3.987765
17	14	0	-6.325016	3.522685	1.012617
18	14	0	-4.162189	5.603517	1.579345
19	14	0	0.647247	5.456625	1.733705
20	14	0	-1.844119	3.714649	0.831632
21	8	0	-3.852639	1.947420	4.023716
22	8	0	-5.455553	4.335445	-2.615539
23	8	0	-0.196048	3.706928	-2.452104
24	8	0	-2.793173	3.900933	-2.803689
25	8	0	-5.589170	1.646619	-2.631827
26	8	0	-1.698777	1.499342	-2.669257
27	8	0	2.308954	4.448864	-2.522715
28	8	0	-6.269602	2.926418	-0.490078
29	8	0	-1.813372	2.853915	-0.526302
30	8	0	-3.748999	0.251337	-3.969426
31	8	0	-5.616053	4.992776	1.131107
32	8	0	-0.385346	4.369102	1.100624
33	8	0	-2.935563	4.910603	0.728056
34	8	0	-5.495699	2.461196	1.947108
35	8	0	-2.291999	2.682986	1.988900
36	8	0	2.165161	4.909265	1.496688
37	14	0	6.780485	0.677694	1.548135
38	14	0	6.841859	0.067637	-1.464736
39	8	0	6.673575	-0.119048	0.136786
40	14	0	0.602829	-2.815265	4.295603
41	14	0	-1.572035	-0.677593	4.421706
42	14	0	-6.329904	-0.897792	4.425424
43	14	0	4.017247	-4.131806	-3.863784
44	14	0	-3.935221	-2.829541	4.094032
45	14	0	6.355895	-2.030171	-3.577387
46	14	0	-3.111284	-5.538819	-0.941442
47	14	0	-0.019541	-5.444803	-0.850162
48	14	0	1.006983	-4.044179	-3.392566
49	14	0	-1.343922	-2.233583	-4.254575
50	14	0	-6.292596	-2.086035	-4.377071
51	14	0	3.642899	-2.810217	4.910927
52	14	0	-3.910466	-3.843129	-3.380541
53	14	0	5.948281	-0.985787	4.022283
54	14	0	-3.194874	-4.971360	2.178074
55	14	0	-0.081139	-4.953548	2.246890
56	8	0	-0.193399	-1.435767	4.007335
57	8	0	-1.590601	0.636218	3.467445
58	8	0	-5.820502	0.272837	3.392739

59	8	0	-5.398772	-2.233705	4.365794
60	8	0	4.922090	-2.770367	-3.799928
61	8	0	-2.840453	-1.631038	4.124129
62	8	0	-1.534463	-5.578413	-1.422316
63	8	0	0.670232	-3.665218	2.895334
64	8	0	-3.879741	-3.567260	2.635022
65	8	0	6.280101	-1.308340	-2.106962
66	8	0	2.543171	-3.539950	-3.483370
67	8	0	-3.182692	-4.929426	0.559847
68	8	0	0.022078	-4.666733	0.616671
69	8	0	0.109769	-2.760394	-3.753797
70	8	0	-1.272571	-0.649314	-3.961857
71	8	0	-6.314041	-0.478013	-4.052524
72	8	0	-5.176013	-2.834701	-3.432770
73	8	0	4.630959	-1.940246	3.952709
74	8	0	-2.499941	-3.013967	-3.408778
75	8	0	-1.634089	-5.053782	2.725675
76	8	0	0.843508	-4.476713	-1.819466
77	8	0	-3.997299	-4.637177	-1.950980
78	8	0	5.890294	-0.116370	2.643886
79	8	0	2.104319	-2.343442	4.649933
80	1	0	7.026510	4.463393	1.909920
81	1	0	7.097567	3.596955	-1.883683
82	1	0	8.140905	0.802810	2.005781
83	1	0	8.225701	0.361532	-1.804090
84	1	0	7.180969	-1.726815	4.228729
85	1	0	7.375289	-3.034924	-3.464830
86	1	0	4.414070	-5.213143	-2.898776
87	1	0	3.924171	-4.181568	4.608744
88	1	0	0.650385	-6.129653	2.664164
89	1	0	0.632891	-6.737527	-0.755434
90	1	0	4.152279	6.574453	1.645670
91	1	0	4.432617	5.819631	-2.949046
92	1	0	0.561280	6.750176	1.062389
93	1	0	0.524811	6.189555	-2.425399
94	1	0	-4.123798	6.960020	1.115329
95	1	0	-3.832282	6.194513	-2.535189
96	1	0	-7.704077	3.719788	1.403073
97	1	0	-7.629735	3.219996	-2.613516
98	1	0	-7.567178	-1.419054	3.978537
99	1	0	-7.592835	-2.616603	-4.050210
100	1	0	-3.870889	-6.137612	2.741204
101	1	0	-3.575335	-6.893743	-0.905044
102	1	0	5.869247	-0.103312	5.153708
103	1	0	5.810604	3.360397	3.648124
104	1	0	3.798555	-2.585983	6.317274
105	1	0	-0.014001	-3.635302	5.359673
106	1	0	-3.709241	-3.797041	5.129991
107	1	0	-1.522488	-0.354863	5.841818
108	1	0	-6.372490	-0.414994	5.799593
109	1	0	-6.202215	2.614721	4.358694
110	1	0	0.455178	5.548066	3.183233
111	1	0	-3.966767	5.439796	3.048813
112	1	0	-1.612853	2.973767	4.378245
113	1	0	-4.057872	4.999621	-4.612451
114	1	0	0.780887	4.965830	-4.433286
115	1	0	-5.501396	1.630258	-5.159166
116	1	0	-1.876169	1.478224	-5.182474
117	1	0	6.235739	2.912514	-4.005738
118	1	0	-5.979860	-2.325398	-5.789180

119	1	0	-3.949227	-4.814869	-4.478804
120	1	0	0.677673	-5.153208	-4.298206
121	1	0	3.948977	-4.480533	-5.275071
122	1	0	6.579729	-1.065482	-4.657641
123	1	0	-1.515632	-2.426046	-5.679197
124	14	0	-1.623941	3.016735	-2.123888
125	79	0	1.998516	-0.422865	-1.222480
126	79	0	0.783108	-2.262583	0.260116
127	79	0	1.055133	0.187248	1.269023
128	6	0	2.842240	1.286765	4.129439
129	1	0	2.971649	0.404196	3.500963
130	1	0	2.558199	0.979513	5.144934
131	1	0	4.190027	0.722614	-2.550634
132	6	0	1.789160	2.194743	3.605966
133	1	0	3.783929	1.839053	4.224351
134	1	0	1.646869	3.152822	4.133768
135	8	0	1.048795	1.969417	2.652545
136	1	0	3.514231	-1.158699	-3.801782
137	8	0	3.277018	0.493617	-2.844855
138	8	0	3.500453	-0.223351	-4.087460

Zero-point correction= 0.395705 (Hartree/Particle)
Thermal correction to Energy= 0.483220
Thermal correction to Enthalpy= 0.484164
Thermal correction to Gibbs Free Energy= 0.281745
Sum of electronic and zero-point Energies= -14045.214097
Sum of electronic and thermal Energies= -14045.126582
Sum of electronic and thermal Enthalpies= -14045.125638
Sum of electronic and thermal Free Energies= -14045.328057

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -14048.5873605

INT3a

Charge: 1 multiplicity: 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.300953	5.071405	0.754302
2	14	0	6.545396	3.131835	1.705435
3	14	0	4.180974	4.635722	-2.348097
4	14	0	6.249509	2.494198	-3.032703
5	8	0	5.128963	3.770313	1.244057
6	8	0	6.674846	1.767369	0.818368
7	8	0	4.304754	5.301031	-0.858019
8	8	0	4.908578	3.197274	-2.428955
9	8	0	6.108822	0.933549	-2.574453
10	14	0	-1.677087	2.123752	3.596437
11	14	0	-4.748507	2.060632	3.772899
12	14	0	-5.988215	3.382095	-1.673856
13	14	0	-3.717188	5.144307	-2.882130
14	14	0	1.145904	4.841597	-3.065782
15	14	0	-2.181894	0.839930	-3.915374
16	14	0	-5.285300	1.125840	-3.650496
17	14	0	-5.761596	3.828339	1.440110
18	14	0	-3.444865	5.767777	1.872366
19	14	0	1.358927	5.344296	1.671173
20	14	0	-1.288249	3.759540	0.940215
21	8	0	-3.175249	2.059720	4.232948

22	8	0	-5.124984	4.649506	-2.225745
23	8	0	0.081448	3.730532	-2.496019
24	8	0	-2.544160	4.014472	-2.665452
25	8	0	-5.409402	1.970443	-2.267702
26	8	0	-1.518704	1.584707	-2.595072
27	8	0	2.633097	4.313115	-2.710284
28	8	0	-5.853799	3.244437	-0.067042
29	8	0	-1.437512	2.950258	-0.452904
30	8	0	-3.762375	0.508715	-3.747050
31	8	0	-4.958505	5.251679	1.506673
32	8	0	0.228583	4.297408	1.109220
33	8	0	-2.312800	5.016320	0.940202
34	8	0	-4.916648	2.715292	2.293871
35	8	0	-1.703428	2.706733	2.091114
36	8	0	2.812952	4.714910	1.310042
37	14	0	7.172460	0.229371	0.948561
38	14	0	6.969614	-0.338723	-2.049674
39	8	0	6.945571	-0.566677	-0.435915
40	14	0	1.027371	-2.949440	4.129364
41	14	0	-0.994468	-0.708720	4.442092
42	14	0	-5.770093	-0.633865	4.783858
43	14	0	3.754070	-4.314921	-4.285128
44	14	0	-3.495574	-2.721387	4.242059
45	14	0	6.211903	-2.360518	-4.136659
46	14	0	-3.222124	-5.379998	-0.860738
47	14	0	-0.143357	-5.465663	-1.005861
48	14	0	0.798594	-4.081310	-3.588471
49	14	0	-1.516178	-2.145238	-4.249388
50	14	0	-6.448391	-1.698952	-4.006542
51	14	0	4.110867	-3.128054	4.506917
52	14	0	-4.109531	-3.604121	-3.204499
53	14	0	6.429304	-1.404970	3.468891
54	14	0	-3.051528	-4.862917	2.262864
55	14	0	0.042323	-5.014696	2.114169
56	8	0	0.392821	-1.449540	3.983101
57	8	0	-1.060722	0.614764	3.509799
58	8	0	-5.303056	0.529791	3.723189
59	8	0	-4.850677	-1.966563	4.636834
60	8	0	4.753354	-3.042311	-4.301307
61	8	0	-2.244478	-1.685905	4.171341
62	8	0	-1.701163	-5.507651	-1.474662
63	8	0	0.877103	-3.750075	2.710722
64	8	0	-3.648793	-3.439316	2.782459
65	8	0	6.305928	-1.686492	-2.649868
66	8	0	2.337633	-3.680310	-3.777133
67	8	0	-3.136143	-4.790365	0.648082
68	8	0	0.004540	-4.728603	0.480722
69	8	0	-0.068432	-2.744074	-3.865939
70	8	0	-1.357864	-0.555455	-3.910724
71	8	0	-6.357755	-0.094528	-3.660259
72	8	0	-5.310388	-2.517223	-3.153258
73	8	0	5.060261	-2.293445	3.489378
74	8	0	-2.666371	-2.841877	-3.332752
75	8	0	-1.470573	-5.042509	2.718121
76	8	0	0.688910	-4.521391	-2.011604
77	8	0	-4.135091	-4.407432	-1.780933
78	8	0	6.301486	-0.500534	2.119083
79	8	0	2.581049	-2.586325	4.346337
80	1	0	7.649686	3.993677	1.358310
81	1	0	7.393469	3.187015	-2.440346

82	1	0	8.556865	0.275265	1.326889
83	1	0	8.337465	-0.107518	-2.483930
84	1	0	7.618939	-2.232572	3.583647
85	1	0	7.175021	-3.423175	-4.118653
86	1	0	4.143362	-5.440690	-3.361878
87	1	0	4.263566	-4.506492	4.173385
88	1	0	0.750182	-6.235418	2.452509
89	1	0	0.448121	-6.785378	-0.963626
90	1	0	4.889246	6.266908	1.333354
91	1	0	4.789295	5.573011	-3.278532
92	1	0	1.281214	6.653520	1.019240
93	1	0	0.957793	6.153097	-2.462899
94	1	0	-3.367763	7.125188	1.420995
95	1	0	-3.388238	6.404485	-2.250184
96	1	0	-7.096883	4.086837	1.933027
97	1	0	-7.345147	3.649598	-2.083879
98	1	0	-7.066226	-1.093135	4.428319
99	1	0	-7.747361	-2.155520	-3.590596
100	1	0	-3.746316	-5.990913	2.863541
101	1	0	-3.761905	-6.702521	-0.803589
102	1	0	6.473382	-0.553360	4.622848
103	1	0	6.503071	2.932507	3.168177
104	1	0	4.354687	-2.934598	5.905897
105	1	0	0.428580	-3.752344	5.220035
106	1	0	-3.276774	-3.702597	5.262242
107	1	0	-0.850493	-0.400712	5.852448
108	1	0	-5.686103	-0.187723	6.168203
109	1	0	-5.448612	2.850855	4.755791
110	1	0	1.261866	5.424647	3.127276
111	1	0	-3.156989	5.567066	3.318851
112	1	0	-0.857081	2.951299	4.440383
113	1	0	-3.833072	5.258360	-4.319445
114	1	0	0.995933	4.950039	-4.499044
115	1	0	-5.503066	1.984790	-4.799132
116	1	0	-1.904007	1.630040	-5.092394
117	1	0	6.341033	2.586934	-4.501076
118	1	0	-6.251845	-1.926866	-5.440368
119	1	0	-4.276570	-4.547574	-4.314220
120	1	0	0.324225	-5.148097	-4.480373
121	1	0	3.548424	-4.644242	-5.688150
122	1	0	6.408324	-1.392871	-5.225213
123	1	0	-1.804615	-2.279827	-5.662017
124	14	0	-1.343702	3.134753	-2.052373
125	79	0	-0.537136	-0.100969	-1.219048
126	79	0	0.097228	-2.312353	0.075712
127	79	0	0.909560	0.100472	1.006456
128	6	0	3.728705	1.321893	4.596413
129	1	0	4.743544	1.726727	4.596176
130	1	0	3.126969	1.929394	5.291829
131	1	0	3.769239	0.304153	5.002280
132	6	0	3.162498	1.347412	3.218318
133	1	0	3.273578	2.215967	2.573996
134	1	0	4.079396	0.434619	1.484844
135	8	0	1.918264	0.763895	3.038855
136	8	0	3.029939	1.117058	0.100468
137	8	0	4.040518	0.338475	0.495998
138	1	0	1.765657	-0.004392	3.621529

Zero-point correction= 0.393613 (Hartree/Particle)
Thermal correction to Energy= 0.477250

Thermal correction to Enthalpy= 0.478994
Thermal correction to Gibbs Free Energy= 0.279061
Sum of electronic and zero-point Energies= -14045.111616
Sum of electronic and thermal Energies= -14045.027979
Sum of electronic and thermal Enthalpies= -14045.026235
Sum of electronic and thermal Free Energies= -14045.226168

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -14048.492639

INT3b

Charge: 1 multiplicity: 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	3.480317	5.431010	0.921789
2	14	0	5.828223	3.735172	2.100156
3	14	0	3.576936	4.853758	-2.147900
4	14	0	5.869548	2.895297	-2.617383
5	8	0	4.422897	4.234822	1.466372
6	8	0	6.109351	2.330512	1.298585
7	8	0	3.545814	5.605263	-0.698890
8	8	0	4.441342	3.480789	-2.102040
9	8	0	5.842743	1.329649	-2.119756
10	14	0	-2.365739	2.050988	3.581567
11	14	0	-5.422105	1.690885	3.590743
12	14	0	-6.447906	2.686180	-1.979331
13	14	0	-4.268668	4.590759	-3.139834
14	14	0	0.589748	4.738316	-3.039725
15	14	0	-2.277537	0.423189	-3.870518
16	14	0	-5.414665	0.427854	-3.806759
17	14	0	-6.446013	3.265699	1.121737
18	14	0	-4.336841	5.438963	1.582998
19	14	0	0.478659	5.448211	1.673368
20	14	0	-1.962910	3.600700	0.875216
21	8	0	-3.885715	1.867691	4.131696
22	8	0	-5.665619	4.003330	-2.539970
23	8	0	-0.397361	3.570899	-2.459303
24	8	0	-3.021406	3.566252	-2.802998
25	8	0	-5.709166	1.313657	-2.478175
26	8	0	-1.704342	1.266195	-2.568953
27	8	0	2.100872	4.351252	-2.587957
28	8	0	-6.399808	2.621566	-0.364259
29	8	0	-1.952429	2.708450	-0.477627
30	8	0	-3.831038	-0.031336	-3.766497
31	8	0	-5.764194	4.753035	1.158318
32	8	0	-0.501203	4.272542	1.082473
33	8	0	-3.076106	4.774192	0.750617
34	8	0	-5.572475	2.259990	2.071350
35	8	0	-2.364989	2.575500	2.050272
36	8	0	2.006800	4.939758	1.401647
37	14	0	6.752726	0.862233	1.538567
38	14	0	6.784692	0.193707	-1.459978
39	8	0	6.636246	0.012706	0.149615
40	14	0	0.725468	-2.745611	4.469097
41	14	0	-1.518252	-0.676509	4.584741
42	14	0	-6.257199	-1.048020	4.665799
43	14	0	4.060046	-4.195306	-3.678083
44	14	0	-3.812259	-2.905676	4.349109

45	14	0	6.333620	-2.014416	-3.496414
46	14	0	-2.939516	-5.744771	-0.598801
47	14	0	0.112252	-5.542784	-0.549385
48	14	0	1.061550	-4.207132	-3.142266
49	14	0	-1.360288	-2.509071	-4.042777
50	14	0	-6.306206	-2.512901	-4.096433
51	14	0	3.763910	-2.607515	5.055607
52	14	0	-3.865932	-4.164578	-3.065983
53	14	0	6.001313	-0.745493	4.080926
54	14	0	-2.997440	-5.076033	2.511380
55	14	0	0.087219	-4.952197	2.517117
56	8	0	-0.138386	-1.408838	4.142055
57	8	0	-1.588245	0.608483	3.571323
58	8	0	-5.805210	0.108457	3.586836
59	8	0	-5.298890	-2.362448	4.625619
60	8	0	4.948391	-2.827373	-3.648588
61	8	0	-2.788343	-1.642974	4.339582
62	8	0	-1.393558	-5.744529	-1.160776
63	8	0	0.829319	-3.626934	3.101608
64	8	0	-3.750070	-3.682397	2.912276
65	8	0	6.238597	-1.259591	-2.012380
66	8	0	2.574137	-3.651835	-3.283779
67	8	0	-2.995898	-5.102227	0.888336
68	8	0	0.068828	-4.803294	0.896178
69	8	0	0.112810	-2.958354	-3.549270
70	8	0	-1.324936	-0.893353	-3.773366
71	8	0	-6.358771	-0.892742	-3.822449
72	8	0	-5.165393	-3.198534	-3.140145
73	8	0	4.714143	-1.737821	4.053272
74	8	0	-2.504219	-3.252145	-3.165498
75	8	0	-1.449201	-5.059454	3.083410
76	8	0	0.929941	-4.566870	-1.561249
77	8	0	-3.892078	-4.895445	-1.609349
78	8	0	5.906314	0.058057	2.658275
79	8	0	2.210261	-2.194097	4.798251
80	1	0	6.875466	4.675414	1.775297
81	1	0	6.920826	3.691955	-1.989938
82	1	0	8.111631	1.058050	1.968388
83	1	0	8.156468	0.499217	-1.826676
84	1	0	7.267952	-1.429711	4.283681
85	1	0	7.395321	-2.974127	-3.367331
86	1	0	4.516273	-5.228812	-2.688148
87	1	0	4.100028	-3.976215	4.790143
88	1	0	0.865129	-6.090835	2.957850
89	1	0	0.818706	-6.807146	-0.440434
90	1	0	3.929309	6.682116	1.489657
91	1	0	4.168773	5.791582	-3.083153
92	1	0	0.326562	6.721920	0.956262
93	1	0	0.258680	6.050080	-2.511336
94	1	0	-4.361672	6.780273	1.074569
95	1	0	-4.097225	5.909350	-2.554343
96	1	0	-7.828175	3.435630	1.518278
97	1	0	-7.794867	2.811426	-2.481393
98	1	0	-7.484351	-1.611753	4.250480
99	1	0	-7.585297	-3.063479	-3.735584
100	1	0	-3.651883	-6.243905	3.104494
101	1	0	-3.383722	-7.105304	-0.520431
102	1	0	5.916585	0.178584	5.177634
103	1	0	5.721764	3.589144	3.565657
104	1	0	3.946148	-2.332261	6.449788

105	1	0	0.157079	-3.535392	5.584012
106	1	0	-3.533645	-3.824786	5.416260
107	1	0	-1.452034	-0.292089	5.986706
108	1	0	-6.297586	-0.512036	6.020760
109	1	0	-6.248360	2.474472	4.483570
110	1	0	0.290705	5.584840	3.114979
111	1	0	-4.126708	5.328062	3.051937
112	1	0	-1.673564	2.983541	4.421350
113	1	0	-4.312911	4.642391	-4.589525
114	1	0	0.526439	4.772350	-4.483735
115	1	0	-5.651729	1.212105	-5.008575
116	1	0	-2.024151	1.177831	-5.082782
117	1	0	6.051824	2.912791	-4.076104
118	1	0	-6.007913	-2.775060	-5.507361
119	1	0	-3.877408	-5.154102	-4.151222
120	1	0	0.760273	-5.335315	-4.031239
121	1	0	3.993191	-4.587496	-5.078733
122	1	0	6.517987	-1.070523	-4.608699
123	1	0	-1.541684	-2.726380	-5.462843
124	14	0	-1.780366	2.837758	-2.074387
125	79	0	0.181000	-0.089655	-1.606354
126	79	0	2.242873	-1.480214	-0.700066
127	79	0	1.545526	0.862249	0.569035
128	6	0	2.760605	1.570195	2.194353
129	1	0	3.742015	1.173208	1.941176
130	1	0	5.339025	-2.154355	-0.772921
131	1	0	2.635853	2.631793	1.963278
132	6	0	2.265428	1.173082	3.550122
133	1	0	2.286781	0.084984	3.689351
134	1	0	2.983603	1.587418	4.280583
135	8	0	0.999764	1.717931	3.868265
136	8	0	5.121714	-2.888349	-0.128564
137	8	0	3.804918	-2.977337	0.013394
138	1	0	0.317174	1.133971	3.505272

Zero-point correction= 0.395270 (Hartree/Particle)
Thermal correction to Energy= 0.481764
Thermal correction to Enthalpy= 0.482708
Thermal correction to Gibbs Free Energy= 0.282185
Sum of electronic and zero-point Energies= -14045.127671
Sum of electronic and thermal Energies= -14045.041177
Sum of electronic and thermal Enthalpies= -14045.040233
Sum of electronic and thermal Free Energies= -14045.240757

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -14048.4979998

TS4

Charge: 1 multiplicity: 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.157209	5.178496	0.687655
2	14	0	6.440932	3.319026	1.700663
3	14	0	4.077965	4.671247	-2.399195
4	14	0	6.202204	2.570374	-3.026392
5	8	0	5.019126	3.917104	1.213021
6	8	0	6.607011	1.940513	0.834115
7	8	0	4.192731	5.377423	-0.931417

8	8	0	4.834771	3.243288	-2.448921
9	8	0	6.096628	1.013126	-2.542546
10	14	0	-1.755942	2.135895	3.549010
11	14	0	-4.830942	2.020015	3.699790
12	14	0	-6.060119	3.171955	-1.768886
13	14	0	-3.824142	4.955704	-2.998350
14	14	0	1.043602	4.781738	-3.141196
15	14	0	-2.164264	0.677389	-3.922264
16	14	0	-5.280619	0.889156	-3.684014
17	14	0	-5.868951	3.714626	1.334135
18	14	0	-3.622619	5.693861	1.744255
19	14	0	1.202466	5.388928	1.580818
20	14	0	-1.409916	3.719186	0.861653
21	8	0	-3.260410	2.002265	4.175871
22	8	0	-5.233269	4.446879	-2.354185
23	8	0	-0.000775	3.664931	-2.550440
24	8	0	-2.636024	3.848332	-2.745070
25	8	0	-5.447664	1.757739	-2.320176
26	8	0	-1.501625	1.461391	-2.627181
27	8	0	2.540273	4.297152	-2.760996
28	8	0	-5.922763	3.090494	-0.157668
29	8	0	-1.512144	2.862771	-0.506719
30	8	0	-3.738717	0.317902	-3.744688
31	8	0	-5.142759	5.177519	1.395941
32	8	0	0.061929	4.353552	1.023913
33	8	0	-2.513916	4.908793	0.816906
34	8	0	-4.970277	2.665033	2.216965
35	8	0	-1.797605	2.679454	2.038098
36	8	0	2.665350	4.799448	1.201991
37	14	0	7.151325	0.425688	1.011159
38	14	0	6.988979	-0.219602	-1.977109
39	8	0	6.933225	-0.404109	-0.359168
40	14	0	1.100958	-2.893922	4.216215
41	14	0	-0.994828	-0.654614	4.472340
42	14	0	-5.776821	-0.664862	4.760220
43	14	0	3.897025	-4.329992	-4.145957
44	14	0	-3.383921	-2.746620	4.280481
45	14	0	6.302163	-2.308654	-4.022921
46	14	0	-3.075919	-5.503358	-0.754353
47	14	0	0.012616	-5.507084	-0.870472
48	14	0	0.931714	-4.156582	-3.477561
49	14	0	-1.428379	-2.297189	-4.193716
50	14	0	-6.372433	-1.973951	-3.990646
51	14	0	4.195658	-2.949906	4.619409
52	14	0	-3.989963	-3.798922	-3.137066
53	14	0	6.448289	-1.174970	3.555064
54	14	0	-2.951143	-4.922670	2.352223
55	14	0	0.141123	-4.995920	2.218939
56	8	0	0.543443	-1.287775	4.113302
57	8	0	-1.140093	0.611569	3.507095
58	8	0	-5.432962	0.505473	3.664312
59	8	0	-4.644158	-1.830863	4.630131
60	8	0	4.863272	-3.032693	-4.180814
61	8	0	-1.989622	-1.877543	4.171453
62	8	0	-1.543732	-5.601624	-1.339639
63	8	0	0.868662	-3.644907	2.802319
64	8	0	-3.586939	-3.504025	2.852980
65	8	0	6.367922	-1.599875	-2.550860
66	8	0	2.461595	-3.720155	-3.663173
67	8	0	-3.037607	-4.871829	0.741457

68	8	0	0.151863	-4.745763	0.596519
69	8	0	0.032519	-2.851601	-3.793672
70	8	0	-1.309496	-0.697968	-3.902429
71	8	0	-6.319128	-0.361850	-3.677775
72	8	0	-5.220501	-2.745762	-3.112843
73	8	0	5.105435	-2.108882	3.585542
74	8	0	-2.565542	-3.004476	-3.267320
75	8	0	-1.371130	-5.074428	2.816718
76	8	0	0.825083	-4.562313	-1.891250
77	8	0	-4.008991	-4.579832	-1.700798
78	8	0	6.306803	-0.318440	2.185876
79	8	0	2.633901	-2.515843	4.423938
80	1	0	7.534078	4.197377	1.341025
81	1	0	7.325840	3.302417	-2.440751
82	1	0	8.537880	0.504159	1.396509
83	1	0	8.355506	0.033534	-2.406417
84	1	0	7.649548	-1.978019	3.701192
85	1	0	7.291316	-3.345938	-3.976076
86	1	0	4.307881	-5.425251	-3.195311
87	1	0	4.350368	-4.325669	4.318438
88	1	0	0.895544	-6.182808	2.612796
89	1	0	0.631907	-6.813965	-0.792484
90	1	0	4.715677	6.396538	1.248573
91	1	0	4.666477	5.600800	-3.347654
92	1	0	1.101129	6.681763	0.902613
93	1	0	0.815500	6.097958	-2.569829
94	1	0	-3.561278	7.040236	1.263700
95	1	0	-3.536989	6.240101	-2.390949
96	1	0	-7.213633	3.917099	1.817483
97	1	0	-7.421995	3.386842	-2.190476
98	1	0	-7.065901	-1.205171	4.425145
99	1	0	-7.662364	-2.458005	-3.573000
100	1	0	-3.608692	-6.047054	2.989061
101	1	0	-3.579805	-6.837903	-0.661718
102	1	0	6.453366	-0.307294	4.696089
103	1	0	6.402669	3.145919	3.166067
104	1	0	4.388300	-2.714872	6.016869
105	1	0	0.489748	-3.649666	5.323393
106	1	0	-3.215853	-3.695980	5.340371
107	1	0	-0.880529	-0.319775	5.874325
108	1	0	-5.722160	-0.226596	6.153854
109	1	0	-5.553793	2.785942	4.677179
110	1	0	1.098820	5.498608	3.036733
111	1	0	-3.323484	5.529488	3.196369
112	1	0	-0.964319	2.999631	4.389562
113	1	0	-3.937215	5.038311	-4.437705
114	1	0	0.899352	4.852575	-4.578979
115	1	0	-5.518066	1.712568	-4.856799
116	1	0	-1.908895	1.445686	-5.118691
117	1	0	6.303994	2.630631	-4.494737
118	1	0	-6.160238	-2.230309	-5.417532
119	1	0	-4.125479	-4.773513	-4.221738
120	1	0	0.490445	-5.256902	-4.344783
121	1	0	3.708919	-4.695087	-5.542206
122	1	0	6.479919	-1.360766	-5.131569
123	1	0	-1.703877	-2.471504	-5.602440
124	14	0	-1.405924	3.024453	-2.106719
125	79	0	-0.265812	-0.124719	-1.297589
126	79	0	0.547090	-2.198853	0.085003
127	79	0	1.067622	0.312634	1.019950

128	8	0	1.676453	1.607555	2.577571
129	6	0	2.585205	1.168049	3.424382
130	6	0	3.054895	2.198414	4.441561
131	1	0	3.412128	0.573345	3.006625
132	1	0	2.200952	2.676149	4.928690
133	1	0	3.706144	1.750843	5.198927
134	1	0	3.615929	2.967679	3.901465
135	1	0	1.427007	-0.480786	4.152106
136	1	0	2.119974	0.259996	4.207989

Zero-point correction= 0.382929 (Hartree/Particle)
Thermal correction to Energy= 0.466140
Thermal correction to Enthalpy= 0.467084
Thermal correction to Gibbs Free Energy= 0.275303
Sum of electronic and zero-point Energies= -13894.769590
Sum of electronic and thermal Energies= -13894.686379
Sum of electronic and thermal Enthalpies= -13894.685435
Sum of electronic and thermal Free Energies= -13894.877216

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -13898.0877956

TS1

Charge: 1 multiplicity: 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.192967	5.040150	1.442341
2	14	0	-6.374709	3.051356	2.434545
3	14	0	-4.283969	4.786446	-1.674102
4	14	0	-6.410635	2.688255	-2.345011
5	8	0	-5.018362	3.733467	1.880435
6	8	0	-6.568455	1.741079	1.472670
7	8	0	-4.301005	5.372598	-0.157433
8	8	0	-5.011279	3.343277	-1.813480
9	8	0	-6.232852	1.100340	-1.999641
10	14	0	1.936353	1.915972	3.702190
11	14	0	5.017285	1.819681	3.675378
12	14	0	5.903098	3.460788	-1.759442
13	14	0	3.563239	5.289777	-2.715520
14	14	0	-1.305535	5.024109	-2.587575
15	14	0	1.913791	1.064127	-3.868014
16	14	0	5.041937	1.325963	-3.807576
17	14	0	5.887238	3.722113	1.385652
18	14	0	3.619896	5.644897	2.072630
19	14	0	-1.195835	5.253409	2.175239
20	14	0	1.389926	3.703960	1.177843
21	8	0	3.473759	1.800334	4.227113
22	8	0	5.008022	4.754952	-2.185978
23	8	0	-0.217032	3.876076	-2.147711
24	8	0	2.401706	4.142873	-2.485237
25	8	0	5.281106	2.085258	-2.392685
26	8	0	1.294343	1.726623	-2.482685
27	8	0	-2.768761	4.465396	-2.176748
28	8	0	5.869635	3.233256	-0.159090
29	8	0	1.425798	2.955411	-0.263259
30	8	0	3.502116	0.737459	-3.805218
31	8	0	5.106028	5.143680	1.592007
32	8	0	-0.097599	4.254664	1.470327

33	8	0	2.441712	4.938874	1.159982
34	8	0	5.103342	2.554925	2.224843
35	8	0	1.874307	2.581790	2.231379
36	8	0	-2.670249	4.671243	1.856608
37	14	0	-7.064041	0.202373	1.571534
38	14	0	-7.075779	-0.190933	-1.469463
39	8	0	-6.914731	-0.498222	0.115700
40	14	0	-0.746936	-3.181134	4.119995
41	14	0	1.321556	-0.952413	4.429319
42	14	0	6.093180	-0.934221	4.459787
43	14	0	-4.046821	-4.051489	-4.142864
44	14	0	3.796387	-2.947873	3.966649
45	14	0	-6.476811	-2.098720	-3.717834
46	14	0	3.139777	-5.327825	-1.254690
47	14	0	0.064578	-5.400113	-1.202656
48	14	0	-1.043956	-3.868929	-3.630736
49	14	0	1.234107	-1.901665	-4.341563
50	14	0	6.168180	-1.483730	-4.407431
51	14	0	-3.791305	-3.357286	4.706104
52	14	0	3.879837	-3.427676	-3.554026
53	14	0	-6.166796	-1.583099	3.928863
54	14	0	3.173161	-4.981915	1.901818
55	14	0	0.079012	-5.130090	1.947820
56	8	0	-0.001714	-1.749853	3.914863
57	8	0	1.272185	0.427523	3.564197
58	8	0	5.536186	0.283747	3.506732
59	8	0	5.230222	-2.305183	4.287402
60	8	0	-5.029093	-2.768522	-4.014152
61	8	0	2.650360	-1.801946	4.075181
62	8	0	1.583250	-5.418652	-1.784959
63	8	0	-0.741498	-3.919870	2.651448
64	8	0	3.783445	-3.577320	2.454517
65	8	0	-6.456829	-1.499340	-2.198759
66	8	0	-2.591335	-3.456901	-3.693867
67	8	0	3.148894	-4.824776	0.287041
68	8	0	0.032291	-4.752379	0.329154
69	8	0	-0.191831	-2.516375	-3.893958
70	8	0	1.091764	-0.333672	-3.909666
71	8	0	6.091770	0.096689	-3.966296
72	8	0	5.088065	-2.350327	-3.526476
73	8	0	-4.814842	-2.487383	3.798810
74	8	0	2.436039	-2.648773	-3.540642
75	8	0	1.626410	-5.187771	2.451847
76	8	0	-0.820556	-4.379276	-2.087213
77	8	0	3.991475	-4.303080	-2.178892
78	8	0	-6.142812	-0.627280	2.613585
79	8	0	-2.265866	-2.814637	4.482750
80	1	0	-7.497952	3.936517	2.209481
81	1	0	-7.503063	3.345918	-1.637187
82	1	0	-8.430045	0.228497	2.029572
83	1	0	-8.469861	0.061999	-1.802843
84	1	0	-7.359366	-2.406060	4.072782
85	1	0	-7.442147	-3.158904	-3.696796
86	1	0	-4.380047	-5.224820	-3.261387
87	1	0	-3.987241	-4.719418	4.305479
88	1	0	-0.609207	-6.358080	2.256695
89	1	0	-0.540974	-6.713996	-1.197608
90	1	0	-4.730225	6.199554	2.126555
91	1	0	-4.945277	5.768147	-2.513410
92	1	0	-1.149018	6.593056	1.592067

93	1	0	-1.063638	6.290112	-1.926550
94	1	0	3.519511	7.027801	1.705178
95	1	0	3.288218	6.516556	-1.994000
96	1	0	7.254173	3.954513	1.792077
97	1	0	7.228948	3.745230	-2.250671
98	1	0	7.356645	-1.358597	3.987454
99	1	0	7.490136	-1.966173	-4.106289
100	1	0	3.906009	-6.150103	2.376219
101	1	0	3.671020	-6.652560	-1.317850
102	1	0	-6.135338	-0.791835	5.125399
103	1	0	-6.239401	2.771050	3.875055
104	1	0	-3.951175	-3.248123	6.126111
105	1	0	-0.085585	-4.036924	5.131801
106	1	0	3.614463	-4.000201	4.926568
107	1	0	1.255445	-0.730327	5.864437
108	1	0	6.102676	-0.549433	5.864793
109	1	0	5.791091	2.565015	4.645410
110	1	0	-0.996239	5.246381	3.621169
111	1	0	3.426355	5.365036	3.521944
112	1	0	1.189621	2.696457	4.646368
113	1	0	3.585546	5.488278	-4.149905
114	1	0	-1.246705	5.204575	-4.020011
115	1	0	5.197433	2.242478	-4.925142
116	1	0	1.584478	1.915264	-4.993710
117	1	0	-6.595626	2.860866	-3.794875
118	1	0	5.875226	-1.628605	-5.835074
119	1	0	3.962557	-4.303316	-4.727811
120	1	0	-0.642826	-4.880170	-4.616736
121	1	0	-3.937493	-4.299343	-5.573839
122	1	0	-6.737990	-1.071280	-4.736253
123	1	0	1.420861	-1.955576	-5.775505
124	14	0	1.232792	3.246368	-1.836667
125	79	0	-0.132249	-2.326522	0.109571
126	79	0	-0.869863	-0.136976	1.516046
127	79	0	0.029352	0.024741	-1.142855
128	6	0	-2.632509	0.133776	-3.758261
129	1	0	-2.955946	0.673328	-4.655907
130	1	0	-3.370567	-0.637615	-3.530184
131	1	0	-1.683605	-0.360447	-3.979917
132	6	0	-2.495762	1.109424	-2.607979
133	1	0	-3.442766	1.621345	-2.392881
134	1	0	-1.763269	1.897433	-2.820307
135	8	0	-2.151833	0.440846	-1.381487
136	1	0	-2.446171	1.136577	-0.440202
137	8	0	-2.838091	1.868931	0.462786
138	8	0	-2.331762	1.535688	1.630900

Zero-point correction= 0.390407 (Hartree/Particle)
Thermal correction to Energy= 0.476797
Thermal correction to Enthalpy= 0.477741
Thermal correction to Gibbs Free Energy= 0.276760
Sum of electronic and zero-point Energies= -14045.106548
Sum of electronic and thermal Energies= -14045.020159
Sum of electronic and thermal Enthalpies= -14045.019215
Sum of electronic and thermal Free Energies= -14045.220195

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -14048.491806

TS1a

Charge: 1 multiplicity: 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.333521	5.054345	0.748815
2	14	0	6.572015	3.109474	1.701847
3	14	0	4.211291	4.613085	-2.354434
4	14	0	6.272244	2.462105	-3.034083
5	8	0	5.154203	3.751381	1.244346
6	8	0	6.711274	1.751254	0.811616
7	8	0	4.333277	5.279230	-0.863926
8	8	0	4.933795	3.172012	-2.430945
9	8	0	6.124315	0.902477	-2.576273
10	14	0	-1.660009	2.139263	3.595450
11	14	0	-4.730440	2.088997	3.769547
12	14	0	-5.962390	3.400428	-1.681000
13	14	0	-3.684077	5.152143	-2.891942
14	14	0	1.176716	4.828410	-3.073597
15	14	0	-2.171607	0.838664	-3.917921
16	14	0	-5.271118	1.136354	-3.652085
17	14	0	-5.735469	3.853402	1.432098
18	14	0	-3.410740	5.784746	1.861396
19	14	0	1.390094	5.343092	1.662186
20	14	0	-1.261588	3.765153	0.933351
21	8	0	-3.158349	2.093168	4.231674
22	8	0	-5.094016	4.662637	-2.236222
23	8	0	0.109866	3.719024	-2.504243
24	8	0	-2.512866	4.022465	-2.670034
25	8	0	-5.388782	1.984652	-2.270983
26	8	0	-1.510737	1.586131	-2.600078
27	8	0	2.662174	4.295678	-2.716095
28	8	0	-5.828649	3.267033	-0.073922
29	8	0	-1.412068	2.953331	-0.457659
30	8	0	-3.752262	0.509272	-3.751844
31	8	0	-4.926010	5.273287	1.496524
32	8	0	0.258070	4.298537	1.100818
33	8	0	-2.280730	5.026152	0.932131
34	8	0	-4.896686	2.737505	2.287706
35	8	0	-1.677143	2.716347	2.087377
36	8	0	2.843568	4.703905	1.310079
37	14	0	7.182342	0.205685	0.955005
38	14	0	6.979781	-0.370370	-2.042346
39	8	0	6.938618	-0.590728	-0.428440
40	14	0	1.026946	-2.940133	4.139301
41	14	0	-0.985297	-0.697924	4.447220
42	14	0	-5.760829	-0.600376	4.786900
43	14	0	3.750520	-4.339754	-4.270889
44	14	0	-3.494007	-2.700792	4.249769
45	14	0	6.216002	-2.394526	-4.126175
46	14	0	-3.230356	-5.370173	-0.846111
47	14	0	-0.152848	-5.468435	-0.990001
48	14	0	0.795819	-4.093504	-3.574954
49	14	0	-1.511964	-2.151468	-4.241562
50	14	0	-6.442449	-1.683832	-4.001083
51	14	0	4.111163	-3.134347	4.518272
52	14	0	-4.111424	-3.596565	-3.193420
53	14	0	6.438229	-1.422494	3.478988
54	14	0	-3.059334	-4.846900	2.276478
55	14	0	0.032710	-5.010943	2.131548

56	8	0	0.404667	-1.433813	3.986255
57	8	0	-1.063726	0.622951	3.513125
58	8	0	-5.286815	0.558859	3.724442
59	8	0	-4.842821	-1.934001	4.642616
60	8	0	4.754588	-3.070997	-4.289513
61	8	0	-2.230600	-1.681100	4.178646
62	8	0	-1.710452	-5.505181	-1.460852
63	8	0	0.867970	-3.744030	2.722530
64	8	0	-3.653612	-3.420337	2.791712
65	8	0	6.312769	-1.717442	-2.641272
66	8	0	2.336217	-3.698510	-3.764704
67	8	0	-3.140579	-4.777844	0.661366
68	8	0	-0.005062	-4.732271	0.496904
69	8	0	-0.065799	-2.752860	-3.857190
70	8	0	-1.350567	-0.560192	-3.904130
71	8	0	-6.349474	-0.078540	-3.658548
72	8	0	-5.306590	-2.503064	-3.145734
73	8	0	5.063442	-2.302871	3.502158
74	8	0	-2.664471	-2.841532	-3.323694
75	8	0	-1.480323	-5.032471	2.735362
76	8	0	0.683598	-4.529924	-1.997608
77	8	0	-4.140583	-4.396026	-1.767925
78	8	0	6.327871	-0.512091	2.138462
79	8	0	2.583045	-2.589464	4.353788
80	1	0	7.676837	3.966561	1.354078
81	1	0	7.418377	3.152068	-2.442755
82	1	0	8.569578	0.244592	1.331520
83	1	0	8.349583	-0.146197	-2.478452
84	1	0	7.621394	-2.254330	3.593874
85	1	0	7.174654	-3.461109	-4.105745
86	1	0	4.135007	-5.465072	-3.345018
87	1	0	4.257078	-4.513828	4.188082
88	1	0	0.737409	-6.233097	2.470378
89	1	0	0.434013	-6.789823	-0.944543
90	1	0	4.925251	6.250428	1.323168
91	1	0	4.823684	5.546202	-3.287116
92	1	0	1.318821	6.650314	1.007282
93	1	0	0.994273	6.143055	-2.473763
94	1	0	-3.328383	7.140961	1.406812
95	1	0	-3.350799	6.411808	-2.262687
96	1	0	-7.069392	4.118311	1.925000
97	1	0	-7.318414	3.672698	-2.090938
98	1	0	-7.059433	-1.055925	4.432334
99	1	0	-7.742816	-2.134302	-3.584255
100	1	0	-3.758201	-5.970181	2.879750
101	1	0	-3.775697	-6.690249	-0.785720
102	1	0	6.482123	-0.568271	4.628891
103	1	0	6.525688	2.914062	3.166129
104	1	0	4.353898	-2.938275	5.916958
105	1	0	0.424806	-3.742364	5.232046
106	1	0	-3.280337	-3.678133	5.273239
107	1	0	-0.841391	-0.384330	5.856357
108	1	0	-5.676211	-0.151834	6.170443
109	1	0	-5.426592	2.882506	4.751029
110	1	0	1.294209	5.426431	3.118164
111	1	0	-3.124104	5.586450	3.308335
112	1	0	-0.834633	2.964389	4.436502
113	1	0	-3.799597	5.262610	-4.329386
114	1	0	1.028216	4.935126	-4.507097
115	1	0	-5.482178	1.994442	-4.801868

116	1	0	-1.884455	1.625040	-5.093431
117	1	0	6.364100	2.551288	-4.502339
118	1	0	-6.245991	-1.915758	-5.434191
119	1	0	-4.281171	-4.541489	-4.301475
120	1	0	0.317297	-5.160255	-4.465116
121	1	0	3.543710	-4.671732	-5.673279
122	1	0	6.416105	-1.430422	-5.217207
123	1	0	-1.800114	-2.286497	-5.653940
124	14	0	-1.319120	3.133287	-2.057653
125	79	0	-0.568963	-0.147985	-1.249744
126	79	0	0.072044	-2.320646	0.099741
127	79	0	0.836338	0.123665	0.988161
128	6	0	3.811183	1.263499	4.389713
129	1	0	4.820295	1.676063	4.327842
130	1	0	3.286789	1.778920	5.208601
131	1	0	3.889425	0.204795	4.656908
132	6	0	3.087959	1.451180	3.093900
133	1	0	3.069658	2.439012	2.631475
134	1	0	3.816478	0.832382	1.805748
135	8	0	1.822545	0.879407	3.015962
136	8	0	3.048282	1.027619	0.059072
137	8	0	4.028308	0.548689	0.787200
138	1	0	1.740144	0.070246	3.558089

Zero-point correction=	0.390750 (Hartree/Particle)
Thermal correction to Energy=	0.477657
Thermal correction to Enthalpy=	0.478202
Thermal correction to Gibbs Free Energy=	0.277916
Sum of electronic and zero-point Energies=	-14045.112770
Sum of electronic and thermal Energies=	-14045.016863
Sum of electronic and thermal Enthalpies=	-14045.015918
Sum of electronic and thermal Free Energies=	-14045.225604

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -14048.490316

TS1b

Charge: 1 multiplicity: 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.318908	5.165968	1.050690
2	14	0	6.563373	3.215441	2.002980
3	14	0	4.277347	4.824971	-2.062157
4	14	0	6.389583	2.728171	-2.761271
5	8	0	5.165254	3.861735	1.496508
6	8	0	6.694953	1.865700	1.083954
7	8	0	4.357755	5.450009	-0.553906
8	8	0	5.023045	3.390810	-2.157212
9	8	0	6.246179	1.154676	-2.342438
10	14	0	-1.688929	2.056285	3.654425
11	14	0	-4.764516	1.941359	3.753461
12	14	0	-5.885204	3.420505	-1.681888
13	14	0	-3.607197	5.259130	-2.777179
14	14	0	1.255584	5.006080	-2.848228
15	14	0	-2.010839	0.996498	-3.918341
16	14	0	-5.114713	1.238052	-3.715442
17	14	0	-5.741891	3.769051	1.449424
18	14	0	-3.456258	5.728201	2.000333

19	14	0	1.354649	5.366385	1.905937
20	14	0	-1.250691	3.777906	1.061137
21	8	0	-3.201765	1.958344	4.246603
22	8	0	-5.014926	4.710672	-2.167403
23	8	0	0.210828	3.837062	-2.354385
24	8	0	-2.400325	4.167227	-2.567841
25	8	0	-5.271419	2.036645	-2.307520
26	8	0	-1.446719	1.714553	-2.536784
27	8	0	2.743276	4.485220	-2.466226
28	8	0	-5.793487	3.231325	-0.077446
29	8	0	-1.355252	3.017549	-0.364454
30	8	0	-3.589102	0.628277	-3.813017
31	8	0	-4.947092	5.193871	1.574260
32	8	0	0.260956	4.319366	1.274297
33	8	0	-2.280794	5.029144	1.079354
34	8	0	-4.913225	2.634191	2.288801
35	8	0	-1.683689	2.682920	2.163915
36	8	0	2.823181	4.763447	1.546453
37	14	0	7.241789	0.336833	1.177331
38	14	0	7.119686	-0.129060	-1.854480
39	8	0	7.027411	-0.391199	-0.248141
40	14	0	1.057033	-3.008950	4.085044
41	14	0	-1.003465	-0.798536	4.428904
42	14	0	-5.777510	-0.798692	4.654023
43	14	0	4.006480	-4.070793	-4.288910
44	14	0	-3.478034	-2.827737	4.103905
45	14	0	6.436983	-2.096634	-4.023722
46	14	0	-3.033323	-5.323193	-1.076460
47	14	0	0.040644	-5.377342	-1.155412
48	14	0	1.033823	-3.892408	-3.658204
49	14	0	-1.283089	-1.960415	-4.318545
50	14	0	-6.227899	-1.581912	-4.183632
51	14	0	4.122706	-3.157636	4.543126
52	14	0	-3.883386	-3.481573	-3.382517
53	14	0	6.456346	-1.389067	3.626047
54	14	0	-2.940316	-4.901975	2.071415
55	14	0	0.151195	-5.018508	1.994326
56	8	0	0.367585	-1.537915	3.943272
57	8	0	-1.038064	0.564173	3.544872
58	8	0	-5.281152	0.400733	3.646525
59	8	0	-4.874826	-2.140870	4.485639
60	8	0	4.991945	-2.785367	-4.245057
61	8	0	-2.282349	-1.727283	4.114345
62	8	0	-1.502748	-5.418541	-1.673832
63	8	0	0.974670	-3.781288	2.647277
64	8	0	-3.564506	-3.498443	2.615401
65	8	0	6.490506	-1.459297	-2.517199
66	8	0	2.571345	-3.466615	-3.801727
67	8	0	-2.980650	-4.787544	0.454929
68	8	0	0.100610	-4.699477	0.364596
69	8	0	0.160170	-2.554589	-3.913745
70	8	0	-1.157893	-0.375843	-3.948836
71	8	0	-6.178802	0.013413	-3.786075
72	8	0	-5.098868	-2.409506	-3.328120
73	8	0	5.092050	-2.276971	3.581006
74	8	0	-2.449113	-2.694887	-3.451192
75	8	0	-1.373152	-5.073023	2.572101
76	8	0	0.889971	-4.392147	-2.103746
77	8	0	-3.936417	-4.327352	-1.983542
78	8	0	6.368544	-0.459683	2.290015

79	8	0	2.594814	-2.615088	4.365255
80	1	0	7.665102	4.099464	1.707236
81	1	0	7.511915	3.410983	-2.120136
82	1	0	8.618072	0.394497	1.581350
83	1	0	8.496816	0.130480	-2.243887
84	1	0	7.655768	-2.194294	3.734011
85	1	0	7.415313	-3.144621	-4.010578
86	1	0	4.390887	-5.219632	-3.393345
87	1	0	4.314940	-4.523956	4.168202
88	1	0	0.866320	-6.237473	2.306895
89	1	0	0.654576	-6.681890	-1.131273
90	1	0	4.878538	6.340622	1.685167
91	1	0	4.900141	5.792519	-2.947337
92	1	0	1.274859	6.695790	1.293701
93	1	0	1.042952	6.302583	-2.209418
94	1	0	-3.387980	7.101353	1.594317
95	1	0	-3.309628	6.497485	-2.097115
96	1	0	-7.091168	4.005847	1.917520
97	1	0	-7.235586	3.693637	-2.116060
98	1	0	-7.058516	-1.250078	4.248485
99	1	0	-7.529872	-2.064902	-3.814326
100	1	0	-3.641642	-6.057340	2.613392
101	1	0	-3.558678	-6.652302	-1.073482
102	1	0	6.464698	-0.562163	4.796784
103	1	0	6.487502	2.968280	3.453687
104	1	0	4.344422	-3.006984	5.951070
105	1	0	0.446526	-3.847401	5.142429
106	1	0	-3.259063	-3.841246	5.093923
107	1	0	-0.888340	-0.532153	5.848070
108	1	0	-5.732576	-0.384762	6.049825
109	1	0	-5.497591	2.699735	4.740142
110	1	0	1.218868	5.400422	3.360867
111	1	0	-3.204783	5.486208	3.446845
112	1	0	-0.901264	2.862512	4.542265
113	1	0	-3.689701	5.412618	-4.211893
114	1	0	1.145746	5.165345	-4.280835
115	1	0	-5.307352	2.137115	-4.835750
116	1	0	-1.698027	1.832776	-5.050272
117	1	0	6.517689	2.864685	-4.224281
118	1	0	-5.992373	-1.760530	-5.618207
119	1	0	-4.013461	-4.392959	-4.526317
120	1	0	0.596993	-4.935319	-4.596771
121	1	0	3.843454	-4.356547	-5.707478
122	1	0	6.651263	-1.089074	-5.071421
123	1	0	-1.537068	-2.055452	-5.740103
124	14	0	-1.234854	3.245637	-1.956682
125	79	0	-0.899749	-0.051268	-1.049018
126	79	0	-0.241318	-2.365136	-0.006121
127	79	0	0.569376	-0.072669	1.159977
128	6	0	3.350532	1.298314	0.737946
129	1	0	4.300396	1.546278	0.272550
130	1	0	3.338053	-0.238835	-0.043878
131	1	0	2.484067	1.837193	0.360448
132	6	0	3.381320	0.949303	2.184077
133	1	0	3.986242	0.055766	2.363090
134	1	0	3.813363	1.782832	2.758299
135	8	0	2.034174	0.733764	2.688088
136	8	0	3.486160	-1.206915	-0.400986
137	8	0	3.156538	-2.021849	0.574553
138	1	0	2.040821	0.050235	3.377599

Zero-point correction=	0.390962 (Hartree/Particle)
Thermal correction to Energy=	0.477660
Thermal correction to Enthalpy=	0.478605
Thermal correction to Gibbs Free Energy=	0.276420
Sum of electronic and zero-point Energies=	-14045.101926
Sum of electronic and thermal Energies=	-14045.015227
Sum of electronic and thermal Enthalpies=	-14045.014283
Sum of electronic and thermal Free Energies=	-14045.216467

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -14048.479883

TS2

Charge: 1 multiplicity: 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.370312	5.011544	0.777709
2	14	0	6.585517	3.050950	1.752410
3	14	0	4.267759	4.574456	-2.324324
4	14	0	6.319719	2.410028	-2.987435
5	8	0	5.186213	3.701740	1.255653
6	8	0	6.731516	1.690705	0.858097
7	8	0	4.396959	5.238237	-0.839811
8	8	0	4.963100	3.110955	-2.403886
9	8	0	6.141686	0.851812	-2.515608
10	14	0	-1.658803	2.134791	3.569075
11	14	0	-4.733382	2.086279	3.730091
12	14	0	-5.917817	3.421795	-1.734356
13	14	0	-3.615923	5.159734	-2.929071
14	14	0	1.239798	4.806113	-3.068893
15	14	0	-2.118410	0.837241	-3.941345
16	14	0	-5.221931	1.157200	-3.704273
17	14	0	-5.714654	3.859986	1.384449
18	14	0	-3.381771	5.787516	1.827825
19	14	0	1.421593	5.315859	1.667547
20	14	0	-1.235917	3.765462	0.914098
21	8	0	-3.163973	2.116228	4.193281
22	8	0	-5.030397	4.674857	-2.282446
23	8	0	0.170670	3.689764	-2.515291
24	8	0	-2.448842	4.020605	-2.709560
25	8	0	-5.348574	2.003313	-2.323523
26	8	0	-1.458627	1.569440	-2.608903
27	8	0	2.718898	4.255005	-2.696150
28	8	0	-5.798160	3.284885	-0.128032
29	8	0	-1.378716	2.946931	-0.478636
30	8	0	-3.702947	0.524789	-3.786465
31	8	0	-4.894979	5.273564	1.460484
32	8	0	0.279988	4.301885	1.071401
33	8	0	-2.256812	5.024975	0.895251
34	8	0	-4.908581	2.722858	2.241006
35	8	0	-1.666802	2.717132	2.059874
36	8	0	2.871451	4.678433	1.304720
37	14	0	7.183555	0.141935	1.014609
38	14	0	7.004716	-0.427292	-1.989061
39	8	0	6.939920	-0.647909	-0.378590
40	14	0	0.968356	-2.975742	4.126206
41	14	0	-1.054715	-0.703848	4.426857

42	14	0	-5.797198	-0.605171	4.735389
43	14	0	3.765029	-4.377709	-4.252144
44	14	0	-3.574040	-2.684138	4.227434
45	14	0	6.243162	-2.448395	-4.086653
46	14	0	-3.247752	-5.363670	-0.878584
47	14	0	-0.167094	-5.477383	-0.999960
48	14	0	0.806693	-4.112355	-3.580514
49	14	0	-1.480599	-2.154408	-4.266240
50	14	0	-6.409090	-1.657477	-4.066301
51	14	0	4.039177	-3.174133	4.542514
52	14	0	-4.096733	-3.585855	-3.238618
53	14	0	6.397427	-1.488522	3.524951
54	14	0	-3.091623	-4.837052	2.247547
55	14	0	0.005688	-5.029965	2.115210
56	8	0	0.224230	-1.555920	3.896289
57	8	0	-1.083616	0.611550	3.472891
58	8	0	-5.260218	0.543699	3.689676
59	8	0	-4.982131	-2.008844	4.594916
60	8	0	4.776666	-3.111814	-4.256151
61	8	0	-2.412179	-1.554392	4.218600
62	8	0	-1.721863	-5.504321	-1.479985
63	8	0	0.888868	-3.802953	2.709507
64	8	0	-3.654756	-3.396705	2.755729
65	8	0	6.322737	-1.760856	-2.603350
66	8	0	2.352745	-3.723017	-3.757497
67	8	0	-3.170081	-4.773129	0.629465
68	8	0	-0.018296	-4.730629	0.480924
69	8	0	-0.038833	-2.763041	-3.870263
70	8	0	-1.306118	-0.564851	-3.932621
71	8	0	-6.304518	-0.053266	-3.723021
72	8	0	-5.285256	-2.484723	-3.202547
73	8	0	5.016519	-2.358451	3.529475
74	8	0	-2.643759	-2.837209	-3.357336
75	8	0	-1.512636	-5.030320	2.705757
76	8	0	0.682661	-4.545161	-2.004952
77	8	0	-4.139921	-4.383214	-1.813043
78	8	0	6.305284	-0.580528	2.174956
79	8	0	2.517303	-2.605517	4.374396
80	1	0	7.699423	3.900192	1.411641
81	1	0	7.467770	3.090114	-2.387867
82	1	0	8.568554	0.172615	1.393710
83	1	0	8.378179	-0.214008	-2.418283
84	1	0	7.585413	-2.321837	3.646056
85	1	0	7.195876	-3.520168	-4.057986
86	1	0	4.137202	-5.505221	-3.324440
87	1	0	4.201859	-4.560229	4.210155
88	1	0	0.686004	-6.255862	2.461561
89	1	0	0.407666	-6.807976	-0.956259
90	1	0	4.962816	6.201602	1.359334
91	1	0	4.895608	5.501376	-3.252184
92	1	0	1.361809	6.624754	1.013401
93	1	0	1.063367	6.122111	-2.470640
94	1	0	-3.285376	7.144806	1.374167
95	1	0	-3.281519	6.418461	-2.295937
96	1	0	-7.049834	4.145702	1.858495
97	1	0	-7.267860	3.704594	-2.159740
98	1	0	-7.094009	-1.030292	4.361797
99	1	0	-7.716693	-2.098497	-3.661101
100	1	0	-3.811222	-5.964384	2.833233
101	1	0	-3.802441	-6.681699	-0.832806

102	1	0	6.448247	-0.629284	4.672752
103	1	0	6.526356	2.853755	3.213118
104	1	0	4.294164	-2.986580	5.941015
105	1	0	0.365930	-3.765050	5.222399
106	1	0	-3.338944	-3.677194	5.232450
107	1	0	-0.884031	-0.399461	5.838650
108	1	0	-5.719745	-0.136318	6.112195
109	1	0	-5.438815	2.897398	4.697299
110	1	0	1.311596	5.399507	3.123040
111	1	0	-3.107044	5.587611	3.276130
112	1	0	-0.843949	2.950175	4.421491
113	1	0	-3.720233	5.273665	-4.367327
114	1	0	1.106740	4.915429	-4.504536
115	1	0	-5.419611	2.016646	-4.856447
116	1	0	-1.821883	1.624321	-5.117879
117	1	0	6.427074	2.497567	-4.456722
118	1	0	-6.202970	-1.888168	-5.498198
119	1	0	-4.264554	-4.527226	-4.351032
120	1	0	0.331091	-5.175217	-4.476417
121	1	0	3.570620	-4.706444	-5.656984
122	1	0	6.459694	-1.483874	-5.174222
123	1	0	-1.757859	-2.287133	-5.680773
124	14	0	-1.272307	3.124592	-2.075903
125	79	0	-0.579108	-0.132465	-1.179284
126	79	0	0.092123	-2.292388	0.148120
127	79	0	0.778691	0.172244	1.125834
128	6	0	3.577057	1.829115	4.090032
129	1	0	4.588793	1.485754	4.321821
130	1	0	3.622604	2.859482	3.728375
131	1	0	2.987710	1.814301	5.016120
132	6	0	2.938015	0.932843	3.047737
133	1	0	3.713570	0.890954	1.827756
134	1	0	3.039582	-0.153247	3.228117
135	8	0	1.736918	1.319252	2.632807
136	8	0	3.000212	1.197634	0.020525
137	8	0	4.058629	0.660011	0.728669
138	1	0	3.153020	0.845848	-0.880898

Zero-point correction= 0.388432 (Hartree/Particle)
Thermal correction to Energy= 0.475143
Thermal correction to Enthalpy= 0.476087
Thermal correction to Gibbs Free Energy= 0.275291
Sum of electronic and zero-point Energies= -14045.088132
Sum of electronic and thermal Energies= -14045.001421
Sum of electronic and thermal Enthalpies= -14045.000477
Sum of electronic and thermal Free Energies= -14045.218947

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -14048.487693

TS2a

Charge: 1 multiplicity: 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.341202	5.042199	0.681705
2	14	0	6.567140	3.097399	1.673265
3	14	0	4.232912	4.572536	-2.410437
4	14	0	6.290708	2.412400	-3.060955

5	8	0	5.167523	3.745801	1.177333
6	8	0	6.754052	1.735747	0.790148
7	8	0	4.358924	5.260798	-0.933861
8	8	0	4.946624	3.124328	-2.474049
9	8	0	6.134418	0.853967	-2.595175
10	14	0	-1.672595	2.164064	3.525247
11	14	0	-4.745148	2.101826	3.693409
12	14	0	-5.947752	3.387978	-1.779641
13	14	0	-3.659496	5.118898	-2.995664
14	14	0	1.204170	4.787650	-3.148335
15	14	0	-2.128345	0.794653	-3.962357
16	14	0	-5.239542	1.106642	-3.727710
17	14	0	-5.737365	3.854737	1.335400
18	14	0	-3.414692	5.793811	1.754292
19	14	0	1.396503	5.340144	1.581713
20	14	0	-1.263439	3.770525	0.855281
21	8	0	-3.172832	2.126764	4.154724
22	8	0	-5.075409	4.645023	-2.342993
23	8	0	0.124688	3.688596	-2.580210
24	8	0	-2.502765	3.970651	-2.760315
25	8	0	-5.374573	1.967183	-2.355876
26	8	0	-1.465473	1.532836	-2.627400
27	8	0	2.682975	4.248609	-2.771677
28	8	0	-5.817245	3.267458	-0.171707
29	8	0	-1.397478	2.934098	-0.527297
30	8	0	-3.714855	0.489466	-3.795213
31	8	0	-4.929953	5.275527	1.403694
32	8	0	0.244217	4.325484	1.009951
33	8	0	-2.299072	5.017372	0.822413
34	8	0	-4.921066	2.729654	2.201464
35	8	0	-1.687656	2.729406	2.012286
36	8	0	2.842396	4.696711	1.213556
37	14	0	7.178636	0.186342	0.951277
38	14	0	6.985827	-0.413441	-2.045730
39	8	0	6.918435	-0.616707	-0.427579
40	14	0	0.979241	-2.936204	4.118807
41	14	0	-1.061283	-0.669262	4.408793
42	14	0	-5.794019	-0.582810	4.728378
43	14	0	3.761292	-4.399411	-4.252455
44	14	0	-3.569562	-2.657424	4.231628
45	14	0	6.230623	-2.458335	-4.112105
46	14	0	-3.240508	-5.382535	-0.851162
47	14	0	-0.162636	-5.487996	-0.982401
48	14	0	0.802199	-4.138896	-3.574548
49	14	0	-1.492481	-2.194032	-4.272610
50	14	0	-6.423555	-1.717961	-4.061548
51	14	0	4.049634	-3.110172	4.529276
52	14	0	-4.099799	-3.628108	-3.224571
53	14	0	6.400201	-1.426303	3.487281
54	14	0	-3.075281	-4.826579	2.270414
55	14	0	0.019132	-5.009180	2.129482
56	8	0	0.215721	-1.525621	3.877619
57	8	0	-1.055802	0.652153	3.458395
58	8	0	-5.266991	0.557379	3.667875
59	8	0	-4.980259	-1.989338	4.600045
60	8	0	4.767827	-3.131741	-4.273619
61	8	0	-2.425566	-1.505070	4.205176
62	8	0	-1.717803	-5.528865	-1.458358
63	8	0	0.904130	-3.776765	2.711368
64	8	0	-3.643982	-3.383176	2.767195

65	8	0	6.320664	-1.767192	-2.631770
66	8	0	2.346945	-3.753223	-3.754196
67	8	0	-3.155082	-4.777473	0.652158
68	8	0	-0.020604	-4.729515	0.493025
69	8	0	-0.050344	-2.798124	-3.872804
70	8	0	-1.319242	-0.603987	-3.961111
71	8	0	-6.315001	-0.111307	-3.732174
72	8	0	-5.296619	-2.536103	-3.193357
73	8	0	5.016973	-2.296964	3.495896
74	8	0	-2.651694	-2.873142	-3.352115
75	8	0	-1.495304	-5.004868	2.731551
76	8	0	0.675251	-4.549294	-1.990329
77	8	0	-4.137093	-4.411503	-1.789574
78	8	0	6.266604	-0.568122	2.091660
79	8	0	2.524532	-2.556236	4.363400
80	1	0	7.676535	3.947057	1.322646
81	1	0	7.437210	3.100643	-2.468457
82	1	0	8.560816	0.223029	1.336895
83	1	0	8.361006	-0.199900	-2.470757
84	1	0	7.594378	-2.254271	3.615249
85	1	0	7.187471	-3.525976	-4.076124
86	1	0	4.139058	-5.516485	-3.315165
87	1	0	4.221632	-4.501005	4.210079
88	1	0	0.707688	-6.227114	2.487658
89	1	0	0.421729	-6.812206	-0.924042
90	1	0	4.930417	6.236765	1.256917
91	1	0	4.852741	5.493291	-3.347663
92	1	0	1.326728	6.642069	0.917601
93	1	0	1.020273	6.105746	-2.560718
94	1	0	-3.321479	7.146618	1.287112
95	1	0	-3.325263	6.386095	-2.376063
96	1	0	-7.072250	4.136925	1.810375
97	1	0	-7.300084	3.657477	-2.202920
98	1	0	-7.088063	-1.015633	4.361905
99	1	0	-7.729565	-2.161137	-3.648838
100	1	0	-3.789598	-5.950416	2.869764
101	1	0	-3.788483	-6.701853	-0.789444
102	1	0	6.453286	-0.556840	4.629458
103	1	0	6.512959	2.912720	3.137220
104	1	0	4.312515	-2.910919	5.925926
105	1	0	0.385430	-3.711976	5.226098
106	1	0	-3.319727	-3.639053	5.246177
107	1	0	-0.876470	-0.345882	5.814627
108	1	0	-5.712406	-0.099807	6.099868
109	1	0	-5.447951	2.921694	4.655956
110	1	0	1.287614	5.436358	3.038699
111	1	0	-3.131297	5.607967	3.202968
112	1	0	-0.854155	2.990525	4.366216
113	1	0	-3.765285	5.220260	-4.435405
114	1	0	1.062692	4.880333	-4.583403
115	1	0	-5.452763	1.951958	-4.889187
116	1	0	-1.854234	1.571800	-5.157485
117	1	0	6.392966	2.484612	-4.528646
118	1	0	-6.222029	-1.961816	-5.492238
119	1	0	-4.269552	-4.582180	-4.326220
120	1	0	0.328318	-5.212675	-4.459018
121	1	0	3.562482	-4.741803	-5.653380
122	1	0	6.439763	-1.503185	-5.209118
123	1	0	-1.775873	-2.344442	-5.684103
124	14	0	-1.302424	3.104490	-2.128821

125	79	0	-0.570149	-0.027470	-1.058781
126	79	0	0.083980	-2.290766	0.119033
127	79	0	0.968019	-0.014783	1.217496
128	6	0	3.100800	2.483664	4.200151
129	1	0	3.357424	2.195848	5.223820
130	1	0	4.021920	2.565355	3.616523
131	1	0	2.644203	3.485948	4.233016
132	6	0	2.176054	1.459479	3.611597
133	1	0	3.121219	1.581541	1.442407
134	1	0	1.341549	1.100904	4.212011
135	8	0	1.884181	1.597426	2.287369
136	8	0	3.636441	-0.154062	0.857481
137	8	0	3.987770	1.198744	1.043691
138	1	0	4.322027	-0.606620	1.400542

Zero-point correction= 0.391330 (Hartree/Particle)
Thermal correction to Energy= 0.477819
Thermal correction to Enthalpy= 0.478763
Thermal correction to Gibbs Free Energy= 0.279431
Sum of electronic and zero-point Energies= -14045.087908
Sum of electronic and thermal Energies= -14045.001419
Sum of electronic and thermal Enthalpies= -14045.000475
Sum of electronic and thermal Free Energies= -14045.199807

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -14048.4713111

TS3

Charge: 1 multiplicity: 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.324025	5.005414	0.822025
2	14	0	6.528757	3.025800	1.797197
3	14	0	4.223543	4.583852	-2.282892
4	14	0	6.280422	2.409268	-2.948264
5	8	0	5.135385	3.695058	1.301100
6	8	0	6.630764	1.662780	0.898339
7	8	0	4.351562	5.237398	-0.794986
8	8	0	4.912511	3.106546	-2.361159
9	8	0	6.089990	0.858619	-2.464936
10	14	0	-1.726438	2.122838	3.589406
11	14	0	-4.801628	2.078981	3.739469
12	14	0	-5.965330	3.447879	-1.726029
13	14	0	-3.654766	5.180468	-2.906987
14	14	0	1.200691	4.823759	-3.036276
15	14	0	-2.137188	0.865546	-3.917442
16	14	0	-5.252709	1.191891	-3.701720
17	14	0	-5.767531	3.864969	1.393530
18	14	0	-3.421180	5.793562	1.849812
19	14	0	1.369579	5.316940	1.706068
20	14	0	-1.280355	3.766550	0.947282
21	8	0	-3.231850	2.097446	4.207250
22	8	0	-5.071953	4.704866	-2.259010
23	8	0	0.121130	3.729670	-2.475034
24	8	0	-2.502073	4.022777	-2.687746
25	8	0	-5.397974	2.033855	-2.320423
26	8	0	-1.451442	1.581677	-2.583475
27	8	0	2.682106	4.267146	-2.672164

28	8	0	-5.857199	3.295321	-0.119915
29	8	0	-1.428644	2.963886	-0.452285
30	8	0	-3.727073	0.575803	-3.756342
31	8	0	-4.922716	5.265182	1.460564
32	8	0	0.254471	4.259032	1.131904
33	8	0	-2.260629	5.057505	0.935240
34	8	0	-4.971984	2.722420	2.252191
35	8	0	-1.735281	2.722882	2.085410
36	8	0	2.826460	4.685300	1.363577
37	14	0	7.114625	0.118109	1.058363
38	14	0	6.950268	-0.434579	-1.952994
39	8	0	6.878105	-0.656595	-0.345713
40	14	0	0.886960	-2.997732	4.127605
41	14	0	-1.138149	-0.710787	4.430823
42	14	0	-5.873395	-0.613883	4.730392
43	14	0	3.707715	-4.366866	-4.244088
44	14	0	-3.657004	-2.674098	4.225256
45	14	0	6.189114	-2.444389	-4.065985
46	14	0	-3.321093	-5.346035	-0.892607
47	14	0	-0.242816	-5.474453	-1.011333
48	14	0	0.747615	-4.095929	-3.582872
49	14	0	-1.530558	-2.125662	-4.267334
50	14	0	-6.457351	-1.621985	-4.079973
51	14	0	3.947440	-3.194162	4.556905
52	14	0	-4.152318	-3.558037	-3.252547
53	14	0	6.315552	-1.520955	3.556956
54	14	0	-3.163705	-4.828830	2.236596
55	14	0	-0.064166	-5.030166	2.106914
56	8	0	0.081182	-1.619677	3.871173
57	8	0	-1.108887	0.619918	3.491999
58	8	0	-5.328242	0.537891	3.690621
59	8	0	-5.086525	-2.034033	4.584120
60	8	0	4.722975	-3.103627	-4.243718
61	8	0	-2.543999	-1.493227	4.236429
62	8	0	-1.795161	-5.494460	-1.494287
63	8	0	0.840160	-3.828807	2.710206
64	8	0	-3.708351	-3.382110	2.748636
65	8	0	6.267169	-1.757450	-2.582357
66	8	0	2.295976	-3.713427	-3.748443
67	8	0	-3.244779	-4.759925	0.617041
68	8	0	-0.095123	-4.725338	0.468610
69	8	0	-0.094373	-2.746282	-3.868274
70	8	0	-1.341691	-0.541080	-3.938187
71	8	0	-6.332943	-0.020848	-3.731826
72	8	0	-5.343333	-2.460173	-3.215489
73	8	0	4.945618	-2.399796	3.548425
74	8	0	-2.699699	-2.807816	-3.363192
75	8	0	-1.585640	-5.029316	2.691093
76	8	0	0.610703	-4.535786	-2.008626
77	8	0	-4.202989	-4.358832	-1.828756
78	8	0	6.239118	-0.618161	2.201861
79	8	0	2.425525	-2.623590	4.406318
80	1	0	7.645230	3.881381	1.462374
81	1	0	7.423538	3.085975	-2.340826
82	1	0	8.505244	0.151759	1.433313
83	1	0	8.325909	-0.220248	-2.380669
84	1	0	7.508893	-2.348592	3.673278
85	1	0	7.140640	-3.517373	-4.036350
86	1	0	4.074802	-5.497573	-3.319784
87	1	0	4.118088	-4.580693	4.218440

88	1	0	0.603477	-6.261012	2.452515
89	1	0	0.334711	-6.799949	-0.968156
90	1	0	4.914478	6.189732	1.410041
91	1	0	4.860051	5.506782	-3.204239
92	1	0	1.315620	6.623051	1.054391
93	1	0	1.026909	6.134058	-2.432420
94	1	0	-3.331379	7.153222	1.402508
95	1	0	-3.317770	6.440492	-2.270259
96	1	0	-7.104702	4.161690	1.863867
97	1	0	-7.311160	3.736029	-2.156646
98	1	0	-7.169489	-1.023441	4.347769
99	1	0	-7.769557	-2.060324	-3.680955
100	1	0	-3.894071	-5.959951	2.811194
101	1	0	-3.875510	-6.663659	-0.857447
102	1	0	6.372666	-0.657054	4.702687
103	1	0	6.463931	2.831173	3.256259
104	1	0	4.208815	-3.013705	5.955412
105	1	0	0.280960	-3.779805	5.221609
106	1	0	-3.423700	-3.682823	5.220357
107	1	0	-0.962651	-0.413435	5.846426
108	1	0	-5.798538	-0.139358	6.105778
109	1	0	-5.505702	2.898876	4.703048
110	1	0	1.255766	5.390135	3.159302
111	1	0	-3.162865	5.588583	3.299225
112	1	0	-0.909866	2.941322	4.441874
113	1	0	-3.752760	5.304457	-4.347163
114	1	0	1.073703	4.934856	-4.470659
115	1	0	-5.458579	2.053492	-4.853766
116	1	0	-1.861128	1.653413	-5.105482
117	1	0	6.387899	2.503683	-4.415123
118	1	0	-6.249551	-1.846937	-5.512500
119	1	0	-4.321254	-4.495001	-4.369062
120	1	0	0.273153	-5.153893	-4.482450
121	1	0	3.517522	-4.688745	-5.651104
122	1	0	6.412981	-1.475140	-5.147309
123	1	0	-1.804878	-2.256210	-5.682631
124	14	0	-1.315590	3.140178	-2.051018
125	79	0	-0.347576	-0.006005	-1.107538
126	79	0	0.106422	-2.345458	0.019645
127	79	0	1.256406	-0.135628	1.090555
128	6	0	3.448929	2.146143	4.064119
129	1	0	3.874453	3.135449	3.881760
130	1	0	2.824152	2.197164	4.965159
131	1	0	4.257998	1.436641	4.256784
132	6	0	2.627976	1.712887	2.874477
133	1	0	1.904262	2.458578	2.505631
134	1	0	3.224004	1.610667	1.591004
135	8	0	2.183832	0.454910	2.914306
136	8	0	3.078642	2.036176	-0.460823
137	8	0	3.297599	1.055625	0.512387
138	1	0	3.703004	1.779277	-1.171264

Zero-point correction= 0.388809 (Hartree/Particle)
Thermal correction to Energy= 0.475289
Thermal correction to Enthalpy= 0.476233
Thermal correction to Gibbs Free Energy= 0.276689
Sum of electronic and zero-point Energies= -14045.091208
Sum of electronic and thermal Energies= -14045.004728
Sum of electronic and thermal Enthalpies= -14045.003783
Sum of electronic and thermal Free Energies= -14045.203328

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -14048.4912976

Au_3^+

Charge: 1 multiplicity: 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	1.352217	-0.780661	0.000000
2	79	0	0.000000	1.561367	0.000000
3	79	0	-1.352217	-0.780706	0.000000

Zero-point correction= 0.000819 (Hartree/Particle)
Thermal correction to Energy= 0.005748
Thermal correction to Enthalpy= 0.006692
Thermal correction to Gibbs Free Energy= -0.034347
Sum of electronic and zero-point Energies= -406.152748
Sum of electronic and thermal Energies= -406.147819
Sum of electronic and thermal Enthalpies= -406.146875
Sum of electronic and thermal Free Energies= -406.187914

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -407.277437

INT1'

Charge: 1 multiplicity: 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	1.308065	-1.308477	0.067229
2	79	0	1.240271	1.345163	0.044359
3	79	0	-1.095146	-0.040801	-0.167106
4	6	0	-5.622894	-0.153652	0.309305
5	1	0	-6.305205	0.163589	1.104341
6	1	0	-5.979718	0.295275	-0.624283
7	1	0	-5.674268	-1.242077	0.225805
8	6	0	-4.220796	0.305327	0.649400
9	1	0	-4.146081	1.393630	0.734309
10	1	0	-3.850854	-0.151900	1.568191
11	8	0	-3.273824	-0.146892	-0.389210
12	1	0	-3.593182	0.131620	-1.261035

Zero-point correction= 0.082838 (Hartree/Particle)
Thermal correction to Energy= 0.093626
Thermal correction to Enthalpy= 0.094571
Thermal correction to Gibbs Free Energy= 0.038070
Sum of electronic and zero-point Energies= -561.174017
Sum of electronic and thermal Energies= -561.163229
Sum of electronic and thermal Enthalpies= -561.162284
Sum of electronic and thermal Free Energies= -561.218785

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -562.376860

INT2'

Charge: 1 multiplicity: 3

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	79	0	0.499920	1.812697	0.063185
2	79	0	1.369976	-0.695163	0.142520
3	79	0	-1.288280	-0.167564	-0.301522
4	6	0	-4.082356	-1.026303	1.548115
5	1	0	-4.705559	-1.572940	2.262168
6	1	0	-4.484639	-0.014793	1.447006
7	1	0	-3.071240	-0.972526	1.968523
8	6	0	-4.091956	-1.751704	0.222829
9	1	0	-5.100616	-1.805913	-0.196448
10	1	0	-3.675436	-2.760465	0.301997
11	8	0	-3.285426	-0.987379	-0.743835
12	1	0	-3.355204	-1.387395	-1.622934
13	8	0	3.721722	-2.783428	-0.541693
14	8	0	3.000071	-2.462392	0.383475

Zero-point correction= 0.087353 (Hartree/Particle)
Thermal correction to Energy= 0.102023
Thermal correction to Enthalpy= 0.102968
Thermal correction to Gibbs Free Energy= 0.033866
Sum of electronic and zero-point Energies= -711.498337
Sum of electronic and thermal Energies= -711.483667
Sum of electronic and thermal Enthalpies= -711.482722
Sum of electronic and thermal Free Energies= -711.551825

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -712.753289

INT3'

Charge: 1 multiplicity: 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	1.409497	0.742457	-0.134043
2	79	0	0.627912	-1.779112	-0.017449
3	79	0	-1.301222	0.047423	0.146715
4	6	0	-5.287817	1.827407	-0.443065
5	1	0	-6.267793	1.450046	-0.748770
6	1	0	-5.409728	2.450618	0.445495
7	1	0	-4.881008	2.436073	-1.254837
8	6	0	-4.368501	0.643380	-0.160014
9	1	0	-4.796120	0.034314	0.670602
10	1	0	-4.243306	-0.044077	-1.007282
11	8	0	-3.138800	1.049394	0.359612
12	1	0	3.274718	2.564256	1.369457
13	8	0	2.576961	2.607485	-0.373583
14	8	0	3.324639	3.147292	0.579126

Zero-point correction= 0.084292 (Hartree/Particle)
Thermal correction to Energy= 0.098954
Thermal correction to Enthalpy= 0.099898
Thermal correction to Gibbs Free Energy= 0.030993
Sum of electronic and zero-point Energies= -711.434872
Sum of electronic and thermal Energies= -711.420210
Sum of electronic and thermal Enthalpies= -711.419266
Sum of electronic and thermal Free Energies= -711.488171

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -712.691897

INT4'

Charge: 1 multiplicity: 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	-1.595057	1.070140	-0.167374
2	79	0	-1.090618	-1.553354	0.131399
3	79	0	0.957885	0.236197	0.024120
4	6	0	5.126931	-1.409387	-0.499456
5	1	0	5.535589	-2.368143	-0.831187
6	1	0	5.336130	-0.660831	-1.268355
7	1	0	5.623831	-1.115913	0.428009
8	6	0	3.623228	-1.548431	-0.293784
9	1	0	3.076052	-1.891731	-1.184301
10	1	0	3.420104	-2.316450	0.490148
11	8	0	3.044763	-0.406113	0.244828
12	8	0	2.302964	3.053946	0.924835
13	8	0	1.933731	2.565901	-0.251820
14	1	0	2.751115	3.904416	0.718952

Zero-point correction= 0.083603 (Hartree/Particle)
Thermal correction to Energy= 0.098667
Thermal correction to Enthalpy= 0.099611
Thermal correction to Gibbs Free Energy= 0.029462
Sum of electronic and zero-point Energies= -711.420316
Sum of electronic and thermal Energies= -711.405253
Sum of electronic and thermal Enthalpies= -711.404308
Sum of electronic and thermal Free Energies= -711.489703

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -712.681793

INT5'

Charge: 1 multiplicity: 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	-1.451781	0.661855	-0.094852
2	79	0	-0.536576	-1.819343	0.077305
3	79	0	1.278189	0.132715	-0.049238
4	6	0	5.549847	1.600118	0.074397
5	1	0	5.320740	2.583858	-0.336064
6	1	0	6.278564	1.077891	-0.559563
7	1	0	-2.840882	2.894165	-1.088010
8	6	0	4.332170	0.762600	0.198439
9	1	0	6.019884	1.694049	1.062276
10	1	0	4.449175	-0.255190	0.603642
11	8	0	3.214842	1.169591	-0.134465
12	1	0	-3.511491	3.440810	1.182552
13	8	0	-2.937842	2.375643	-0.268585
14	8	0	-2.640096	3.372914	0.749830

Zero-point correction= 0.086743 (Hartree/Particle)
Thermal correction to Energy= 0.101560
Thermal correction to Enthalpy= 0.102505
Thermal correction to Gibbs Free Energy= 0.034639

Sum of electronic and zero-point Energies= -711.538888
Sum of electronic and thermal Energies= -711.524071
Sum of electronic and thermal Enthalpies= -711.523126
Sum of electronic and thermal Free Energies= -711.590992

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -712.776271

INT3a'

Charge: 1 multiplicity: 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	-1.444921	-0.705894	-0.089599
2	79	0	-0.541450	1.791591	0.104524
3	79	0	1.271427	-0.131278	-0.134201
4	6	0	5.620916	-1.299586	0.301096
5	1	0	6.276103	-1.056415	1.141777
6	1	0	5.810650	-2.349462	0.024846
7	1	0	5.924437	-0.668736	-0.544973
8	6	0	4.211095	-1.062006	0.692082
9	1	0	3.798263	-1.334196	1.656383
10	1	0	-3.966531	-3.547593	0.590670
11	8	0	3.229861	-1.203630	-0.317539
12	8	0	-2.906196	-2.343521	-0.308871
13	8	0	-3.322512	-2.849864	0.849839
14	1	0	3.636321	-1.097038	-1.192374

Zero-point correction= 0.084780 (Hartree/Particle)
Thermal correction to Energy= 0.099691
Thermal correction to Enthalpy= 0.100635
Thermal correction to Gibbs Free Energy= 0.023098
Sum of electronic and zero-point Energies= -711.446089
Sum of electronic and thermal Energies= -711.431178
Sum of electronic and thermal Enthalpies= -711.430234
Sum of electronic and thermal Free Energies= -711.498771

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -712.682176

INT3b'

Charge: 1 multiplicity: 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	0.333510	1.840995	0.023470
2	79	0	1.344330	-0.618731	-0.011524
3	79	0	-1.376646	-0.302675	-0.033943
4	6	0	-2.406050	-2.256164	0.004458
5	1	0	-2.203827	-2.614047	-1.005893
6	1	0	4.351209	-1.146163	0.126754
7	1	0	-1.908248	-2.823902	0.788926
8	6	0	-3.802991	-1.758265	0.281821
9	1	0	-4.569405	-2.265633	-0.311601
10	1	0	-4.067452	-1.824169	1.337601
11	8	0	-3.792296	-0.321335	-0.031443
12	8	0	4.176324	-2.111332	0.058505
13	8	0	2.865053	-2.280982	-0.025487
14	1	0	-4.135022	-0.177887	-0.928257

Zero-point correction=	0.086245 (Hartree/Particle)
Thermal correction to Energy=	0.100545
Thermal correction to Enthalpy=	0.101489
Thermal correction to Gibbs Free Energy=	0.034409
Sum of electronic and zero-point Energies=	-711.438879
Sum of electronic and thermal Energies=	-711.424579
Sum of electronic and thermal Enthalpies=	-711.423635
Sum of electronic and thermal Free Energies=	-711.490715

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -712.683793

TS1'

Charge: 1 multiplicity: 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	-1.926810	-0.702578	0.081144
2	79	0	-0.335174	1.453913	0.080668
3	79	0	0.740125	-0.983593	-0.233410
4	6	0	3.825646	-2.131962	0.578946
5	1	0	4.650911	-2.453206	1.221627
6	1	0	4.033824	-2.466084	-0.441375
7	1	0	2.920134	-2.632121	0.946655
8	6	0	3.679456	-0.622957	0.641061
9	1	0	4.603551	-0.125361	0.292528
10	1	0	3.498866	-0.252641	1.662238
11	8	0	2.673114	-0.121243	-0.230835
12	1	0	2.570246	1.360018	-0.288599
13	8	0	2.571561	2.417621	-0.318200
14	8	0	1.370170	2.884527	-0.083069

Zero-point correction=	0.083537 (Hartree/Particle)
Thermal correction to Energy=	0.096212
Thermal correction to Enthalpy=	0.097156
Thermal correction to Gibbs Free Energy=	0.036676
Sum of electronic and zero-point Energies=	-711.427367
Sum of electronic and thermal Energies=	-711.414691
Sum of electronic and thermal Enthalpies=	-711.413747
Sum of electronic and thermal Free Energies=	-711.641711

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -712.678387

TS1a'

Charge: 1 multiplicity: 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	-2.104209	-0.096877	0.071137
2	79	0	0.139202	1.380289	-0.009171
3	79	0	0.225889	-1.362700	-0.086951
4	6	0	4.854044	-0.853746	0.282505
5	1	0	5.107831	-0.822862	-0.783623
6	1	0	5.374871	-0.030742	0.778913
7	1	0	5.237817	-1.794746	0.701728
8	6	0	3.377231	-0.748986	0.514989

9	1	0	3.014532	-0.633642	1.538107
10	1	0	3.098639	0.697637	0.055866
11	8	0	2.579062	-1.684513	-0.141534
12	8	0	2.096927	2.447064	-0.180697
13	8	0	3.221817	1.791862	-0.193522
14	1	0	2.986487	-1.970772	-0.976107

Zero-point correction= 0.081571 (Hartree/Particle)
Thermal correction to Energy= 0.094718
Thermal correction to Enthalpy= 0.095662
Thermal correction to Gibbs Free Energy= 0.034495
Sum of electronic and zero-point Energies= -711.434679
Sum of electronic and thermal Energies= -711.421532
Sum of electronic and thermal Enthalpies= -711.420588
Sum of electronic and thermal Free Energies= -711.460755

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -712.6741146

TS1b'

Charge: 1 multiplicity: 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	-2.026701	-0.217763	0.050044
2	79	0	0.056671	1.435995	-0.023018
3	79	0	0.396799	-1.309346	-0.047378
4	6	0	3.598728	-0.225481	0.774859
5	1	0	4.561498	0.253963	0.959933
6	1	0	3.067846	1.131859	0.198012
7	1	0	2.967510	-0.341650	1.656190
8	6	0	3.651733	-1.367018	-0.184563
9	1	0	3.781797	-1.031742	-1.222334
10	1	0	4.516128	-1.999930	0.069490
11	8	0	2.464476	-2.194312	-0.069553
12	8	0	3.071405	2.195743	-0.122198
13	8	0	1.880288	2.713260	-0.178574
14	1	0	2.558411	-2.977018	-0.632658

Zero-point correction= 0.081217 (Hartree/Particle)
Thermal correction to Energy= 0.094194
Thermal correction to Enthalpy= 0.095138
Thermal correction to Gibbs Free Energy= 0.034295
Sum of electronic and zero-point Energies= -711.427847
Sum of electronic and thermal Energies= -711.414870
Sum of electronic and thermal Enthalpies= -711.413926
Sum of electronic and thermal Free Energies= -711.457169

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -712.665181

TS2'

Charge: 1 multiplicity: 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	-1.512061	1.226025	-0.121650
2	79	0	-1.298266	-1.421227	0.113891

3	79	0	0.950029	0.087107	-0.017816
4	6	0	5.141170	-1.217934	-0.168695
5	1	0	5.940017	-0.604152	-0.593248
6	1	0	5.234019	-1.239678	0.919451
7	1	0	5.242903	-2.240391	-0.549969
8	6	0	3.800598	-0.635156	-0.574710
9	1	0	3.544681	0.660923	-0.275358
10	1	0	3.678126	-0.465315	-1.665726
11	8	0	2.741431	-1.195988	0.003513
12	8	0	2.923287	2.171132	1.113373
13	8	0	2.686720	1.578244	-0.147902
14	1	0	2.861707	3.119595	0.893835

Zero-point correction= 0.079677 (Hartree/Particle)
Thermal correction to Energy= 0.093309
Thermal correction to Enthalpy= 0.094253
Thermal correction to Gibbs Free Energy= 0.031133
Sum of electronic and zero-point Energies= -711.395871
Sum of electronic and thermal Energies= -711.382239
Sum of electronic and thermal Enthalpies= -711.381295
Sum of electronic and thermal Free Energies= -711.444415

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -712.669449

TS2a'

Charge: 1 multiplicity: 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	1.423984	1.308612	-0.095818
2	79	0	1.487852	-1.324916	0.226176
3	79	0	-0.911459	-0.066174	-0.252573
4	6	0	-5.137032	-1.405675	-0.329111
5	1	0	-5.909489	-1.365548	0.443092
6	1	0	-5.451404	-0.814437	-1.192731
7	1	0	-5.018050	-2.448265	-0.651007
8	6	0	-3.823890	-0.885627	0.226210
9	1	0	-4.059558	0.539658	0.795713
10	1	0	-3.512802	-1.296335	1.206365
11	8	0	-2.849269	-0.728567	-0.654496
12	8	0	-2.925314	2.049402	0.475666
13	8	0	-3.928819	1.527379	1.266984
14	1	0	-2.685714	2.862786	0.965703

Zero-point correction= 0.079650 (Hartree/Particle)
Thermal correction to Energy= 0.093450
Thermal correction to Enthalpy= 0.094394
Thermal correction to Gibbs Free Energy= 0.028680
Sum of electronic and zero-point Energies= -711.392502
Sum of electronic and thermal Energies= -711.378702
Sum of electronic and thermal Enthalpies= -711.377757
Sum of electronic and thermal Free Energies= -711.443471

M06-L/def2-TZVP//b3lyp/6-31G(d,p)-LANL2DZ Single point energy: -712.667849