Supporting Information

Mechanistic Insights into Pd(0)-Catalyzed Intermolecular and Intramolecular Hydroamination of Methylenecyclopropanes: A Computational Study

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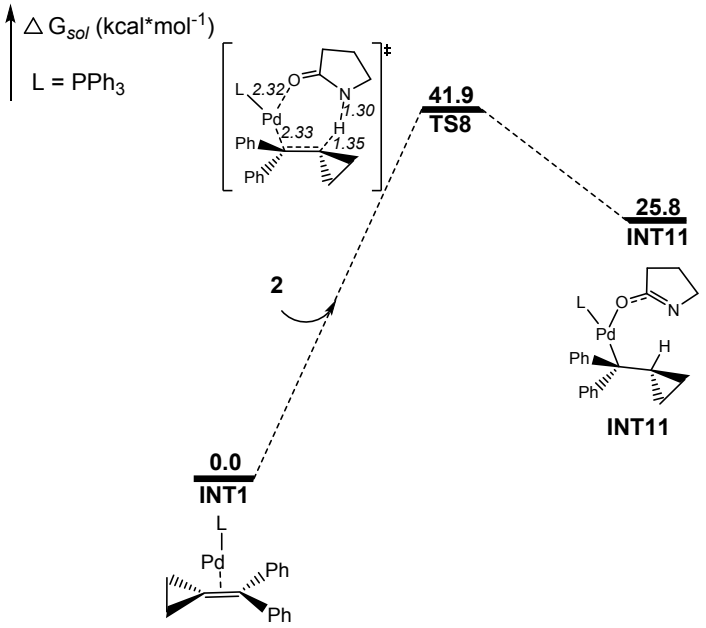

Figure S1. Energy profile for the proton transfer to C^2 from **INT1** in the Pd(0)-catalyzed hydroamination of **1** with **2**. Bond lengths are shown in Å.

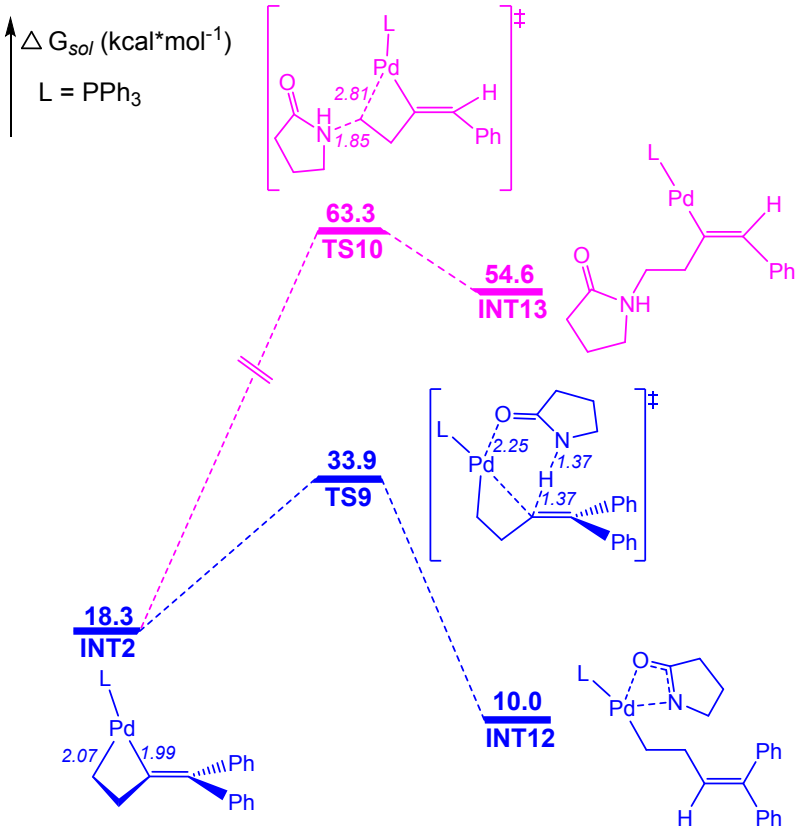

Figure S2. Energy profiles for the proton transfer and nucleophilic attack pathways from **INT2** in the Pd(0)-catalyzed hydroamination of **1** with **2**. Bond lengths are shown in Å.

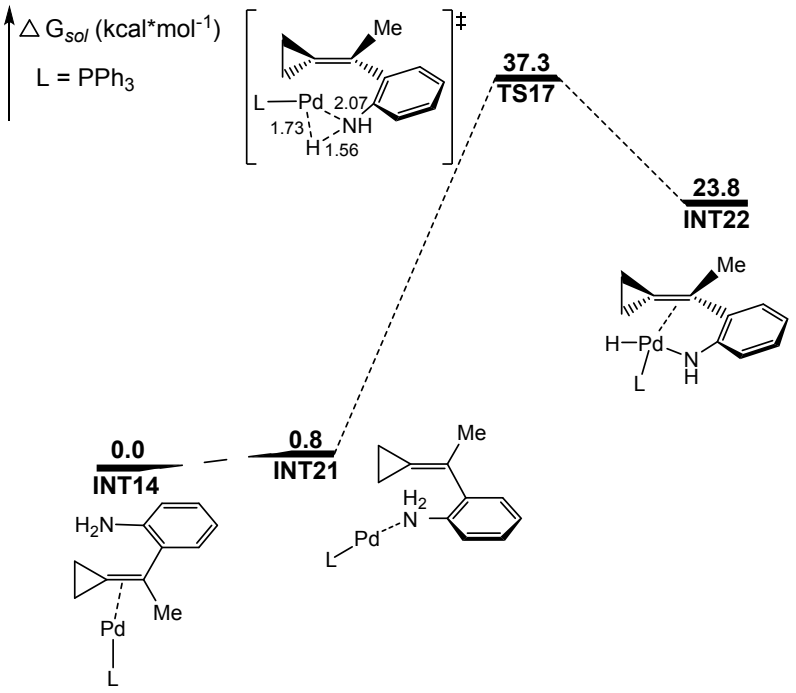

Figure S3. Energy profile for the N-H oxidative addition pathway in the Pd(0)-catalyzed intramolecular hydroamination of **4**. Bond lengths are shown in Å.

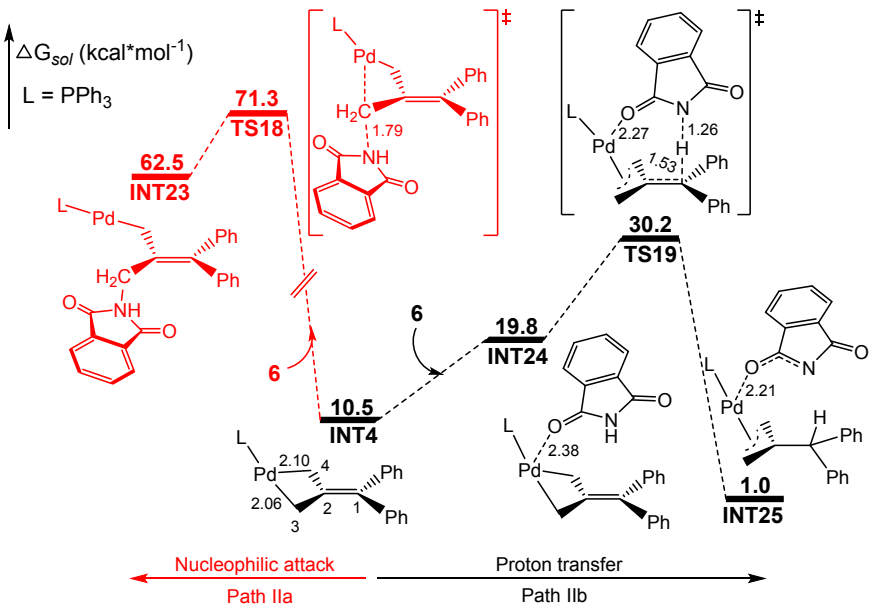

Figure S4. Energy profile for the nucleophilic attack and proton transfer pathways after the formation of **INT4** in the Pd(0)-catalyzed intermolecular hydroamination of **1** with phthalimide. Bond lengths are shown in Å.

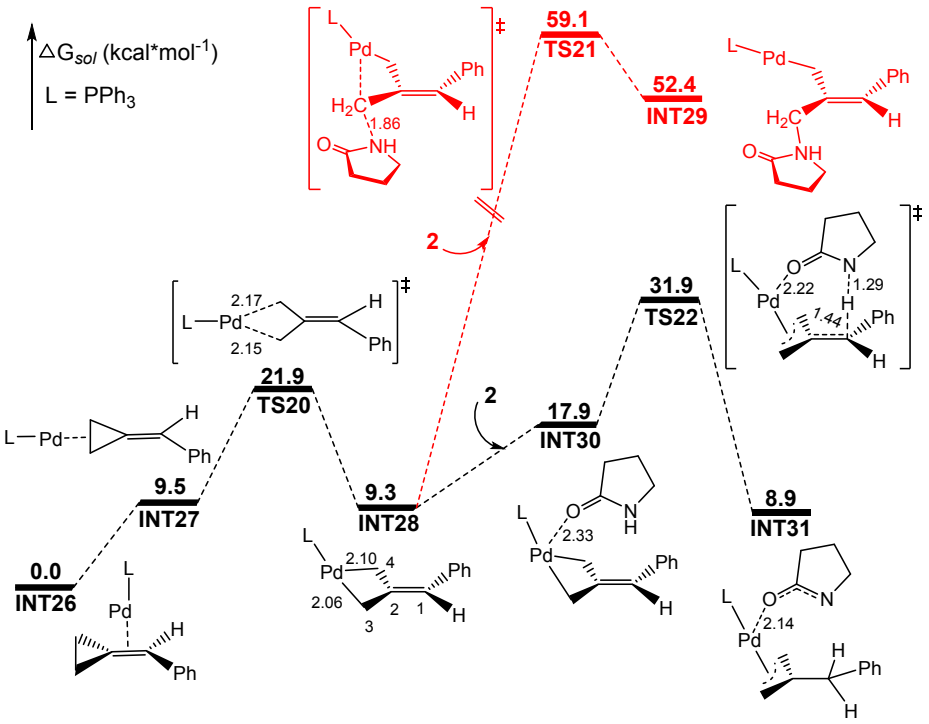

Figure S5. Energy profile for the nucleophilic attack and proton transfer pathways after the cleavage of distal C-C bond in the Pd(0)-catalyzed intermolecular hydroamination of **8**. Bond lengths are shown in Å.

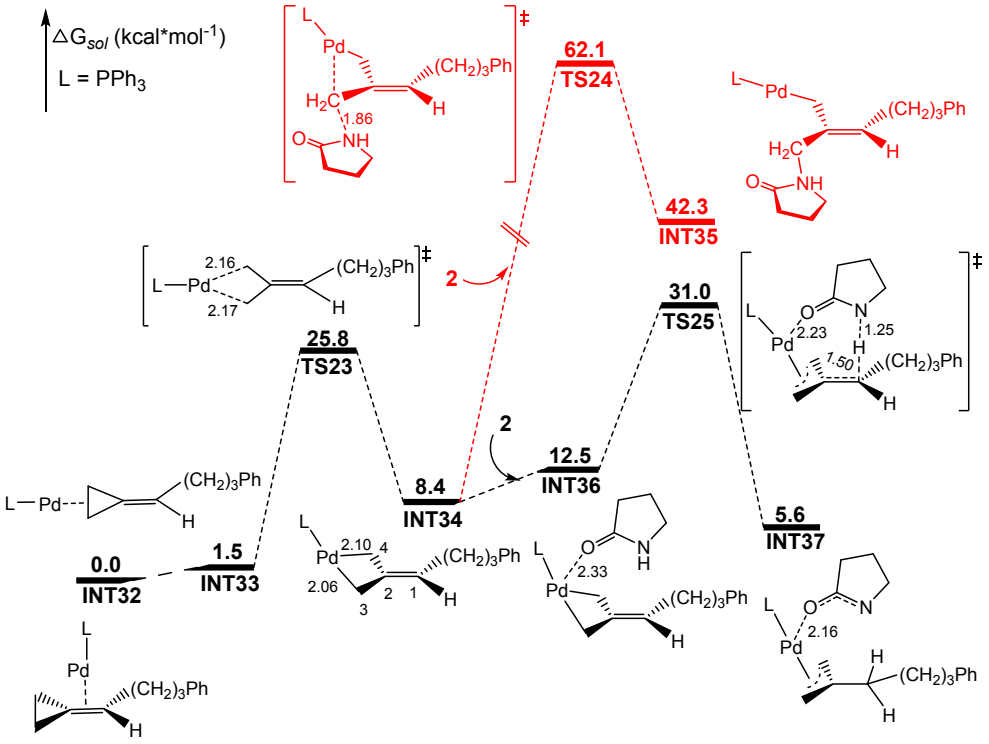

Figure S6. Energy profile for the nucleophilic attack and proton transfer pathways after the cleavage of distal C-C bond in the Pd(0)-catalyzed intermolecular hydroamination of **8**. Bond lengths are shown in Å.

The computational studies for both intra and intermolecular reactions using one electron rich phosphine (PMe_3) were carried out. The results of intermolecular reaction were shown in Figures S7 and S8. The results of intramolecular reaction were shown in Figures S9 and S10. As we can see, the employment of electron rich phosphine (PMe_3) could result in relatively higher energy barrier for the insertion of Pd(0) into distal C-C bond of MCP moiety of **1** in comparison with the PPh_3 ligand. Therefore, the PPh_3 ligand is more efficient in activating the MCP to form the metallacyclobutane intermediate than the electron rich phosphine (PMe_3). Nevertheless, the proposed mechanistic pathways of the reactions are consistent for both ligands.

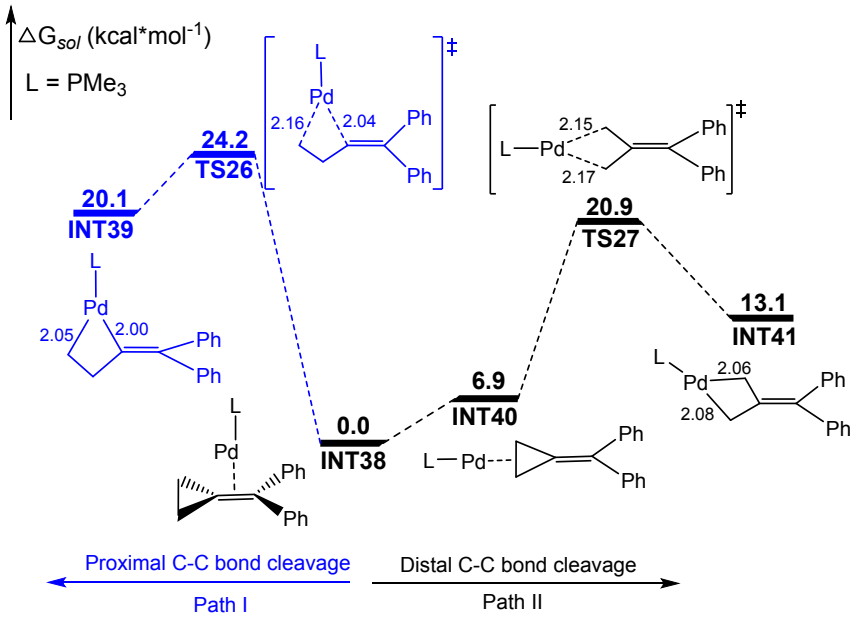

Figure S7. Energy profile for insertion of Pd(0) into proximal and distal C-C bonds of MCP moiety of **1** using PMe_3 as the ligand. Bond lengths are shown in Å.

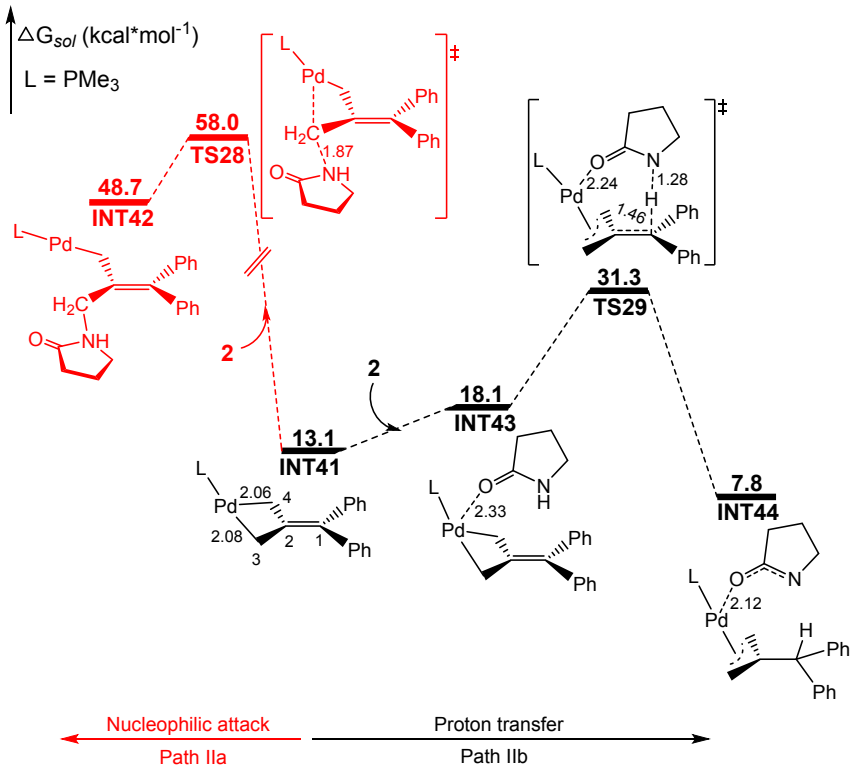

Figure S8. Energy profile for the nucleophilic attack and proton transfer pathways after the formation of **INT41** in the Pd(0)-catalyzed intermolecular hydroamination of **1** using PMe_3 as the ligand. Bond lengths are shown in Å.

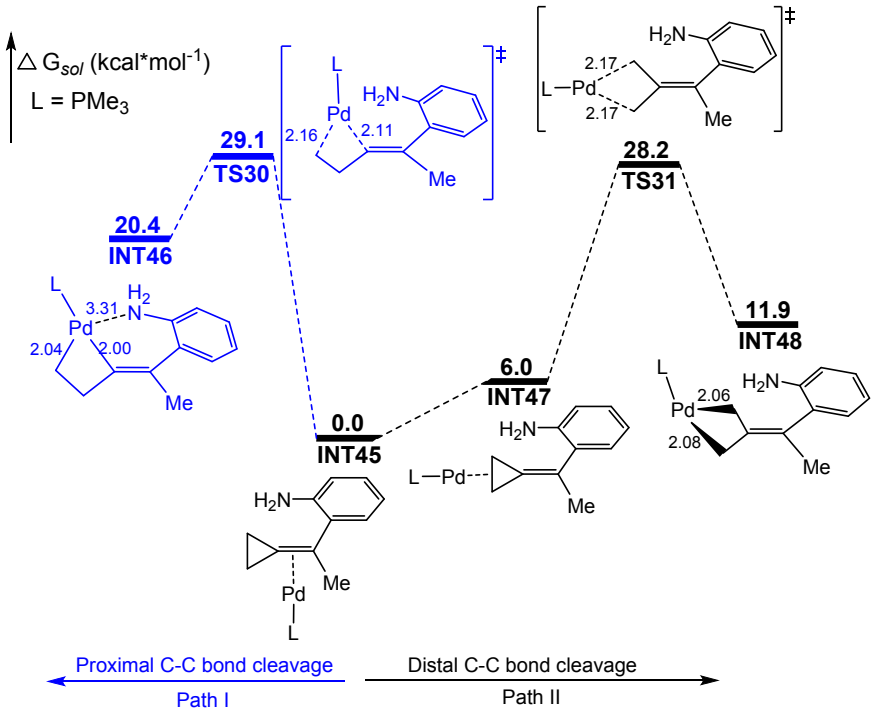

Figure S9. Energy profile for the insertion of Pd(0) into proximal and distal C-C bonds of MCP moiety of **4** using PMe_3 as the ligand. Bond lengths are shown in Å.

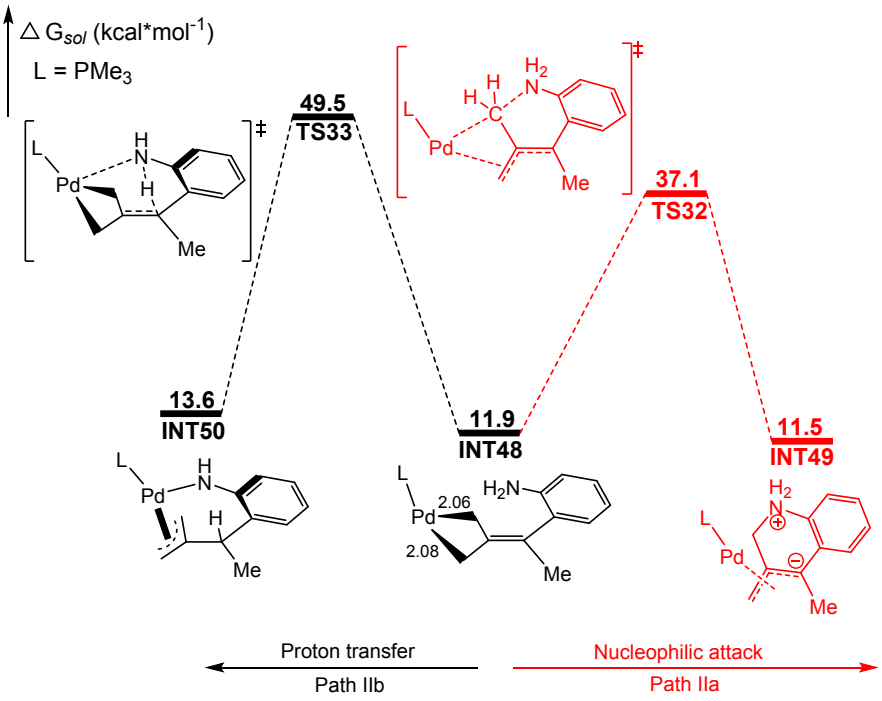

Figure S10. Energy profile for the nucleophilic attack and proton transfer pathways after the formation of **INT48** in the Pd(0)-catalyzed intramolecular hydroa8mination of **4** using PMe_3 as the ligand. Bond lengths are shown in Å.

Cartesian coordinates, energies, and frequencies

MCP 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.764338	3.228517	0.030034
2	6	0	0.764237	3.228643	-0.030029
3	1	0	-1.239111	3.527107	0.962035
4	1	0	-1.300670	3.540826	-0.863033
5	1	0	1.300592	3.540795	0.863078
6	1	0	1.238930	3.527554	-0.961973
7	6	0	0.000073	1.980562	-0.000125
8	6	0	-0.000013	0.648502	-0.000013
9	6	0	-1.282739	-0.106841	0.034966
10	6	0	-1.386717	-1.297422	0.765093
11	6	0	-2.417572	0.368141	-0.631762
12	6	0	-2.593775	-1.984739	0.836869
13	1	0	-0.513005	-1.679620	1.285502
14	6	0	-3.623797	-0.320923	-0.563490
15	1	0	-2.343389	1.279367	-1.216968
16	6	0	-3.717373	-1.499305	0.172752
17	1	0	-2.655906	-2.902080	1.414689
18	1	0	-4.491910	0.059895	-1.093451
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21	6	0	1.386763	-1.297383	-0.765161
22	6	0	2.417520	0.368102	0.631897
23	6	0	2.593837	-1.984654	-0.836967
24	1	0	0.513041	-1.679551	-1.285569
25	6	0	3.623771	-0.320933	0.563603
26	1	0	2.343269	1.279251	1.217217
27	6	0	3.717400	-1.499221	-0.172768
28	1	0	2.656047	-2.901939	-1.414864
29	1	0	4.491863	0.059821	1.093642
30	1	0	4.658480	-2.038242	-0.224231

Zero-point correction= 0.250839 (Hartree/Particle)
Thermal correction to Energy= 0.263911
Thermal correction to Enthalpy= 0.264855
Thermal correction to Gibbs Free Energy= 0.210249
Sum of electronic and zero-point Energies= -617.555306
Sum of electronic and thermal Energies= -617.542234
Sum of electronic and thermal Enthalpies= -617.541290
Sum of electronic and thermal Free Energies= -617.595897
M06-2x/6-311++G(d,p) // M06-2x /6-31G(d) energy= -617.7876245
Frequencies

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83.6397	131.7173	149.0354
224.1379	244.3649	278.5938
300.1831	382.8268	398.5492
417.0230	422.9317	459.8022
522.3686	624.7260	632.2133
635.0658	655.5170	697.6594
715.1516	716.7891	754.7943
775.3855	797.8824	872.9221
873.6132	882.4207	897.7711
930.4598	947.8943	949.5075
993.2804	993.5773	1015.5986
1015.7483	1020.4989	1020.7000
1053.2699	1054.7163	1071.0812
1074.7498	1096.9206	1107.7275
1109.8279	1121.3984	1131.9202
1173.6871	1189.7170	1189.9407
1209.8454	1210.4492	1265.5426
1323.9070	1345.8828	1356.7989
1362.8310	1364.3462	1474.6902
1498.0534	1503.9301	1512.8464
1554.5945	1560.1738	1674.8755
1678.4906	1701.4661	1702.9569
1860.0721	3146.5503	3146.8570
3204.3905	3204.4263	3211.5980
3211.7453	3220.4122	3220.4386
3221.3831	3230.5292	3230.6599

3231.9420 3235.6452 3235.8014

INT1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.863522	0.887040	-3.376251
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9	1	0	4.319505	-0.794388	-3.029692
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14	6	0	1.939272	3.953019	-0.036213
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31	6	0	-2.971398	-1.428810	-0.457997
32	6	0	-3.657782	-1.965239	0.636165
33	6	0	-3.388862	-1.754332	-1.752205
34	6	0	-4.749777	-2.805625	0.435842
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61	1	0	2.154292	-2.404228	-1.209420
62	6	0	4.100224	-3.066434	1.499610
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Zero-point correction= 0.529942 (Hartree/Particle)
Thermal correction to Energy= 0.562277

Thermal correction to Enthalpy= 0.563221
Thermal correction to Gibbs Free Energy= 0.463915
Sum of electronic and zero-point Energies= -1779.914086
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M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1780.420321

Frequencies

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85.1240	96.4449	103.0606
111.5535	119.1573	139.4178
158.3373	161.6021	175.6811
195.5977	219.2803	225.7110
238.8932	255.5724	257.0894
267.7805	272.7588	288.1398
307.3794	390.9186	402.2281
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415.9717	427.1580	431.3925
440.3133	450.8917	461.8611
510.1803	515.2053	523.6039
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3227.2137	3229.5667	3230.5513
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3238.5149	3240.6111	3255.3017

TS1

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
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5	1	0	1.816445	-3.175887	-1.806013
6	6	0	1.798708	-1.029762	-1.445821
7	6	0	2.438690	-0.110015	-0.690882
8	46	0	-0.152492	-0.710511	-1.931964
9	1	0	3.338754	-2.339639	-2.308661
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11	6	0	1.840920	1.905471	0.685310
12	6	0	1.467303	3.241392	0.796896
13	1	0	2.026256	1.313236	1.578936
14	6	0	1.382858	3.419830	-1.603831
15	6	0	1.251561	4.008414	-0.347287
16	1	0	1.348339	3.684160	1.781545
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19	15	0	-1.646721	-0.256504	-0.056014
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21	6	0	0.322517	-1.138613	1.693355
22	6	0	-0.869136	0.809845	2.474144
23	6	0	1.124670	-1.108565	2.830302
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28	1	0	1.911954	-1.845460	2.954917
29	1	0	-0.214953	1.614989	4.356655
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36	6	0	-4.521352	-3.118383	-0.574327
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44	6	0	-3.901793	1.455123	0.372060
45	6	0	-2.458391	3.708603	-0.419916
46	1	0	-0.825842	2.350750	-0.769839
47	6	0	-4.506561	2.711010	0.373502
48	1	0	-4.466270	0.581191	0.684734
49	6	0	-3.786781	3.837437	-0.016719
50	1	0	-1.888100	4.580244	-0.727375
51	1	0	-5.542534	2.808281	0.683797
52	1	0	-4.262021	4.813760	-0.010492
53	6	0	1.735167	2.075935	-1.713822
54	1	0	1.844496	1.615796	-2.692012
55	6	0	3.655083	-0.499267	0.071826
56	6	0	4.674942	0.429570	0.325617
57	6	0	3.816078	-1.802678	0.564954
58	6	0	5.816744	0.064860	1.031469
59	1	0	4.568103	1.446348	-0.040651
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62	6	0	5.965386	-1.235798	1.506864
63	1	0	6.594586	0.801689	1.208795
64	1	0	5.056752	-3.182988	1.644907
65	1	0	6.854179	-1.518406	2.062391

Zero-point correction= 0.529915 (Hartree/Particle)
Thermal correction to Energy= 0.561374
Thermal correction to Enthalpy= 0.562318
Thermal correction to Gibbs Free Energy= 0.464916
Sum of electronic and zero-point Energies= -1779.876702
Sum of electronic and thermal Energies= -1779.845243
Sum of electronic and thermal Enthalpies= -1779.844299

Sum of electronic and thermal Free Energies= -1779.941701
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1780.383028
Frequencies

-228.2702	21.4068	26.2086
33.7786	36.4813	40.2068
55.0575	57.4255	66.0500
71.9163	75.9634	80.3564
89.8284	94.0861	95.6324
108.6949	109.4385	125.5238
146.9294	162.0252	198.6265
202.4561	217.9318	229.6028
243.2211	257.6140	263.5130
270.2490	281.9189	296.3592
329.1851	402.9431	408.0783
411.0236	418.3641	422.4731
426.2161	428.0965	440.7676
447.2918	452.3459	472.1083
508.3472	519.0466	522.0503
528.8178	600.5458	623.1363
629.0085	629.7699	631.7287
632.5813	651.5483	657.4898
703.3582	713.4348	716.0082
717.9628	720.8608	722.1396
724.0077	728.7192	729.4895
761.7730	769.7577	772.5497
777.6975	789.8842	799.0192
843.9574	878.6018	883.9547
886.5333	889.3378	894.6984
937.5450	951.9911	955.2104
955.9825	960.0223	963.1147
966.7457	988.6589	1000.2436
1001.0245	1004.6726	1009.6509
1013.8186	1015.5979	1015.8952
1016.0992	1017.7829	1021.2470
1022.3904	1023.9142	1026.4587
1028.1754	1028.6733	1060.6302
1070.1483	1071.1541	1072.2437
1078.0816	1078.4647	1119.9946
1123.2249	1125.9992	1128.6967
1131.9501	1142.1321	1142.9793
1145.4692	1149.5053	1183.6348
1186.3756	1190.4573	1192.9257
1196.7972	1200.9879	1216.1719
1217.9198	1220.3015	1220.6347
1225.3296	1234.9011	1248.9869
1322.7748	1334.0209	1337.3811
1342.6172	1344.0037	1347.4120
1366.1278	1366.3118	1369.4833
1370.3158	1377.5150	1447.8173
1494.6534	1495.8569	1496.5775
1499.9903	1501.6236	1506.1259
1542.6378	1544.7113	1549.9905
1554.1895	1558.3207	1661.3073
1667.4565	1670.5104	1671.4352
1674.2448	1682.0688	1686.3476
1687.5339	1690.8150	1695.2244
1699.8997	3069.5245	3093.4579
3157.0118	3193.7910	3201.9922
3204.2841	3208.1705	3212.0981
3215.1000	3216.0270	3217.9086
3218.4896	3219.2691	3220.1505
3221.9850	3223.1580	3226.7392
3227.2490	3227.4738	3230.1864
3234.9242	3235.7480	3236.6277
3238.1008	3240.7699	3242.9901
3243.4487	3244.3091	3251.0919

INT2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.175578	-2.453985	-2.777147
2	1	0	1.623591	-2.039001	-3.679367
3	1	0	0.587645	-3.352886	-2.984010

4	6	0	2.161462	-2.546810	-1.597647
5	1	0	1.846124	-3.333160	-0.900916
6	6	0	1.751212	-1.191175	-1.158900
7	6	0	2.400070	-0.162735	-0.589860
8	46	0	-0.116521	-1.137794	-1.836683
9	1	0	3.229527	-2.680208	-1.821172
10	6	0	1.913892	1.244904	-0.669102
11	6	0	1.770897	2.029152	0.482478
12	6	0	1.398150	3.366796	0.389256
13	1	0	1.952183	1.577265	1.455426
14	6	0	1.334801	3.185856	-2.012676
15	6	0	1.195621	3.954865	-0.859123
16	1	0	1.275480	3.953488	1.295163
17	1	0	1.179657	3.633863	-2.989917
18	1	0	0.929502	5.005592	-0.930258
19	15	0	-1.624233	-0.174055	-0.030554
20	6	0	-0.693489	0.047334	1.536107
21	6	0	0.277660	-0.909738	1.854126
22	6	0	-0.882264	1.138929	2.388480
23	6	0	1.051615	-0.774575	3.002417
24	1	0	0.441273	-1.751591	1.185596
25	6	0	-0.107406	1.271050	3.539267
26	1	0	-1.624111	1.895612	2.148965
27	6	0	0.862397	0.319370	3.845254
28	1	0	1.813555	-1.513814	3.229171
29	1	0	-0.259013	2.124092	4.193943
30	1	0	1.472695	0.430279	4.736415
31	6	0	-2.908683	-1.405435	0.420978
32	6	0	-3.274787	-1.676985	1.742581
33	6	0	-3.557458	-2.079948	-0.619300
34	6	0	-4.278203	-2.603654	2.015764
35	1	0	-2.771142	-1.165049	2.558000
36	6	0	-4.564591	-3.000273	-0.345991
37	1	0	-3.271765	-1.881339	-1.650971
38	6	0	-4.924740	-3.264004	0.973671
39	1	0	-4.553399	-2.811322	3.045292
40	1	0	-5.061836	-3.516379	-1.161218
41	1	0	-5.704805	-3.987736	1.188877
42	6	0	-2.569783	1.385129	-0.172014
43	6	0	-1.907241	2.451332	-0.787082
44	6	0	-3.862786	1.567965	0.325620
45	6	0	-2.522745	3.694724	-0.888389
46	1	0	-0.905805	2.302683	-1.182980
47	6	0	-4.481789	2.810621	0.209342
48	1	0	-4.384205	0.742855	0.802954
49	6	0	-3.812645	3.874286	-0.393143
50	1	0	-1.994651	4.517046	-1.361973
51	1	0	-5.488013	2.948514	0.593111
52	1	0	-4.298948	4.841194	-0.480299
53	6	0	1.677717	1.837987	-1.915901
54	1	0	1.795049	1.232789	-2.810942
55	6	0	3.695359	-0.384251	0.111218
56	6	0	4.695462	0.598706	0.107933
57	6	0	3.947848	-1.579504	0.798526
58	6	0	5.909375	0.384612	0.751674
59	1	0	4.515793	1.536418	-0.409955
60	6	0	5.162756	-1.795078	1.441372
61	1	0	3.171236	-2.338125	0.840519
62	6	0	6.150580	-0.813935	1.419671
63	1	0	6.672005	1.157659	0.729070
64	1	0	5.334487	-2.729510	1.967680
65	1	0	7.098302	-0.979092	1.922772

Zero-point correction= 0.529682 (Hartree/Particle)
Thermal correction to Energy= 0.561840
Thermal correction to Enthalpy= 0.562785
Thermal correction to Gibbs Free Energy= 0.462753
Sum of electronic and zero-point Energies= -1779.879515
Sum of electronic and thermal Energies= -1779.847356
Sum of electronic and thermal Enthalpies= -1779.846412
Sum of electronic and thermal Free Energies= -1779.946444

M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1780.39113

Frequencies

16.4442 26.3589 28.3754
32.7808 38.8982 47.1469

51.1499	54.9260	60.6087
64.1616	70.4147	87.2833
89.3213	93.7914	99.0680
105.2615	115.3286	128.8182
163.4005	178.3261	195.8683
216.2982	222.1880	240.3607
253.1037	262.7543	268.7881
271.8591	274.2939	304.1889
380.7224	405.1838	407.7775
409.0376	414.2718	419.8482
425.6045	429.1677	439.2096
448.6952	473.1037	501.5161
508.3970	515.7736	525.7829
533.4235	610.6932	624.1925
627.4911	628.3401	629.0313
629.9683	657.4824	670.5917
695.3984	699.3694	709.6107
713.3619	716.5825	717.9818
720.5990	721.8737	724.3094
766.7603	769.8825	773.6076
776.1004	793.9544	794.9673
863.6429	873.1453	876.0913
878.0713	882.2550	887.0465
934.7557	942.7873	950.6527
952.7222	957.2952	960.7608
984.8323	994.7792	998.1890
1001.5233	1005.2752	1006.0441
1011.5320	1013.6105	1014.5934
1016.1699	1016.7060	1018.1253
1018.9879	1019.4957	1022.8308
1028.8680	1029.8172	1067.8226
1070.1791	1071.2863	1071.7096
1075.0418	1085.9158	1114.2496
1117.2498	1121.5134	1123.8141
1125.2960	1128.0368	1130.8038
1140.3242	1146.2747	1179.8973
1184.7277	1185.1724	1189.6173
1191.2586	1209.8874	1213.0463
1217.1441	1218.1019	1225.2593
1227.8253	1238.8308	1286.5250
1319.6696	1329.7811	1335.0503
1339.4299	1340.4916	1344.4231
1360.8059	1361.5954	1362.7496
1368.3852	1372.5068	1464.2339
1487.8451	1491.0690	1495.9711
1497.3443	1497.8978	1500.9196
1535.9873	1544.6913	1546.8030
1551.1256	1556.0327	1665.3239
1666.2935	1669.1068	1669.6848
1672.5061	1683.4119	1688.3512
1689.2221	1693.5342	1696.8789
1714.5137	3044.8228	3097.2522
3099.4844	3190.5883	3193.1047
3201.6389	3202.2964	3203.5310
3206.9627	3208.0182	3210.6823
3216.2753	3217.6605	3218.3209
3218.7853	3219.4189	3222.6548
3225.2830	3226.8480	3226.9879
3232.0757	3233.1624	3234.0270
3234.5895	3238.6199	3239.8943
3243.5279	3244.3990	3250.1717

INT3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.473748	0.171683	-0.135262
2	6	0	-1.975303	-0.666304	-0.217714
3	6	0	-2.018782	0.901352	-0.159068
4	1	0	-1.622458	-1.199890	0.664664
5	1	0	-1.718075	-1.136903	-1.165942
6	1	0	-1.774623	1.445862	-1.069972
7	6	0	-3.224909	0.080120	-0.131773
8	6	0	-4.554738	0.032281	-0.060648

9	1	0	-1.712064	1.396887	0.762557
10	6	0	-5.354599	1.285090	0.006185
11	6	0	-6.508545	1.347676	0.797747
12	6	0	-4.960051	2.431256	-0.693023
13	6	0	-7.238350	2.527450	0.897226
14	1	0	-6.826660	0.464425	1.344093
15	6	0	-5.692012	3.609932	-0.596720
16	1	0	-4.080363	2.388100	-1.327299
17	6	0	-6.833057	3.663169	0.200243
18	1	0	-8.125761	2.558875	1.521906
19	1	0	-5.375234	4.487146	-1.152603
20	1	0	-7.405562	4.582647	0.272752
21	6	0	-5.258985	-1.279127	-0.048411
22	6	0	-6.476258	-1.439411	-0.722517
23	6	0	-4.708716	-2.384959	0.609336
24	6	0	-7.114862	-2.674644	-0.750591
25	1	0	-6.917822	-0.588412	-1.233112
26	6	0	-5.348763	-3.619343	0.584130
27	1	0	-3.778106	-2.266556	1.155129
28	6	0	-6.553383	-3.769800	-0.098358
29	1	0	-8.054249	-2.781984	-1.284344
30	1	0	-4.908117	-4.464087	1.104849
31	1	0	-7.054340	-4.732706	-0.117590
32	15	0	2.728825	0.047205	-0.020341
33	6	0	3.391398	-0.466649	1.619702
34	6	0	2.775108	0.068839	2.756632
35	6	0	4.475232	-1.334465	1.780703
36	6	0	3.244249	-0.240915	4.028861
37	1	0	1.917135	0.726685	2.633398
38	6	0	4.935992	-1.655019	3.056521
39	1	0	4.959858	-1.766181	0.909392
40	6	0	4.325516	-1.106805	4.180949
41	1	0	2.759776	0.185084	4.902162
42	1	0	5.773929	-2.336319	3.169865
43	1	0	4.686421	-1.358386	5.173576
44	6	0	3.706321	1.570293	-0.360693
45	6	0	4.869762	1.906846	0.337623
46	6	0	3.263129	2.409621	-1.388711
47	6	0	5.580235	3.059144	0.007242
48	1	0	5.221285	1.269413	1.144088
49	6	0	3.979837	3.553618	-1.725944
50	1	0	2.345647	2.160566	-1.917722
51	6	0	5.139770	3.880967	-1.026372
52	1	0	6.479333	3.314037	0.560030
53	1	0	3.628055	4.195382	-2.527949
54	1	0	5.694836	4.778194	-1.282428
55	6	0	3.519366	-1.169916	-1.154982
56	6	0	2.819903	-2.352085	-1.421219
57	6	0	4.776992	-0.979536	-1.736320
58	6	0	3.372382	-3.333591	-2.237973
59	1	0	1.831681	-2.488863	-0.987000
60	6	0	5.324570	-1.957961	-2.563571
61	1	0	5.329668	-0.063400	-1.546804
62	6	0	4.626184	-3.136236	-2.813071
63	1	0	2.820047	-4.247148	-2.435782
64	1	0	6.299118	-1.797635	-3.014874
65	1	0	5.054085	-3.895672	-3.460398

Zero-point correction= 0.529817 (Hartree/Particle)
Thermal correction to Energy= 0.562881
Thermal correction to Enthalpy= 0.563826
Thermal correction to Gibbs Free Energy= 0.456674
Sum of electronic and zero-point Energies= -1779.892421
Sum of electronic and thermal Energies= -1779.859357
Sum of electronic and thermal Enthalpies= -1779.858413
Sum of electronic and thermal Free Energies= -1779.965565
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1780.4142
Frequencies

6.0374	14.5731	17.9031
25.9981	29.2859	34.5347
35.5369	40.1749	46.9833
49.8788	52.9332	58.2818
67.9406	75.2692	78.2928
82.6611	98.4749	104.1196
146.0113	160.1423	176.7400

205.2515	221.6499	223.3397
233.7591	243.5229	259.3253
269.4322	275.2406	291.7554
303.3682	399.2932	408.5277
409.4261	410.1643	414.5758
417.2857	423.2428	442.2753
443.8251	446.3511	461.8065
514.3576	515.7042	525.3202
529.3514	625.0730	629.5723
631.1248	631.8328	632.5712
637.3760	657.9254	697.5614
703.5053	713.6025	713.9963
715.7172	717.1662	717.8757
718.1477	718.6015	741.5737
766.6105	769.9860	772.0775
776.3615	799.1100	841.5252
875.9224	876.0839	879.7473
879.7879	884.5747	900.2161
933.9572	948.9928	950.2031
950.2803	952.6086	953.5247
997.5318	997.9748	999.3492
1001.3576	1005.6036	1015.7825
1015.8843	1016.6689	1018.3089
1019.2024	1020.5248	1021.0770
1021.5688	1022.2146	1023.8814
1046.6155	1056.4768	1068.0508
1071.4179	1073.3509	1075.0558
1075.2432	1081.3310	1091.2992
1107.3409	1122.0097	1123.0067
1130.3401	1130.8455	1131.3657
1137.6494	1141.7390	1144.5277
1156.1012	1186.0470	1187.3836
1193.8107	1195.6968	1197.5147
1209.2927	1219.0930	1220.6251
1230.3645	1230.7462	1266.8051
1326.2017	1333.4370	1337.9065
1340.6558	1348.0901	1359.9795
1364.0543	1364.2917	1370.5424
1372.7874	1374.7409	1458.1264
1480.6594	1494.7455	1501.0582
1502.1931	1505.0197	1512.0879
1542.1870	1547.9650	1551.8679
1556.7040	1565.0492	1673.1599
1673.4355	1674.6874	1676.5958
1678.3178	1689.3796	1690.8780
1692.4644	1703.6161	1705.8186
1867.4967	3127.2554	3128.2746
3193.0478	3196.6367	3205.3131
3205.4080	3207.9438	3208.0801
3213.3093	3213.7949	3214.7509
3214.8979	3215.0885	3215.1217
3218.1945	3218.6580	3221.7919
3222.5788	3224.9539	3229.0977
3229.2024	3229.4610	3230.6686
3230.7371	3235.1029	3241.9155
3242.6063	3242.6886	3247.3677

TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.184018	0.286629	0.026333
2	6	0	-1.688096	-0.815162	-0.016655
3	6	0	-1.795034	1.127791	0.080129
4	1	0	-1.474101	-1.395517	0.882008
5	1	0	-1.514571	-1.350242	-0.953374
6	1	0	-1.652830	1.740098	-0.813280
7	6	0	-2.837147	0.093993	0.024984
8	6	0	-4.173803	0.023497	0.012190
9	1	0	-1.694188	1.671506	1.023549
10	6	0	-5.002639	1.258863	0.049700
11	6	0	-6.151854	1.310457	0.850245
12	6	0	-4.658774	2.392478	-0.695215
13	6	0	-6.919554	2.467456	0.920421

14	1	0	-6.437212	0.432582	1.423238
15	6	0	-5.428599	3.550071	-0.628207
16	1	0	-3.791906	2.355313	-1.346530
17	6	0	-6.559659	3.593435	0.182246
18	1	0	-7.802374	2.489781	1.552141
19	1	0	-5.148469	4.417102	-1.218803
20	1	0	-7.161743	4.495426	0.231856
21	6	0	-4.874117	-1.287769	-0.045409
22	6	0	-6.023616	-1.433503	-0.833570
23	6	0	-4.407376	-2.401634	0.661885
24	6	0	-6.672020	-2.659595	-0.929303
25	1	0	-6.403968	-0.573303	-1.377439
26	6	0	-5.057863	-3.628567	0.569071
27	1	0	-3.540351	-2.297114	1.305734
28	6	0	-6.189862	-3.763733	-0.229784
29	1	0	-7.556762	-2.752515	-1.552032
30	1	0	-4.683752	-4.479169	1.131075
31	1	0	-6.697618	-4.720690	-0.301073
32	15	0	2.594146	0.030220	0.008117
33	6	0	3.330610	-0.606876	1.565762
34	6	0	2.673347	-0.300276	2.761624
35	6	0	4.516459	-1.347486	1.607824
36	6	0	3.202855	-0.709449	3.982420
37	1	0	1.738329	0.255103	2.725516
38	6	0	5.040843	-1.762377	2.829099
39	1	0	5.029479	-1.602906	0.684440
40	6	0	4.387540	-1.440946	4.016909
41	1	0	2.685330	-0.464857	4.904790
42	1	0	5.959556	-2.340436	2.852429
43	1	0	4.797185	-1.768253	4.967629
44	6	0	3.548076	1.571784	-0.299136
45	6	0	4.698054	1.921702	0.413003
46	6	0	3.091976	2.416683	-1.318210
47	6	0	5.385403	3.094166	0.103843
48	1	0	5.058115	1.279870	1.211664
49	6	0	3.785872	3.580287	-1.632704
50	1	0	2.186403	2.156909	-1.862586
51	6	0	4.934441	3.921345	-0.920267
52	1	0	6.275349	3.359526	0.666222
53	1	0	3.425673	4.226006	-2.427596
54	1	0	5.472273	4.833354	-1.159976
55	6	0	3.276098	-1.107056	-1.264046
56	6	0	2.519751	-2.235216	-1.599235
57	6	0	4.508162	-0.899434	-1.892231
58	6	0	2.996338	-3.151822	-2.531812
59	1	0	1.548477	-2.382672	-1.131476
60	6	0	4.979727	-1.813229	-2.831656
61	1	0	5.097782	-0.019156	-1.649954
62	6	0	4.226970	-2.940949	-3.149932
63	1	0	2.402029	-4.024323	-2.784628
64	1	0	5.935999	-1.642440	-3.316618
65	1	0	4.595774	-3.650788	-3.883909

Zero-point correction= 0.527670 (Hartree/Particle)
Thermal correction to Energy= 0.560127
Thermal correction to Enthalpy= 0.561071
Thermal correction to Gibbs Free Energy= 0.455337
Sum of electronic and zero-point Energies= -1779.873740
Sum of electronic and thermal Energies= -1779.841283
Sum of electronic and thermal Enthalpies= -1779.840339
Sum of electronic and thermal Free Energies= -1779.946073
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1780.392926
Frequencies

189.3865	8.1774	12.3193
16.9381	20.4987	24.5282
30.7797	34.5428	41.6902
45.1892	55.6811	58.2142
64.5163	69.2597	69.6011
74.1217	93.6094	116.6665
120.8743	128.0520	193.0514
215.4313	221.5241	223.1529
243.3451	259.0063	264.5232
276.8847	299.7201	304.9921
351.0595	376.1939	407.5711
408.7003	413.4555	417.1268

422.2364	436.0689	441.3221
445.8396	458.9017	472.6502
510.8055	515.7593	518.6964
535.3232	537.6755	579.0317
625.8372	628.5697	631.4340
632.0187	632.3306	642.2291
663.0447	703.5873	708.2022
713.2656	714.7275	717.2781
718.1838	719.2112	721.5032
722.7728	734.9499	767.3903
773.5131	777.2242	784.2327
799.0381	870.6467	877.3583
883.9654	884.2447	887.7693
935.4534	939.4935	945.4367
948.6392	952.5557	955.8434
959.9441	965.3423	985.4934
992.9595	999.4907	1003.3427
1004.7583	1007.6486	1011.5401
1015.2782	1015.4601	1015.9211
1016.4341	1022.1461	1023.1380
1024.1575	1027.7446	1028.0826
1030.1952	1071.1055	1073.2127
1074.8014	1075.6011	1079.5378
1121.5626	1122.0057	1128.3680
1130.5432	1130.8859	1132.0677
1140.4049	1142.2175	1146.3482
1189.2286	1190.2597	1194.1569
1197.8154	1198.8588	1208.5933
1214.8629	1220.4599	1222.5253
1230.8811	1232.2460	1253.2139
1323.5451	1334.4237	1337.6314
1341.5263	1345.2704	1364.6176
1365.6535	1367.3792	1370.9920
1375.3869	1375.8586	1411.2027
1432.0866	1495.9200	1501.7641
1503.1664	1505.0810	1509.2680
1543.6320	1550.6026	1551.6243
1557.2550	1566.0962	1672.9531
1673.7860	1674.0123	1676.1072
1676.6764	1687.8585	1689.6853
1693.3359	1701.7680	1704.8833
1807.2930	3087.3760	3104.0697
3180.2861	3195.4778	3196.6235
3200.8999	3204.3053	3210.8701
3211.6261	3213.3810	3215.4107
3219.0350	3219.9387	3220.3752
3220.6524	3221.1911	3228.3481
3229.4664	3229.5798	3229.9817
3232.5273	3235.4777	3236.6200
3239.7438	3240.3387	3243.5066
3244.4412	3251.0622	3251.3894

INT4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.151578	1.413893	1.207202
2	6	0	-0.838424	-0.292811	1.804517
3	6	0	-1.739349	1.760702	2.057975
4	1	0	-0.552736	-0.408088	2.852876
5	1	0	-0.571530	-1.155607	1.193027
6	1	0	-2.266909	2.633885	1.678458
7	6	0	-2.106289	0.419019	1.548647
8	6	0	-3.110581	0.024605	0.716203
9	1	0	-1.589053	1.787416	3.140049
10	6	0	-4.145237	0.980584	0.244058
11	6	0	-5.507203	0.666711	0.359314
12	6	0	-3.799019	2.194445	-0.361565
13	6	0	-6.485903	1.548304	-0.083548
14	1	0	-5.789375	-0.282833	0.806926
15	6	0	-4.777382	3.081308	-0.805944
16	1	0	-2.746411	2.429741	-0.501464
17	6	0	-6.124694	2.763949	-0.663830
18	1	0	-7.534991	1.289035	0.025581

19	1	0	-4.484681	4.017035	-1.273727
20	1	0	-6.888583	3.453462	-1.010170
21	6	0	-3.182324	-1.356719	0.184989
22	6	0	-3.614112	-1.587353	-1.132521
23	6	0	-2.838063	-2.476553	0.959940
24	6	0	-3.668405	-2.873868	-1.659451
25	1	0	-3.908091	-0.737915	-1.743707
26	6	0	-2.884121	-3.762064	0.431072
27	1	0	-2.550420	-2.329407	1.997452
28	6	0	-3.295164	-3.969434	-0.883719
29	1	0	-4.005404	-3.021153	-2.682106
30	1	0	-2.612724	-4.608575	1.055178
31	1	0	-3.338214	-4.973554	-1.293938
32	15	0	2.015797	0.338372	0.014914
33	6	0	2.585924	-1.133380	0.947952
34	6	0	2.719103	-1.003830	2.335336
35	6	0	2.887516	-2.355807	0.341880
36	6	0	3.167297	-2.074191	3.102529
37	1	0	2.459160	-0.061079	2.812814
38	6	0	3.327881	-3.428939	1.113613
39	1	0	2.770591	-2.473613	-0.731814
40	6	0	3.471249	-3.289024	2.491376
41	1	0	3.268577	-1.963421	4.177686
42	1	0	3.553431	-4.377427	0.636088
43	1	0	3.810156	-4.128615	3.090339
44	6	0	3.569863	1.212231	-0.410624
45	6	0	4.836094	0.633263	-0.288570
46	6	0	3.459206	2.524631	-0.884385
47	6	0	5.972913	1.356828	-0.643272
48	1	0	4.934170	-0.381634	0.086702
49	6	0	4.594430	3.242266	-1.245340
50	1	0	2.476706	2.984208	-0.972876
51	6	0	5.853911	2.658391	-1.123146
52	1	0	6.953269	0.901608	-0.542014
53	1	0	4.497168	4.258075	-1.615228
54	1	0	6.741432	3.220019	-1.397257
55	6	0	1.459060	-0.349446	-1.592225
56	6	0	0.104860	-0.671542	-1.747038
57	6	0	2.348053	-0.597190	-2.644264
58	6	0	-0.345733	-1.258187	-2.926665
59	1	0	-0.609444	-0.461535	-0.953002
60	6	0	1.890827	-1.171697	-3.826990
61	1	0	3.398579	-0.338351	-2.538609
62	6	0	0.545837	-1.507552	-3.966702
63	1	0	-1.395664	-1.517399	-3.021354
64	1	0	2.586953	-1.356608	-4.639434
65	1	0	0.192357	-1.958214	-4.889100

Zero-point correction= 0.529374 (Hartree/Particle)
Thermal correction to Energy= 0.561518
Thermal correction to Enthalpy= 0.562462
Thermal correction to Gibbs Free Energy= 0.460001
Sum of electronic and zero-point Energies= -1779.884752
Sum of electronic and thermal Energies= -1779.852608
Sum of electronic and thermal Enthalpies= -1779.851664
Sum of electronic and thermal Free Energies= -1779.954126
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1780.403592
Frequencies

11.8493	17.3878	22.9474
26.0355	35.4277	36.3906
41.7850	44.2751	50.0011
54.1748	55.4329	67.0533
69.1860	80.4331	89.2048
95.0997	133.7608	144.5530
170.8135	189.8653	216.3569
218.8856	237.0976	256.0967
259.9052	266.4351	269.6251
294.9445	317.8878	373.8091
406.9852	408.6612	413.1466
418.7596	421.0416	429.2101
437.2261	440.1569	443.4718
445.8752	468.4042	503.3875
513.3869	517.3825	525.3426
547.5028	597.8268	627.4739
627.8932	628.3874	629.1875

631.8092 633.7092 663.3716
702.1574 706.2423 713.6076
715.9649 717.0963 718.8058
720.5414 722.5153 723.3320
726.0352 769.7640 772.5000
777.1792 784.8014 790.9522
794.7967 871.5250 878.8335
879.3542 882.9467 885.9112
930.4046 938.9557 945.7268
954.7890 955.7400 957.2067
959.4212 983.0200 988.0597
993.2734 997.8359 1002.1478
1002.9705 1007.9229 1012.9478
1013.2410 1013.7081 1014.8164
1015.3318 1018.2339 1022.3059
1027.1560 1029.9154 1033.5968
1057.4150 1069.8988 1070.8983
1071.3609 1072.2651 1076.5993
1107.9330 1116.6312 1124.0946
1125.6852 1126.7168 1127.9405
1138.7695 1140.2114 1142.6535
1183.3175 1185.0555 1189.2576
1190.4535 1194.1415 1207.8404
1214.9541 1220.7212 1222.0233
1226.3966 1243.0215 1255.9474
1319.6789 1331.3257 1334.4640
1336.5941 1338.8930 1360.5188
1365.9921 1366.1853 1366.6449
1370.6390 1372.2860 1466.9154
1486.5421 1492.6690 1496.0942
1497.1855 1501.3992 1504.4033
1540.1467 1544.1336 1546.7739
1553.7716 1559.0148 1661.6332
1669.9115 1670.8904 1671.6639
1672.1408 1681.5694 1685.0880
1688.1913 1689.1731 1697.7894
1703.2144 3111.9744 3120.6203
3191.4626 3193.7158 3197.9770
3199.5710 3202.5842 3204.0841
3204.8675 3207.4175 3209.0833
3209.3300 3211.6719 3214.6646
3215.9672 3217.7622 3218.0910
3218.2339 3225.2586 3226.6798
3227.0969 3228.9078 3230.4504
3234.4266 3235.5463 3236.4403
3237.1595 3241.6801 3249.9352

2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.403185	0.690458	-0.203622
2	6	0	0.009162	1.217947	0.149558
3	6	0	1.322674	-0.809106	0.142543
4	6	0	-0.902279	0.001582	-0.008112
5	8	0	-2.113283	-0.011765	-0.043631
6	7	0	-0.082684	-1.093508	-0.081008
7	1	0	-0.482278	-2.019429	-0.021976
8	1	0	1.611868	-0.994550	1.186393
9	1	0	1.959847	-1.420127	-0.502291
10	1	0	2.211854	1.193130	0.329854
11	1	0	1.580795	0.801738	-1.277147
12	1	0	-0.053876	1.541792	1.194999
13	1	0	-0.339612	2.040842	-0.475937

Zero-point correction= 0.112782 (Hartree/Particle)
Thermal correction to Energy= 0.118145
Thermal correction to Enthalpy= 0.119089
Thermal correction to Gibbs Free Energy= 0.084004
Sum of electronic and zero-point Energies= -286.388026
Sum of electronic and thermal Energies= -286.382664
Sum of electronic and thermal Enthalpies= -286.381719
Sum of electronic and thermal Free Energies= -286.416804
M06-2x/6-311++G(d,p) // M06-2x /6-31G(d) energy= -286.5314524

Frequencies

141.3443	200.6393	472.1743
489.7955	564.4668	640.8594
700.6062	830.2716	906.3241
921.2958	941.4512	1024.5968
1102.0656	1108.2448	1199.8043
1231.5068	1262.8390	1284.2202
1330.2802	1361.6322	1391.6691
1475.4854	1495.7052	1527.9410
1566.2790	1890.1646	3064.1986
3100.2810	3114.3595	3144.9582
3173.1643	3181.2188	3666.0778

TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.547870	0.201553	-1.903330
2	6	0	1.474222	-1.220130	-1.024386
3	6	0	1.480485	0.381666	-2.779576
4	1	0	1.020041	-1.425505	-0.057055
5	1	0	1.144539	-1.873308	-1.827274
6	1	0	1.731810	1.316027	-3.266223
7	6	0	1.814641	0.168818	-1.399996
8	6	0	2.338529	1.032034	-0.418127
9	1	0	1.554614	-0.492307	-3.424813
10	1	0	3.692324	-1.215342	-0.570639
11	6	0	3.116783	-4.334112	-1.326400
12	6	0	2.437845	-4.192617	0.039921
13	6	0	3.012321	-2.880517	0.589053
14	7	0	3.105043	-2.050911	-0.629446
15	1	0	2.517755	-4.826373	-2.095389
16	1	0	4.070000	-4.871347	-1.257940
17	1	0	1.353589	-4.091544	-0.074339
18	1	0	2.630383	-5.032507	0.709027
19	6	0	2.659858	0.482518	0.937689
20	6	0	1.653919	0.158214	1.860348
21	6	0	3.989625	0.265328	1.340150
22	6	0	1.955703	-0.378449	3.111075
23	1	0	0.617880	0.336832	1.584294
24	6	0	4.300721	-0.265175	2.590946
25	1	0	4.789190	0.531652	0.649770
26	6	0	3.281174	-0.595794	3.481704
27	1	0	1.150403	-0.618459	3.800100
28	1	0	5.339526	-0.417631	2.870498
29	1	0	3.518072	-1.007934	4.457933
30	6	0	2.433252	2.484549	-0.564241
31	6	0	1.654035	3.205696	-1.498645
32	6	0	3.234056	3.264545	0.304279
33	6	0	1.705418	4.593900	-1.581332
34	1	0	0.947802	2.678900	-2.130120
35	6	0	3.288151	4.647508	0.210789
36	1	0	3.822120	2.775076	1.073353
37	6	0	2.531782	5.332240	-0.740581
38	1	0	1.079039	5.100379	-2.311069
39	1	0	3.928884	5.199410	0.893632
40	1	0	2.579286	6.413976	-0.815286
41	15	0	-2.184591	-0.035054	-0.244342
42	6	0	-2.137284	1.401368	0.902031
43	6	0	-1.041253	2.267265	0.809027
44	6	0	-3.129206	1.653507	1.856539
45	6	0	-0.923588	3.355665	1.670895
46	1	0	-0.273063	2.091146	0.057997
47	6	0	-3.013671	2.743495	2.713861
48	1	0	-3.996595	1.001350	1.922970
49	6	0	-1.910363	3.592765	2.624005
50	1	0	-0.062111	4.011467	1.580678
51	1	0	-3.788297	2.934087	3.450589
52	1	0	-1.827350	4.443349	3.293935
53	6	0	-1.736668	-1.458843	0.840933
54	6	0	-1.465027	-1.353216	2.206997
55	6	0	-1.607987	-2.711650	0.222375
56	6	0	-1.064679	-2.473788	2.938021
57	1	0	-1.558406	-0.390536	2.703620

58	6	0	-1.229477	-3.831167	0.955096
59	1	0	-1.804701	-2.799854	-0.844676
60	6	0	-0.946012	-3.712522	2.317171
61	1	0	-0.853915	-2.375168	3.999024
62	1	0	-1.153215	-4.798245	0.465449
63	1	0	-0.643006	-4.583830	2.889793
64	6	0	-3.984419	-0.314960	-0.494587
65	6	0	-4.574850	0.292268	-1.607743
66	6	0	-4.777694	-1.083470	0.364034
67	6	0	-5.938661	0.153081	-1.847625
68	1	0	-3.954633	0.869557	-2.290015
69	6	0	-6.140987	-1.228269	0.119067
70	1	0	-4.327111	-1.574967	1.222774
71	6	0	-6.723040	-0.607857	-0.983911
72	1	0	-6.387000	0.630029	-2.713611
73	1	0	-6.749024	-1.828791	0.788913
74	1	0	-7.785633	-0.724137	-1.174106
75	6	0	3.433330	-2.907923	-1.742192
76	8	0	3.852215	-2.490800	-2.782965
77	1	0	4.011730	-3.013975	1.016076
78	1	0	2.377057	-2.390186	1.330299

Zero-point correction= 0.644393 (Hartree/Particle)
Thermal correction to Energy= 0.682410
Thermal correction to Enthalpy= 0.683354
Thermal correction to Gibbs Free Energy= 0.570149
Sum of electronic and zero-point Energies= -2066.232635
Sum of electronic and thermal Energies= -2066.194617
Sum of electronic and thermal Enthalpies= -2066.193673
Sum of electronic and thermal Free Energies= -2066.306878
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -2066.861069
Frequencies

-482.8560	18.0746	24.7330
5.2071	29.8586	34.1489
38.3805	42.3169	47.9486
54.7550	61.1255	62.6974
69.9837	70.1624	72.7255
82.6688	85.8342	90.1649
100.8559	104.3824	109.5893
122.1419	140.4147	151.9830
160.0835	192.8379	193.2934
208.3771	218.2480	225.5720
255.6429	259.1660	266.2729
278.4450	283.5482	289.7983
323.6908	342.6382	369.8404
393.4662	409.1122	411.3395
417.9290	425.8077	431.9854
437.4119	438.6499	449.8974
457.4782	488.7291	507.5260
508.3116	519.7342	527.7644
531.2993	547.1570	577.4480
616.0809	622.6003	628.9079
629.3222	630.7588	633.2037
636.4611	650.6809	676.0526
681.8859	701.5590	714.3044
714.7780	715.8386	717.0757
719.2275	722.1812	724.3718
731.8021	767.9793	773.1308
776.2500	778.0690	792.1762
815.8412	831.6515	859.0081
869.9285	878.8414	881.9460
885.4141	887.9943	907.9870
925.0893	926.1633	940.4812
950.8034	953.2698	954.8164
956.3266	959.5266	982.2724
987.4797	997.3903	1003.1887
1003.5397	1006.0806	1007.1392
1008.4342	1010.3299	1011.1985
1014.9269	1015.6111	1016.4378
1021.2521	1026.3436	1026.7842
1030.4080	1051.5062	1064.9453
1069.2624	1071.2010	1071.6184
1075.2617	1077.1412	1082.8040
1105.5790	1107.4318	1121.9916
1124.6439	1131.6490	1133.8052

1136.2035	1137.5170	1140.9454
1144.2385	1178.0632	1178.9812
1182.9981	1188.0474	1192.4218
1198.9543	1205.1206	1212.5679
1221.2566	1222.8394	1224.2120
1224.8767	1234.4600	1234.8521
1250.2151	1279.5796	1290.4722
1308.3666	1321.6745	1327.0332
1331.8478	1338.1015	1340.2315
1349.3279	1354.9054	1366.0850
1366.4068	1368.9134	1369.9432
1374.0048	1377.5663	1413.1618
1474.9327	1481.5275	1483.3593
1491.6890	1492.1357	1498.2835
1499.7389	1520.0136	1525.7596
1541.0102	1541.2751	1543.7279
1545.3477	1546.2211	1548.9644
1557.7863	1651.4342	1658.5591
1668.2597	1669.9218	1672.9623
1682.3102	1686.1151	1688.5325
1689.5596	1692.8366	1932.9042
3100.9843	3113.0928	3121.6865
3159.8335	3165.4041	3178.1246
3178.9416	3184.7022	3188.5994
3194.3302	3194.6729	3200.4064
3201.3048	3203.3786	3208.4220
3208.8323	3209.3098	3209.7350
3215.3956	3216.6964	3217.1578
3222.9835	3224.3194	3225.6232
3227.2833	3228.9753	3229.6857
3230.8788	3233.0931	3234.0763
3236.5714	3239.2316	3241.9081
3266.6674	3280.4572	3505.3480

INT5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.688143	0.192650	-1.960131
2	6	0	1.695182	-1.310845	-0.826949
3	6	0	1.470831	0.217031	-2.709446
4	1	0	1.156238	-1.429063	0.115333
5	1	0	1.249934	-1.974504	-1.571497
6	1	0	1.734426	1.104843	-3.270434
7	6	0	1.794902	0.115604	-1.332053
8	6	0	2.274746	1.067320	-0.406369
9	1	0	1.511487	-0.705561	-3.286428
10	1	0	3.717699	-1.007890	-0.438458
11	6	0	3.340566	-4.135027	-1.311645
12	6	0	2.712142	-4.086095	0.086313
13	6	0	3.195103	-2.748418	0.657377
14	7	0	3.131831	-1.848926	-0.530329
15	1	0	2.721010	-4.609513	-2.076564
16	1	0	4.312253	-4.641130	-1.319425
17	1	0	1.619796	-4.082822	0.025570
18	1	0	3.014020	-4.922746	0.717468
19	6	0	2.648506	0.608733	0.970566
20	6	0	1.674508	0.239366	1.910266
21	6	0	3.993909	0.497177	1.368909
22	6	0	2.020423	-0.251977	3.167976
23	1	0	0.629230	0.345652	1.634452
24	6	0	4.349200	0.011614	2.627260
25	1	0	4.768186	0.811976	0.669304
26	6	0	3.360739	-0.374585	3.531064
27	1	0	1.237485	-0.527660	3.869696
28	1	0	5.397706	-0.058985	2.903436
29	1	0	3.632902	-0.750690	4.512573
30	6	0	2.287782	2.512964	-0.626318
31	6	0	1.531884	3.135668	-1.647710
32	6	0	2.977527	3.386054	0.249910
33	6	0	1.505781	4.518568	-1.799343
34	1	0	0.900831	2.536485	-2.292193
35	6	0	2.955763	4.763661	0.085065
36	1	0	3.538914	2.976781	1.083323

37	6	0	2.227085	5.350317	-0.949506
38	1	0	0.899342	4.946783	-2.593263
39	1	0	3.514499	5.387350	0.778204
40	1	0	2.213795	6.427730	-1.079529
41	15	0	-2.246077	-0.060016	-0.313842
42	6	0	-2.143703	1.286809	0.940519
43	6	0	-1.065438	2.173785	0.842861
44	6	0	-3.066540	1.446831	1.980486
45	6	0	-0.893340	3.187641	1.783710
46	1	0	-0.354983	2.067831	0.024490
47	6	0	-2.899526	2.464752	2.915235
48	1	0	-3.920194	0.777495	2.055298
49	6	0	-1.811052	3.332284	2.820694
50	1	0	-0.043882	3.858723	1.690347
51	1	0	-3.622601	2.584717	3.716610
52	1	0	-1.685684	4.124490	3.552813
53	6	0	-1.676201	-1.537585	0.650170
54	6	0	-1.286356	-1.503327	1.991906
55	6	0	-1.542717	-2.745482	-0.053222
56	6	0	-0.751210	-2.637482	2.608845
57	1	0	-1.389927	-0.582333	2.560540
58	6	0	-1.038996	-3.882601	0.567519
59	1	0	-1.828754	-2.778925	-1.102749
60	6	0	-0.624916	-3.828083	1.901721
61	1	0	-0.445565	-2.589203	3.650214
62	1	0	-0.965750	-4.814256	0.012100
63	1	0	-0.221495	-4.713034	2.385851
64	6	0	-4.062607	-0.366381	-0.394967
65	6	0	-4.779960	0.367791	-1.346038
66	6	0	-4.750987	-1.262670	0.428840
67	6	0	-6.159548	0.227370	-1.457060
68	1	0	-4.243543	1.045991	-2.006369
69	6	0	-6.131200	-1.412210	0.309442
70	1	0	-4.208098	-1.848406	1.166576
71	6	0	-6.837565	-0.665117	-0.629626
72	1	0	-6.704182	0.805701	-2.197151
73	1	0	-6.655467	-2.113000	0.952583
74	1	0	-7.913071	-0.783245	-0.721275
75	6	0	3.591572	-2.689709	-1.690038
76	8	0	4.065738	-2.200748	-2.659975
77	1	0	4.236474	-2.790198	0.989400
78	1	0	2.576225	-2.335036	1.456738

Zero-point correction= 0.646705 (Hartree/Particle)
Thermal correction to Energy= 0.684699
Thermal correction to Enthalpy= 0.685643
Thermal correction to Gibbs Free Energy= 0.573186
Sum of electronic and zero-point Energies= -2066.237884
Sum of electronic and thermal Energies= -2066.199890
Sum of electronic and thermal Enthalpies= -2066.198946
Sum of electronic and thermal Free Energies= -2066.311402
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -2066.871976
Frequencies

19.7343	22.8630	29.3459
35.1781	39.6073	42.9764
45.8605	52.5798	55.7289
60.6368	64.2986	68.0296
68.4783	74.3203	85.2287
86.4197	90.9258	96.8891
99.6027	114.7719	118.0941
134.2250	164.3172	166.6215
195.9962	197.8023	213.5985
221.0708	227.5275	254.0400
256.5239	267.1068	278.3187
284.3600	294.4975	315.5936
352.5048	378.0169	403.1581
408.8394	411.9988	418.9591
424.8236	431.0115	435.0347
437.1409	448.2935	460.6917
486.3210	508.2965	518.0230
520.9748	526.0799	534.0126
553.0458	582.8572	606.8790
621.3954	628.9161	629.2729
631.1846	633.4312	634.1266
642.0919	663.2413	668.5700

698.9777	710.0586	712.5621
715.6877	715.8160	717.3334
719.3608	721.3183	735.1847
754.0281	765.9224	770.7601
774.2661	778.3605	791.6472
796.6864	817.3557	856.3367
866.8392	876.8249	879.7942
884.1778	887.0921	915.7643
924.9541	927.6881	938.7720
947.6115	948.4777	949.4077
958.8523	960.3675	983.6065
988.9830	997.6106	998.3798
1002.8986	1004.0104	1005.8385
1008.1835	1011.2142	1013.9306
1014.0795	1015.4149	1016.1962
1016.9155	1020.1888	1022.4836
1028.7543	1062.1477	1067.7652
1069.8511	1070.6457	1072.5438
1076.6550	1087.9745	1105.9944
1107.5902	1119.2570	1121.2576
1129.1439	1132.3240	1133.3713
1135.2050	1135.4257	1142.1574
1177.9149	1184.3228	1186.2486
1187.8571	1197.6315	1204.7113
1208.7010	1219.0932	1222.5100
1224.1626	1227.0341	1232.5736
1235.9223	1243.7966	1274.6142
1293.9548	1309.4341	1315.7098
1328.1687	1329.1646	1333.4447
1334.8384	1341.0763	1349.5995
1357.7014	1363.1820	1363.9676
1367.4246	1372.8109	1373.7405
1377.7877	1397.8607	1418.2691
1474.6699	1484.1690	1487.9289
1491.3995	1494.5417	1495.8773
1499.4052	1520.0433	1526.8928
1532.2282	1539.5330	1541.8441
1544.9356	1546.7469	1550.5773
1567.0869	1649.1522	1656.4140
1662.0975	1672.6254	1673.3029
1683.1926	1685.1385	1685.7232
1687.5963	1694.2282	1993.8781
3106.0847	3123.2041	3132.4529
3140.6453	3158.3599	3163.3788
3178.3639	3186.5785	3194.0472
3195.7944	3197.7859	3198.6483
3200.0537	3200.1832	3201.2162
3202.8977	3205.9192	3207.2550
3210.0790	3211.1196	3212.0300
3213.3672	3217.7196	3218.7330
3218.9862	3222.1375	3223.6325
3225.4569	3228.4110	3229.2388
3232.4939	3234.6528	3237.6416
3262.3955	3286.4720	3418.2346

INT6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.283193	-0.475158	-1.696870
2	6	0	-0.500798	1.402057	-1.984760
3	6	0	-1.551175	-0.438392	-2.798201
4	1	0	-0.218145	1.730873	-2.986829
5	1	0	-0.230813	2.119718	-1.211329
6	1	0	-2.180001	-1.320408	-2.786805
7	6	0	-1.800597	0.696807	-1.905412
8	6	0	-2.765226	0.871694	-0.929103
9	1	0	-1.222466	-0.159642	-3.800096
10	1	0	-1.452290	-0.960763	0.127286
11	6	0	-0.523155	-3.999882	1.009447
12	6	0	-1.909441	-3.860948	1.649824
13	6	0	-2.151955	-2.340840	1.664479
14	7	0	-1.343439	-1.887992	0.539937
15	1	0	-0.371760	-4.912469	0.431127

16	1	0	0.281378	-3.923292	1.751187
17	1	0	-2.659713	-4.338153	1.011464
18	1	0	-1.977171	-4.302271	2.645505
19	6	0	-2.643667	2.003658	0.027758
20	6	0	-2.859328	1.797701	1.401557
21	6	0	-2.324672	3.307916	-0.381609
22	6	0	-2.742280	2.835620	2.320688
23	1	0	-3.133609	0.801387	1.744252
24	6	0	-2.188495	4.345198	0.536701
25	1	0	-2.192643	3.504537	-1.442059
26	6	0	-2.393616	4.116293	1.895162
27	1	0	-2.925379	2.644291	3.375222
28	1	0	-1.937066	5.341955	0.185815
29	1	0	-2.296724	4.926290	2.611220
30	6	0	-3.985349	0.038103	-0.797410
31	6	0	-5.194962	0.662861	-0.426733
32	6	0	-4.040665	-1.351678	-1.010814
33	6	0	-6.378567	-0.047350	-0.288793
34	1	0	-5.194761	1.734922	-0.253398
35	6	0	-5.230939	-2.065949	-0.875936
36	1	0	-3.137295	-1.902363	-1.240840
37	6	0	-6.409306	-1.423405	-0.515318
38	1	0	-7.286990	0.478954	-0.009627
39	1	0	-5.226945	-3.139045	-1.049108
40	1	0	-7.334794	-1.980923	-0.410305
41	15	0	2.138049	0.075117	-0.227223
42	6	0	2.703737	1.813642	-0.181968
43	6	0	2.749887	2.508591	-1.394817
44	6	0	3.101127	2.458501	0.994403
45	6	0	3.204271	3.823827	-1.435002
46	1	0	2.416461	2.015170	-2.305198
47	6	0	3.548659	3.776005	0.952797
48	1	0	3.052374	1.930991	1.943570
49	6	0	3.602654	4.457959	-0.260990
50	1	0	3.236289	4.356034	-2.380472
51	1	0	3.852213	4.271795	1.869672
52	1	0	3.948258	5.486711	-0.289988
53	6	0	3.681920	-0.908826	-0.296150
54	6	0	4.915971	-0.412625	0.135652
55	6	0	3.598089	-2.214823	-0.794443
56	6	0	6.052091	-1.214293	0.072805
57	1	0	4.992753	0.603642	0.511278
58	6	0	4.737359	-3.014892	-0.847007
59	1	0	2.638382	-2.604834	-1.124896
60	6	0	5.964054	-2.515508	-0.416995
61	1	0	7.007704	-0.820921	0.405505
62	1	0	4.665239	-4.026692	-1.233722
63	1	0	6.852494	-3.137688	-0.465853
64	6	0	1.497317	-0.215563	1.466736
65	6	0	0.465454	0.613605	1.930649
66	6	0	1.903495	-1.302260	2.243549
67	6	0	-0.122837	0.375408	3.167477
68	1	0	0.115597	1.450338	1.326094
69	6	0	1.297953	-1.547881	3.477138
70	1	0	2.693871	-1.957997	1.888322
71	6	0	0.294161	-0.705793	3.945446
72	1	0	-0.912156	1.034914	3.514673
73	1	0	1.624176	-2.392946	4.076612
74	1	0	-0.166928	-0.891009	4.911127
75	1	0	-3.200168	-2.075045	1.501475
76	1	0	-1.800765	-1.875982	2.592744
77	6	0	-0.428305	-2.773539	0.117548
78	8	0	0.368835	-2.633697	-0.819869

Zero-point correction= 0.645039 (Hartree/Particle)
Thermal correction to Energy= 0.683278
Thermal correction to Enthalpy= 0.684222
Thermal correction to Gibbs Free Energy= 0.571032
Sum of electronic and zero-point Energies= -2066.311727
Sum of electronic and thermal Energies= -2066.273488
Sum of electronic and thermal Enthalpies= -2066.272543
Sum of electronic and thermal Free Energies= -2066.385733
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -2066.928091
Frequencies
17.6869 21.9122 24.9279

30.3841	36.2790	42.6427
45.9414	48.1667	52.6581
64.1035	65.7596	66.5010
69.1363	74.4131	78.1451
88.0380	96.1674	104.6586
108.6541	125.0070	138.3635
143.6385	150.8711	173.2930
186.8923	199.0330	206.3291
211.1169	227.0145	250.9480
253.4309	258.5522	260.5163
264.3141	283.7681	305.4836
335.4700	373.1153	408.3681
409.4120	411.1619	415.1937
421.1851	429.4042	435.1288
438.6931	441.2253	459.7766
468.7421	506.7512	517.2131
518.4361	522.9940	534.4419
542.0438	547.9070	591.5373
628.0250	628.1563	628.5484
629.7428	631.1970	637.7492
638.8688	672.0036	699.0862
701.4288	708.9307	714.9414
716.4591	718.6979	719.0897
721.6074	722.7748	725.6032
731.4390	736.9578	767.8361
770.7363	779.0018	781.2914
788.1211	790.3823	835.7480
871.8963	877.4085	877.7430
882.2810	892.1589	913.8132
916.0788	927.9720	929.2166
938.6723	944.3868	945.9916
950.2774	958.8014	968.5603
975.5586	991.9308	993.8149
998.3926	999.7594	1005.7038
1008.7277	1011.5862	1012.6548
1013.2508	1015.6502	1015.8597
1016.5544	1018.1975	1019.7771
1024.6593	1027.3346	1033.6915
1034.1084	1070.0432	1070.4232
1071.2460	1072.7677	1079.8139
1100.6488	1103.5559	1121.3013
1123.2390	1126.8969	1127.3541
1129.3530	1131.2519	1140.4107
1143.0725	1145.4839	1184.4228
1186.4266	1191.4496	1192.1652
1193.6282	1204.4422	1212.7470
1221.8109	1225.7923	1225.9123
1232.0277	1232.9753	1243.1613
1257.3441	1269.1658	1306.9791
1308.9531	1332.0345	1336.1943
1337.8279	1340.7496	1344.4879
1361.9907	1363.1910	1367.9756
1372.2771	1372.5345	1372.6697
1377.2825	1410.4386	1476.3145
1488.4761	1493.6118	1494.2658
1495.8117	1499.0101	1499.4667
1502.3031	1516.6205	1526.9710
1543.3817	1544.6363	1549.5346
1552.3565	1552.4853	1558.4110
1599.8124	1661.6900	1667.3450
1670.3538	1672.1446	1674.0197
1685.3393	1687.3523	1688.8298
1692.2726	1700.1243	1778.1328
3099.6539	3101.3918	3108.3727
3122.3352	3146.0451	3156.8990
3170.3790	3177.4393	3185.6967
3191.9076	3195.4553	3202.0365
3203.3120	3205.6154	3206.9476
3208.4463	3208.7795	3210.7585
3216.0129	3218.5117	3218.8282
3219.7510	3220.7761	3221.0389
3225.0648	3228.0828	3229.1406
3231.1491	3231.9586	3237.5748
3238.1371	3239.9149	3244.5710
3256.8701	3287.7029	3525.9570

TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.215821	-0.519751	-1.530762
2	6	0	-0.580023	1.339075	-1.975112
3	6	0	-1.669760	-0.573100	-2.731052
4	1	0	-0.265321	1.569363	-2.993016
5	1	0	-0.368391	2.123797	-1.254318
6	1	0	-2.330331	-1.428083	-2.663630
7	6	0	-1.772557	0.514106	-1.833149
8	6	0	-2.617989	0.486817	-0.637496
9	1	0	-1.198345	-0.411749	-3.697893
10	1	0	-1.941196	-0.584734	0.050487
11	6	0	-0.508737	-3.620559	1.450439
12	6	0	-1.891895	-3.503263	2.088681
13	6	0	-2.216868	-2.015730	1.874148
14	7	0	-1.500893	-1.650693	0.653736
15	1	0	-0.274573	-4.593246	1.013720
16	1	0	0.292261	-3.357799	2.154756
17	1	0	-2.609456	-4.117633	1.534479
18	1	0	-1.926225	-3.798984	3.139571
19	6	0	-2.611562	1.712709	0.229980
20	6	0	-2.758637	1.567295	1.618384
21	6	0	-2.527906	3.020537	-0.270102
22	6	0	-2.788020	2.668166	2.469357
23	1	0	-2.862567	0.565670	2.029279
24	6	0	-2.544198	4.126372	0.577069
25	1	0	-2.462294	3.173304	-1.344373
26	6	0	-2.668347	3.956856	1.952915
27	1	0	-2.906939	2.519514	3.539489
28	1	0	-2.473270	5.125339	0.156344
29	1	0	-2.683781	4.818147	2.613346
30	6	0	-3.991821	-0.126457	-0.783069
31	6	0	-5.145052	0.670866	-0.707394
32	6	0	-4.177950	-1.506741	-0.966702
33	6	0	-6.417321	0.123262	-0.832186
34	1	0	-5.037409	1.740137	-0.549240
35	6	0	-5.451493	-2.056541	-1.096808
36	1	0	-3.314609	-2.165636	-0.971158
37	6	0	-6.579740	-1.245404	-1.033463
38	1	0	-7.287015	0.771950	-0.777016
39	1	0	-5.558863	-3.128501	-1.237635
40	1	0	-7.572300	-1.673943	-1.132713
41	15	0	2.119619	0.076666	-0.243250
42	6	0	2.703937	1.807731	-0.305622
43	6	0	2.700331	2.452643	-1.546619
44	6	0	3.172281	2.487967	0.822194
45	6	0	3.169998	3.757450	-1.661838
46	1	0	2.321855	1.927676	-2.421242
47	6	0	3.634572	3.796694	0.705519
48	1	0	3.170045	1.995661	1.791050
49	6	0	3.635621	4.430594	-0.534476
50	1	0	3.164185	4.251160	-2.628555
51	1	0	3.991919	4.321937	1.585840
52	1	0	3.994765	5.451340	-0.621634
53	6	0	3.625583	-0.920793	-0.531549
54	6	0	4.910021	-0.372162	-0.481574
55	6	0	3.461181	-2.287970	-0.792889
56	6	0	6.022676	-1.183505	-0.689922
57	1	0	5.044125	0.687599	-0.284823
58	6	0	4.579407	-3.092431	-0.992002
59	1	0	2.459684	-2.713310	-0.824601
60	6	0	5.858963	-2.542484	-0.943979
61	1	0	7.018012	-0.751456	-0.653506
62	1	0	4.448679	-4.151408	-1.192115
63	1	0	6.727937	-3.172621	-1.107996
64	6	0	1.717862	-0.193023	1.520599
65	6	0	0.553912	0.414012	2.009426
66	6	0	2.496981	-0.977877	2.373176
67	6	0	0.189860	0.257797	3.341690
68	1	0	-0.075921	1.007794	1.348214
69	6	0	2.116228	-1.149470	3.704273

70	1	0	3.398238	-1.456711	2.000559
71	6	0	0.967977	-0.530824	4.190216
72	1	0	-0.708242	0.747796	3.707465
73	1	0	2.723937	-1.764462	4.360953
74	1	0	0.678249	-0.662187	5.228373
75	1	0	-3.288601	-1.821843	1.753576
76	1	0	-1.851877	-1.412279	2.718668
77	6	0	-0.550843	-2.534108	0.383858
78	8	0	0.258476	-2.533656	-0.584071

Zero-point correction= 0.640116 (Hartree/Particle)
Thermal correction to Energy= 0.677699
Thermal correction to Enthalpy= 0.678643
Thermal correction to Gibbs Free Energy= 0.567627
Sum of electronic and zero-point Energies= -2066.294174
Sum of electronic and thermal Energies= -2066.256591
Sum of electronic and thermal Enthalpies= -2066.255647
Sum of electronic and thermal Free Energies= -2066.366663
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -2066.905128
Frequencies

-1351.3915	21.3308	24.5023
27.9438	34.1604	39.1572
42.8766	46.9924	49.7260
51.4825	57.1621	60.8507
66.0535	71.3967	80.8575
86.5303	91.3414	104.6013
115.3841	129.9383	136.7385
153.1579	158.3872	171.7905
197.7362	201.6355	205.7221
215.3789	225.6996	249.1753
255.7169	258.6358	266.8928
269.4973	277.2313	300.0265
304.5479	308.9664	354.2187
392.0570	409.1039	410.5274
414.4927	421.7035	430.6878
436.1554	447.0091	450.2337
459.1830	487.2198	511.9591
516.4269	517.6770	535.0010
548.9779	553.0574	565.3556
606.6458	627.2462	628.1213
628.4961	629.1227	632.7506
643.9146	661.9772	702.7851
711.4028	712.2299	714.7846
715.8045	716.7430	721.8437
723.9849	726.3776	730.6853
752.8810	766.3720	768.6691
770.4406	773.6678	791.5723
798.0645	810.9939	871.2915
873.2906	878.0531	883.2280
884.0804	888.7132	913.2076
921.6969	924.6668	944.3929
949.4985	952.0334	953.6007
955.2643	961.5674	963.3566
982.9703	994.8523	997.2725
1003.8751	1006.8122	1011.1811
1013.1908	1014.4114	1014.9944
1015.2572	1016.1818	1017.7838
1019.7427	1020.4271	1023.1231
1025.2721	1027.3470	1028.6460
1036.5147	1069.5574	1069.9952
1071.9792	1073.7936	1079.8108
1086.5478	1099.6026	1122.3978
1122.6384	1126.1141	1129.3680
1129.8078	1137.0636	1140.6882
1142.8372	1144.8453	1185.7630
1185.9115	1188.2920	1189.6921
1191.5713	1191.7048	1217.3965
1222.2172	1222.7485	1223.6083
1231.4632	1233.5580	1238.0851
1269.0604	1277.9008	1312.9170
1316.8055	1322.5663	1334.2725
1339.4892	1340.5257	1344.6490
1358.2523	1361.2793	1366.1141
1367.6575	1369.5154	1370.6462
1378.8508	1408.3219	1436.3094

1485.6160	1491.8159	1493.5150
1496.4826	1497.9670	1499.4004
1508.0489	1508.9692	1523.8856
1541.6813	1545.6945	1547.0993
1549.4228	1552.0934	1555.9626
1562.2918	1599.4706	1666.5972
1668.4767	1669.6451	1673.0073
1675.1559	1687.8642	1689.4121
1690.3541	1693.8174	1698.5981
1721.2899	3056.3222	3077.5192
3097.0530	3121.8572	3152.5159
3161.2723	3167.5891	3190.8262
3198.8763	3201.5198	3204.7933
3206.0712	3206.3697	3206.7088
3208.0509	3212.5787	3212.7168
3212.8807	3215.1165	3218.3117
3219.2613	3219.6658	3223.7405
3223.9398	3224.7945	3225.6197
3228.3438	3230.9447	3233.7873
3234.6725	3237.7097	3239.8235
3243.5958	3252.6410	3297.5834

INT7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.011076	-0.228575	-1.083557
2	6	0	-1.028839	1.568067	-1.295859
3	6	0	-1.918173	-0.382249	-2.350190
4	1	0	-0.672208	1.987881	-2.236862
5	1	0	-1.022624	2.262719	-0.459292
6	1	0	-2.516481	-1.285805	-2.360537
7	6	0	-2.068568	0.572424	-1.359618
8	6	0	-2.996480	0.360235	-0.156710
9	1	0	-1.356698	-0.150363	-3.253132
10	1	0	-2.366745	-0.106757	0.615080
11	6	0	0.875246	-3.999787	0.771798
12	6	0	-0.221451	-4.421637	1.750025
13	6	0	-0.994493	-3.099251	1.970220
14	7	0	-0.738776	-2.258802	0.806237
15	1	0	1.137524	-4.748253	0.020127
16	1	0	1.799497	-3.697114	1.283465
17	1	0	-0.878154	-5.160890	1.279476
18	1	0	0.157285	-4.852976	2.680771
19	6	0	-3.524072	1.671778	0.397762
20	6	0	-3.722655	1.801126	1.773611
21	6	0	-3.869936	2.743446	-0.430638
22	6	0	-4.251124	2.970412	2.312772
23	1	0	-3.462297	0.970420	2.424976
24	6	0	-4.400746	3.914345	0.104214
25	1	0	-3.717777	2.660794	-1.504525
26	6	0	-4.592198	4.031870	1.478421
27	1	0	-4.394154	3.053186	3.385917
28	1	0	-4.664113	4.736653	-0.554217
29	1	0	-5.002245	4.946088	1.896033
30	6	0	-4.118881	-0.631749	-0.449652
31	6	0	-5.371419	-0.222965	-0.911353
32	6	0	-3.873877	-1.997678	-0.273329
33	6	0	-6.361598	-1.161146	-1.193106
34	1	0	-5.584159	0.834661	-1.037032
35	6	0	-4.864920	-2.933940	-0.556352
36	1	0	-2.887158	-2.310089	0.066053
37	6	0	-6.112870	-2.519309	-1.015343
38	1	0	-7.332214	-0.826609	-1.546952
39	1	0	-4.660686	-3.991041	-0.413128
40	1	0	-6.887709	-3.249351	-1.229283
41	15	0	2.062339	0.398533	-0.119084
42	6	0	2.308216	2.111809	0.474415
43	6	0	1.880938	3.155644	-0.354720
44	6	0	2.932462	2.412373	1.687363
45	6	0	2.080180	4.479588	0.019868
46	1	0	1.396430	2.924411	-1.300474
47	6	0	3.120880	3.740461	2.065689
48	1	0	3.271293	1.610429	2.336693

49	6	0	2.697780	4.773441	1.234542
50	1	0	1.748192	5.281758	-0.631741
51	1	0	3.603009	3.965427	3.011943
52	1	0	2.847019	5.806721	1.532086
53	6	0	3.431278	0.149577	-1.309874
54	6	0	4.476818	1.066386	-1.447824
55	6	0	3.417540	-1.017241	-2.087802
56	6	0	5.499118	0.824928	-2.363190
57	1	0	4.495434	1.969445	-0.845093
58	6	0	4.447200	-1.251594	-2.994456
59	1	0	2.611455	-1.737356	-1.958779
60	6	0	5.484749	-0.331705	-3.137272
61	1	0	6.305966	1.543390	-2.469663
62	1	0	4.435796	-2.156059	-3.594712
63	1	0	6.281112	-0.516617	-3.851789
64	6	0	2.506405	-0.643519	1.314451
65	6	0	1.561356	-0.799534	2.335548
66	6	0	3.751445	-1.267886	1.424224
67	6	0	1.871410	-1.556075	3.462337
68	1	0	0.576875	-0.349693	2.234128
69	6	0	4.050936	-2.037175	2.547166
70	1	0	4.487227	-1.156933	0.633488
71	6	0	3.114283	-2.178988	3.567092
72	1	0	1.136831	-1.668210	4.253632
73	1	0	5.018400	-2.523633	2.623587
74	1	0	3.350340	-2.776817	4.442057
75	1	0	-2.071898	-3.265413	2.099673
76	1	0	-0.646268	-2.594133	2.884908
77	6	0	0.266794	-2.752854	0.142138
78	8	0	0.786792	-2.241450	-0.918609

Zero-point correction= 0.645410 (Hartree/Particle)
Thermal correction to Energy= 0.683600
Thermal correction to Enthalpy= 0.684544
Thermal correction to Gibbs Free Energy= 0.570879
Sum of electronic and zero-point Energies= -2066.317539
Sum of electronic and thermal Energies= -2066.279349
Sum of electronic and thermal Enthalpies= -2066.278405
Sum of electronic and thermal Free Energies= -2066.392070
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -2066.934074
Frequencies

14.4668	19.4350	27.2477
33.4898	38.6554	42.7413
47.0272	48.1159	52.6268
56.5572	59.1068	61.2912
70.2222	74.2838	76.4711
82.9140	91.5069	104.8316
108.1020	123.9374	135.2600
143.4125	146.1011	165.3545
190.3844	206.5505	220.6051
223.9251	229.3045	248.4743
256.4972	262.0914	268.3078
274.6788	276.4695	285.4894
305.7387	324.1189	382.8410
410.2531	411.4176	416.4083
417.1464	421.0650	433.5215
436.7589	452.7981	457.8709
470.6205	498.0332	511.9897
516.9581	525.4543	537.2377
555.4581	568.0527	600.3219
623.0157	628.9077	629.2592
631.7390	632.7760	634.1644
656.0445	694.7056	704.6838
713.9471	715.0756	717.6182
722.2804	723.6166	724.8977
726.9928	727.6139	763.3683
769.3667	772.2480	774.6581
774.9750	786.0733	801.2793
837.6475	851.8941	878.2624
878.5569	883.6112	890.5215
894.4713	894.7935	900.5654
925.5147	927.6090	946.6303
947.9125	954.1565	955.4489
958.3914	968.5268	969.2273
992.7680	995.9247	1000.9343

1006.0485	1011.2225	1013.1215
1013.2492	1015.7009	1016.2732
1017.2307	1020.6224	1021.7389
1022.0258	1026.0071	1027.1288
1031.0405	1041.0236	1048.0882
1060.0971	1070.0337	1072.6790
1074.3701	1074.5206	1078.5333
1091.5888	1116.6558	1121.2383
1122.5485	1126.4855	1129.4858
1134.4904	1139.5454	1144.6270
1150.2925	1183.0953	1187.2869
1188.3857	1189.0117	1196.7220
1200.9933	1211.7044	1217.5274
1222.0014	1227.9101	1231.4160
1233.6064	1236.3843	1239.0083
1255.2726	1286.5396	1303.2185
1310.4699	1333.7681	1339.9768
1342.4941	1344.2678	1346.7013
1355.9455	1363.6685	1365.5007
1370.0158	1372.4576	1377.4681
1382.1986	1384.8483	1428.1072
1481.2768	1495.1503	1496.6639
1498.2620	1503.3986	1511.7835
1515.8445	1520.7062	1523.2306
1541.2055	1541.4831	1550.9400
1552.3694	1558.1780	1560.3799
1593.7716	1671.7923	1672.4605
1674.0528	1676.9888	1683.2558
1685.1080	1687.3319	1689.6959
1690.9509	1701.9135	1705.8895
3038.7482	3069.9449	3078.3397
3080.2515	3097.4263	3143.6624
3150.5008	3153.7235	3186.2751
3198.4653	3201.2148	3204.6208
3205.3166	3209.6939	3211.5947
3212.9537	3216.3461	3217.1522
3218.0989	3219.8719	3220.1228
3224.7631	3224.9693	3227.5887
3227.6903	3229.0630	3234.7485
3235.7946	3236.4259	3240.3768
3240.9331	3240.9968	3241.2217
3244.9733	3248.5638	3297.4649

TS5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.057213	0.890375	-0.404379
2	6	0	1.164137	-0.222657	-1.736774
3	6	0	2.410784	1.847080	-1.301128
4	1	0	0.910405	0.129523	-2.737478
5	1	0	1.109121	-1.302944	-1.620813
6	1	0	3.297384	2.323051	-0.891231
7	6	0	2.177338	0.495886	-1.009434
8	6	0	2.979108	-0.143447	0.127363
9	1	0	2.052461	2.249770	-2.242216
10	1	0	3.109607	0.639900	0.887304
11	6	0	0.990992	4.647962	1.702422
12	6	0	1.586651	5.639818	0.702691
13	6	0	2.229975	4.701662	-0.338989
14	7	0	1.427362	3.485468	-0.305936
15	1	0	0.058707	4.967666	2.172473
16	1	0	1.697101	4.390328	2.502134
17	1	0	0.783524	6.210980	0.226431
18	1	0	2.295380	6.348304	1.138944
19	6	0	2.240723	-1.285768	0.824222
20	6	0	1.291269	-0.990756	1.810946
21	6	0	2.467350	-2.623048	0.491961
22	6	0	0.585275	-2.007713	2.449022
23	1	0	1.092651	0.049663	2.068975
24	6	0	1.764849	-3.644359	1.133498
25	1	0	3.212022	-2.867443	-0.261126
26	6	0	0.823274	-3.340102	2.112824
27	1	0	-0.155355	-1.757120	3.204291

28	1	0	1.961754	-4.679503	0.868911
29	1	0	0.274330	-4.133581	2.610890
30	6	0	4.377965	-0.562676	-0.312252
31	6	0	5.366794	-0.737225	0.661950
32	6	0	4.703297	-0.813734	-1.645110
33	6	0	6.648566	-1.146445	0.314582
34	1	0	5.118882	-0.552637	1.705019
35	6	0	5.987358	-1.229477	-1.997160
36	1	0	3.948629	-0.677685	-2.414217
37	6	0	6.963747	-1.395057	-1.020799
38	1	0	7.403717	-1.270918	1.084811
39	1	0	6.222629	-1.420987	-3.039880
40	1	0	7.964494	-1.713173	-1.296073
41	15	0	-2.006919	-0.158772	-0.283695
42	6	0	-2.119801	-1.782066	-1.125081
43	6	0	-3.143924	-2.138352	-2.003320
44	6	0	-1.100507	-2.701903	-0.845332
45	6	0	-3.147495	-3.402020	-2.594657
46	1	0	-3.940100	-1.434592	-2.228083
47	6	0	-1.114630	-3.963877	-1.425509
48	1	0	-0.298071	-2.424668	-0.164281
49	6	0	-2.138855	-4.315374	-2.305551
50	1	0	-3.945365	-3.671092	-3.280190
51	1	0	-0.321364	-4.668161	-1.192064
52	1	0	-2.147897	-5.298744	-2.765888
53	6	0	-3.488044	0.749213	-0.859718
54	6	0	-4.775383	0.439669	-0.407601
55	6	0	-3.315259	1.765365	-1.803121
56	6	0	-5.875158	1.131944	-0.903839
57	1	0	-4.912425	-0.339944	0.337675
58	6	0	-4.418059	2.454988	-2.301632
59	1	0	-2.310235	2.017203	-2.134616
60	6	0	-5.697045	2.137873	-1.852990
61	1	0	-6.871848	0.890042	-0.547799
62	1	0	-4.276517	3.243280	-3.034236
63	1	0	-6.556913	2.678540	-2.236776
64	6	0	-2.394804	-0.583139	1.459966
65	6	0	-2.051273	0.352253	2.444649
66	6	0	-2.977202	-1.797872	1.833601
67	6	0	-2.303900	0.072687	3.785466
68	1	0	-1.561822	1.283600	2.164386
69	6	0	-3.218267	-2.074688	3.177787
70	1	0	-3.231385	-2.536015	1.077703
71	6	0	-2.883787	-1.140215	4.154623
72	1	0	-2.033365	0.800497	4.544507
73	1	0	-3.666115	-3.022673	3.460634
74	1	0	-3.070002	-1.358631	5.201911
75	1	0	2.242749	5.138520	-1.343558
76	1	0	3.277549	4.483299	-0.069033
77	6	0	0.776474	3.406527	0.838895
78	8	0	0.063865	2.438333	1.227766

Zero-point correction= 0.644745 (Hartree/Particle)
Thermal correction to Energy= 0.682263
Thermal correction to Enthalpy= 0.683207
Thermal correction to Gibbs Free Energy= 0.571126
Sum of electronic and zero-point Energies= -2066.297755
Sum of electronic and thermal Energies= -2066.260236
Sum of electronic and thermal Enthalpies= -2066.259292
Sum of electronic and thermal Free Energies= -2066.371373
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -2066.910057
Frequencies

-240.1726	16.4857	17.8416
27.9031	30.0569	36.0337
38.0638	43.0135	51.0735
53.1556	56.4783	59.7760
69.7772	71.1069	78.3091
83.0505	89.3093	95.5122
112.5621	117.1046	135.2374
147.4031	150.1676	178.5575
182.0371	196.6525	218.3844
228.0456	230.0963	235.5192
252.0602	253.2030	258.1652
261.9554	277.0734	282.5044
294.6466	321.3810	366.1880

408.3734	409.9810	417.3108
418.9029	425.3700	435.5912
445.5706	454.7445	458.5560
464.6002	494.7256	508.9288
520.0164	529.5680	531.7753
539.0256	554.4161	583.2112
627.1136	629.0002	629.4881
629.5326	630.2222	647.2637
651.8581	681.0687	703.9554
710.9185	712.8861	715.5500
720.1187	722.3815	723.4318
724.7481	726.6657	761.0040
767.5065	770.7542	773.6827
782.7492	811.8279	832.0767
842.0209	879.8706	882.7747
883.8096	884.6069	887.5429
889.3751	892.6099	902.4913
917.0472	925.2896	949.8098
954.9935	956.4890	956.7566
959.9492	962.6873	1000.1411
1002.6165	1004.2974	1005.0340
1009.0554	1013.8121	1014.6874
1015.8963	1017.5485	1018.5880
1020.6871	1023.7881	1023.9865
1025.4630	1027.3647	1029.0390
1030.7636	1033.6133	1068.5695
1069.2721	1070.5115	1071.1790
1073.7861	1077.2548	1089.7838
1100.2132	1120.5011	1121.6638
1122.4641	1125.8399	1126.7452
1129.1017	1140.5954	1142.3217
1143.9206	1183.3165	1186.3324
1186.6175	1187.0552	1189.2646
1191.1723	1214.9497	1219.2950
1220.3506	1221.1761	1223.4761
1228.6222	1233.1451	1233.7888
1262.2719	1290.0682	1308.0627
1311.1996	1333.7227	1336.3005
1340.7479	1347.7726	1351.2399
1359.3847	1365.6490	1366.4220
1367.4318	1368.1275	1371.3210
1375.4788	1378.9120	1414.1608
1484.5244	1490.2857	1495.2552
1497.5965	1498.0478	1504.7734
1513.2460	1519.0074	1526.7940
1538.6568	1540.7297	1544.3072
1546.3495	1548.9586	1552.6131
1561.9754	1668.1475	1670.8213
1672.1402	1673.3005	1676.9020
1682.3766	1684.8883	1688.4368
1690.6996	1692.3461	1707.2446
3014.4410	3059.5812	3079.9129
3099.1274	3110.8564	3139.6511
3156.7544	3165.6259	3184.3079
3191.4385	3201.5785	3201.6884
3204.4761	3204.8455	3206.3811
3208.8180	3209.5849	3212.2728
3214.7111	3214.9854	3216.9861
3218.0982	3220.6915	3221.9103
3222.2775	3224.8946	3228.8436
3229.9738	3232.6936	3235.7028
3238.4594	3240.7243	3241.2030
3241.7162	3245.4490	3291.7744

Product 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.750739	0.741528	1.610467
2	6	0	-1.526388	-1.152810	0.221603
3	1	0	-1.631047	0.589704	2.231445
4	1	0	-0.080651	1.555556	1.868570
5	1	0	-1.123841	-1.806885	-0.561367
6	6	0	-0.524911	-0.057137	0.568557

7	6	0	0.676010	0.046585	-0.356809
8	1	0	-1.749146	-1.766385	1.098828
9	1	0	0.271983	0.092213	-1.381524
10	6	0	-4.877785	0.431263	-0.051533
11	6	0	-4.413511	0.473515	-1.510547
12	6	0	-2.900408	0.218748	-1.408278
13	7	0	-2.794996	-0.611257	-0.222581
14	1	0	-5.880666	0.028579	0.099330
15	1	0	-4.840535	1.420585	0.419416
16	1	0	-4.879764	-0.338549	-2.075401
17	1	0	-4.640787	1.414639	-2.014446
18	6	0	1.480934	1.317526	-0.143940
19	6	0	1.110532	2.482461	-0.819454
20	6	0	2.550152	1.372211	0.751612
21	6	0	1.792865	3.676660	-0.611800
22	1	0	0.274472	2.449107	-1.515254
23	6	0	3.233372	2.567073	0.964992
24	1	0	2.852849	0.471475	1.278751
25	6	0	2.858606	3.721850	0.283838
26	1	0	1.494825	4.570919	-1.150958
27	1	0	4.064937	2.593395	1.662851
28	1	0	3.394893	4.651501	0.447602
29	6	0	1.539804	-1.208431	-0.294765
30	6	0	2.317502	-1.560392	-1.401717
31	6	0	1.608184	-2.000192	0.852551
32	6	0	3.141333	-2.679403	-1.366421
33	1	0	2.278057	-0.942229	-2.295992
34	6	0	2.433200	-3.123568	0.890812
35	1	0	1.012125	-1.733326	1.721611
36	6	0	3.200120	-3.466919	-0.217592
37	1	0	3.736746	-2.939971	-2.236293
38	1	0	2.471666	-3.731130	1.789942
39	1	0	3.839223	-4.344016	-0.189939
40	1	0	-2.494936	-0.303444	-2.281958
41	1	0	-2.336505	1.155667	-1.275688
42	6	0	-3.837833	-0.436864	0.648816
43	8	0	-3.891896	-0.873854	1.782025

Zero-point correction= 0.368222 (Hartree/Particle)
Thermal correction to Energy= 0.387302
Thermal correction to Enthalpy= 0.388247
Thermal correction to Gibbs Free Energy= 0.317522
Sum of electronic and zero-point Energies= -903.991090
Sum of electronic and thermal Energies= -903.972010
Sum of electronic and thermal Enthalpies= -903.971066
Sum of electronic and thermal Free Energies= -904.041791
M06-2x/6-311++G(d,p) /SMD// M06-2x /6-31G(d) energy= -904.332214
Frequencies

24.1973	27.5411	31.4007
36.8922	45.6817	62.5128
90.9549	94.5044	131.0549
151.7901	189.5464	203.4877
241.4111	256.0613	291.1009
301.5293	333.4813	382.2136
415.0779	417.4069	447.3260
467.5303	495.8293	521.0837
556.4723	604.5264	611.2220
631.7699	631.8909	641.7210
662.6588	718.9986	725.5286
729.0649	740.3968	771.3402
785.2955	800.4394	859.9619
870.7074	877.7648	887.0772
897.9998	902.6593	924.9400
942.7784	954.1285	958.8030
977.1354	984.8385	990.7397
1003.0705	1005.5385	1018.6239
1020.9622	1022.4176	1027.3345
1048.3401	1077.1057	1078.6428
1086.6634	1104.7459	1124.4321
1130.1973	1185.8707	1192.5696
1195.2077	1218.6528	1221.3029
1224.0731	1225.7057	1235.0330
1238.3109	1257.9356	1265.8450
1305.5628	1308.3464	1327.5016
1333.9446	1361.8880	1364.1817

1366.9711	1373.3460	1378.0427
1383.1634	1406.7263	1458.0169
1480.4653	1494.7773	1502.5429
1511.6346	1515.5000	1525.5405
1555.5279	1561.7402	1562.6650
1681.5504	1685.2839	1703.2182
1707.2390	1757.4838	1854.2249
3022.3189	3038.6703	3088.8778
3099.0587	3108.5718	3118.7286
3164.3593	3167.2260	3176.3479
3179.2805	3190.4756	3206.8265
3209.3903	3217.6350	3221.6198
3225.5881	3231.2007	3233.7018
3238.9049	3248.7036	3267.3635

INT8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.811906	0.848369	-1.930644
2	46	0	1.459291	0.139112	-0.638713
3	6	0	4.993033	-1.338803	0.176057
4	6	0	4.507732	-0.198842	1.079534
5	6	0	4.264656	-1.121026	-1.173237
6	6	0	4.151434	0.904773	0.093494
7	8	0	4.189540	2.098361	0.255132
8	7	0	3.768792	0.266216	-1.100246
9	1	0	3.428670	-1.811558	-1.303619
10	1	0	4.943719	-1.238364	-2.022881
11	1	0	4.790104	-2.328652	0.587680
12	1	0	6.073424	-1.254630	0.027461
13	1	0	3.598089	-0.467524	1.628088
14	1	0	5.251100	0.162370	1.790792
15	15	0	-0.719994	0.003098	-0.064759
16	6	0	-1.621615	1.606133	0.009881
17	6	0	-0.894051	2.738003	0.394289
18	6	0	-2.982241	1.739016	-0.285955
19	6	0	-1.519801	3.976511	0.501431
20	1	0	0.170749	2.639919	0.595816
21	6	0	-3.605247	2.980996	-0.186043
22	1	0	-3.556405	0.871597	-0.601044
23	6	0	-2.876590	4.099621	0.210835
24	1	0	-0.944374	4.847161	0.800379
25	1	0	-4.661136	3.074650	-0.421644
26	1	0	-3.363337	5.067336	0.286082
27	6	0	-1.066357	-0.727528	1.589993
28	6	0	-2.116992	-0.313516	2.414053
29	6	0	-0.239781	-1.772565	2.017485
30	6	0	-2.342002	-0.942173	3.637185
31	1	0	-2.759197	0.505857	2.102636
32	6	0	-0.471541	-2.407483	3.233758
33	1	0	0.593242	-2.076621	1.386614
34	6	0	-1.523715	-1.991587	4.046830
35	1	0	-3.158096	-0.609463	4.271476
36	1	0	0.174018	-3.220511	3.551868
37	1	0	-1.700128	-2.478831	5.000913
38	6	0	-1.811896	-0.995109	-1.161055
39	6	0	-1.591468	-0.897206	-2.539932
40	6	0	-2.844681	-1.814184	-0.695742
41	6	0	-2.399989	-1.586220	-3.437577
42	1	0	-0.772057	-0.278893	-2.900880
43	6	0	-3.646691	-2.513915	-1.595649
44	1	0	-3.023459	-1.911296	0.371594
45	6	0	-3.429416	-2.398438	-2.965664
46	1	0	-2.220553	-1.497900	-4.504770
47	1	0	-4.442639	-3.151940	-1.223315
48	1	0	-4.055656	-2.945855	-3.663593

Zero-point correction= 0.392073 (Hartree/Particle)
Thermal correction to Energy= 0.417186
Thermal correction to Enthalpy= 0.418130
Thermal correction to Gibbs Free Energy= 0.329913
Sum of electronic and zero-point Energies= -1448.734168
Sum of electronic and thermal Energies= -1448.709055

Sum of electronic and thermal Enthalpies= -1448.708110
Sum of electronic and thermal Free Energies= -1448.796328
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1449.159745
Frequencies

11.5970	18.0532	24.0503
24.7687	34.3276	36.7087
47.2423	52.1134	55.4345
65.2200	72.0853	84.8080
98.9862	120.4182	135.4196
179.6509	203.0221	219.9748
223.3819	255.2973	259.2969
270.0672	271.4245	408.3972
409.6493	413.9565	439.6737
443.7673	449.0343	481.6599
515.4005	516.7045	522.9964
528.5660	618.6274	629.0910
629.7737	632.4103	683.3082
704.5411	713.0398	714.9584
717.0580	717.9374	719.8626
753.5167	766.2997	769.7337
775.3058	817.8034	874.0345
879.0132	884.5761	887.5158
916.5204	939.8253	950.1799
950.8705	959.7497	996.4453
1000.4025	1007.5843	1015.3222
1016.2088	1016.4526	1019.3351
1019.6720	1021.4923	1029.1301
1070.7519	1073.0171	1075.0613
1075.9988	1122.5626	1122.9263
1123.7615	1130.0478	1139.2946
1142.9710	1145.5833	1186.6983
1188.7652	1198.1389	1206.2687
1221.9385	1223.1966	1228.8757
1235.7507	1246.0138	1270.8158
1331.7631	1332.8987	1336.5407
1340.4040	1346.2114	1366.5945
1366.9314	1373.6289	1380.6070
1435.2118	1492.5693	1494.6734
1495.2472	1502.8748	1527.1358
1543.8905	1544.7220	1550.0058
1555.9163	1670.7966	1672.6592
1676.5052	1687.5442	1690.2838
1691.8784	1908.3559	3101.7795
3103.6572	3114.1554	3148.0136
3173.3289	3187.9049	3194.8685
3196.8045	3199.9998	3205.6504
3209.9381	3210.1645	3217.0879
3218.0753	3224.6559	3225.3844
3225.7082	3231.8920	3233.3828
3237.4082	3244.6108	3610.5387

TS6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.167316	-0.629414	-0.696651
2	46	0	1.374352	-0.543471	0.614303
3	6	0	5.690949	-1.083964	-0.166205
4	6	0	5.579472	0.404925	0.166601
5	6	0	4.396732	-1.663146	0.440242
6	6	0	4.066244	0.639505	0.204840
7	8	0	3.512078	1.723560	0.079946
8	7	0	3.449173	-0.557476	0.406455
9	1	0	4.560560	-1.994318	1.475702
10	1	0	4.015469	-2.523346	-0.120019
11	1	0	6.591151	-1.562651	0.226633
12	1	0	5.679400	-1.221457	-1.252564
13	1	0	5.989178	0.632248	1.158112
14	1	0	6.049106	1.076297	-0.554268
15	15	0	-0.858996	-0.091157	0.047815
16	6	0	-0.896362	1.347294	-1.083646
17	6	0	0.215796	2.197089	-1.105348
18	6	0	-1.998599	1.622677	-1.901441
19	6	0	0.210725	3.321943	-1.928447

20	1	0	1.097675	1.977716	-0.503502
21	6	0	-1.994521	2.745571	-2.722904
22	1	0	-2.856338	0.954435	-1.900775
23	6	0	-0.890506	3.597342	-2.733523
24	1	0	1.079091	3.972627	-1.942312
25	1	0	-2.850021	2.953768	-3.358146
26	1	0	-0.887845	4.471222	-3.377917
27	6	0	-1.946473	0.386883	1.444845
28	6	0	-2.680325	1.574534	1.478585
29	6	0	-2.020675	-0.496364	2.529377
30	6	0	-3.483757	1.868542	2.579458
31	1	0	-2.622186	2.273332	0.649472
32	6	0	-2.829467	-0.204815	3.621636
33	1	0	-1.441894	-1.418021	2.513688
34	6	0	-3.562239	0.981118	3.648021
35	1	0	-4.048022	2.795708	2.599512
36	1	0	-2.882073	-0.897449	4.455743
37	1	0	-4.187338	1.214985	4.504117
38	6	0	-1.835353	-1.382434	-0.810283
39	6	0	-1.153100	-2.272059	-1.646081
40	6	0	-3.222669	-1.495267	-0.673633
41	6	0	-1.849975	-3.249416	-2.350034
42	1	0	-0.071749	-2.198056	-1.735978
43	6	0	-3.916690	-2.478692	-1.374183
44	1	0	-3.759679	-0.818520	-0.013724
45	6	0	-3.232257	-3.354056	-2.213733
46	1	0	-1.311753	-3.935600	-2.996422
47	1	0	-4.993108	-2.563026	-1.260345
48	1	0	-3.774719	-4.122882	-2.755130

Zero-point correction= 0.386098 (Hartree/Particle)
Thermal correction to Energy= 0.410645
Thermal correction to Enthalpy= 0.411590
Thermal correction to Gibbs Free Energy= 0.326519
Sum of electronic and zero-point Energies= -1448.686897
Sum of electronic and thermal Energies= -1448.662349
Sum of electronic and thermal Enthalpies= -1448.661405
Sum of electronic and thermal Free Energies= -1448.746476
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1449.112478
Frequencies

-751.9024	15.9653	17.0605
26.4357	35.5296	38.4952
49.2114	53.1656	60.7725
65.4445	71.0085	92.6228
121.9321	142.8087	155.8448
172.0539	191.9851	212.8144
225.6514	253.0816	256.0761
256.4039	267.6649	278.1765
405.3824	410.7832	412.7967
440.4068	443.5060	452.2078
501.3069	510.0508	521.4976
530.1252	539.1699	574.7217
627.8749	629.4365	631.0723
655.0040	704.5604	713.0072
714.5898	716.2464	718.2631
722.0063	724.4224	767.3043
771.7464	778.5971	856.4446
873.5592	882.3954	892.5449
910.5510	929.8521	947.5353
948.3210	958.9422	970.2873
996.4495	1004.6120	1012.6198
1014.4793	1015.0880	1015.6942
1023.8876	1028.6575	1029.1933
1047.2016	1069.5747	1070.8425
1073.3810	1096.8761	1123.4321
1129.8582	1130.3392	1141.0264
1144.0974	1145.8472	1156.4790
1191.3823	1193.9387	1195.8541
1198.3431	1219.7614	1224.1060
1229.4709	1233.2830	1261.5742
1308.1820	1325.0387	1331.8037
1335.9717	1341.2045	1356.9898
1365.3795	1374.4093	1376.3643
1419.2349	1495.9700	1497.4283
1499.8271	1501.5543	1522.3029

1541.5242	1547.9229	1549.8231
1550.1157	1670.8363	1672.3963
1676.8097	1685.0203	1687.4106
1690.8257	1805.0539	2056.1907
3053.0624	3091.0090	3094.6377
3114.2239	3151.1275	3170.9340
3197.1271	3202.7451	3209.4727
3210.0929	3212.3165	3216.5592
3223.4945	3223.6281	3224.6523
3229.8127	3230.8490	3236.3433
3242.9062	3243.1913	3249.5512

INT9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.884661	-1.995955	-0.216270
2	46	0	1.433208	-0.575800	-0.115014
3	6	0	5.902382	-0.453838	-0.228321
4	6	0	5.211521	0.837582	0.233163
5	6	0	4.806942	-1.535715	-0.051239
6	6	0	3.748240	0.486289	0.027620
7	8	0	2.766421	1.289929	0.055316
8	7	0	3.560972	-0.802018	-0.156276
9	1	0	4.887951	-2.025155	0.930354
10	1	0	4.873610	-2.319330	-0.812074
11	1	0	6.815211	-0.685067	0.325626
12	1	0	6.161700	-0.371786	-1.288387
13	1	0	5.375722	1.043932	1.297549
14	1	0	5.493015	1.731523	-0.327185
15	15	0	-0.778526	-0.071839	-0.024651
16	6	0	-1.117989	1.674190	-0.444983
17	6	0	-0.129824	2.625264	-0.165764
18	6	0	-2.337722	2.076271	-1.001447
19	6	0	-0.377007	3.971561	-0.426300
20	1	0	0.835810	2.315834	0.228021
21	6	0	-2.574545	3.422996	-1.258816
22	1	0	-3.099785	1.338365	-1.237649
23	6	0	-1.595442	4.371036	-0.968044
24	1	0	0.393317	4.706191	-0.214606
25	1	0	-3.521434	3.731534	-1.691083
26	1	0	-1.780961	5.420908	-1.173667
27	6	0	-1.507739	-0.303810	1.636933
28	6	0	-2.432739	0.596789	2.173347
29	6	0	-1.148268	-1.442091	2.367679
30	6	0	-3.000236	0.353229	3.421768
31	1	0	-2.705931	1.490345	1.619680
32	6	0	-1.722698	-1.684105	3.611301
33	1	0	-0.412619	-2.131079	1.960700
34	6	0	-2.649580	-0.787213	4.139143
35	1	0	-3.714842	1.058588	3.834131
36	1	0	-1.439648	-2.568882	4.172544
37	1	0	-3.092112	-0.973043	5.112893
38	6	0	-1.875313	-1.030314	-1.129969
39	6	0	-1.372499	-1.433514	-2.370562
40	6	0	-3.195118	-1.336753	-0.785897
41	6	0	-2.187013	-2.120661	-3.264815
42	1	0	-0.337069	-1.218102	-2.624308
43	6	0	-4.005345	-2.030888	-1.681138
44	1	0	-3.587657	-1.040137	0.183304
45	6	0	-3.503728	-2.419747	-2.920308
46	1	0	-1.790498	-2.432963	-4.225673
47	1	0	-5.027864	-2.271740	-1.407515
48	1	0	-4.136123	-2.964266	-3.614705

Zero-point correction= 0.389134 (Hartree/Particle)
Thermal correction to Energy= 0.413465
Thermal correction to Enthalpy= 0.414410
Thermal correction to Gibbs Free Energy= 0.330874
Sum of electronic and zero-point Energies= -1448.713200
Sum of electronic and thermal Energies= -1448.688869
Sum of electronic and thermal Enthalpies= -1448.687925
Sum of electronic and thermal Free Energies= -1448.771461
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1449.13157

Frequencies

21.0918	25.3548	33.1990
36.6304	41.3817	47.5900
50.3214	64.3364	68.3974
70.2876	98.8674	133.7639
159.3010	165.5155	194.0938
208.2266	222.5654	226.0891
237.5662	259.6571	265.2290
273.7019	284.0511	407.6458
409.1811	412.2054	448.1588
450.6279	455.5237	510.1347
519.9158	522.3431	540.2466
550.4588	571.6399	626.8505
628.9905	630.1850	652.1104
709.7538	712.8375	714.3172
716.8886	727.4043	728.7141
732.2631	769.6625	775.0387
780.0079	839.9478	853.8227
881.3206	885.3538	890.8570
914.1520	931.7936	941.7910
954.1824	963.8180	964.9084
1004.9360	1010.6275	1012.1395
1014.6296	1015.7582	1016.1029
1026.7438	1029.9754	1035.5528
1037.5890	1070.9005	1071.3712
1073.8138	1100.7933	1126.7624
1128.7269	1130.9515	1143.7879
1146.9983	1151.5475	1176.4127
1188.1551	1191.4958	1192.4640
1196.3871	1224.3472	1228.3806
1228.8655	1232.4435	1252.6780
1310.2363	1335.3855	1337.4155
1339.4452	1347.0313	1356.5775
1368.2525	1374.5474	1375.3286
1496.0237	1498.9431	1500.1436
1500.6808	1517.4933	1539.3214
1544.7275	1546.1584	1550.0970
1558.4638	1667.3372	1672.3670
1672.4634	1673.0828	1685.4558
1689.4286	1690.5860	2142.5847
3051.1246	3091.8968	3100.2237
3123.2125	3156.7047	3168.8000
3210.7827	3211.6196	3215.9339
3220.8106	3221.8593	3224.7021
3227.6551	3230.2854	3233.8779
3235.1271	3235.8956	3242.2119
3243.3850	3246.8715	3254.0340

TS7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.411437	-1.750984	-2.543580
2	6	0	2.147649	-0.529194	-3.092644
3	1	0	1.910656	-2.706996	-2.405839
4	1	0	1.553744	0.120237	-3.732249
5	6	0	1.826960	-0.627785	-1.656799
6	6	0	2.703556	-0.644176	-0.488763
7	1	0	0.364775	-1.832737	-2.861974
8	1	0	3.195811	-0.614642	-3.372339
9	6	0	2.721205	-1.979234	0.209712
10	6	0	3.722589	-2.932315	-0.017438
11	6	0	1.652282	-2.328849	1.041538
12	6	0	3.657951	-4.189447	0.578371
13	1	0	4.555493	-2.683242	-0.670826
14	6	0	1.579526	-3.587902	1.631616
15	1	0	0.871443	-1.595383	1.231169
16	6	0	2.586631	-4.522156	1.405704
17	1	0	4.443304	-4.915547	0.389059
18	1	0	0.736056	-3.829959	2.272345
19	1	0	2.537417	-5.503681	1.867253
20	6	0	3.952972	0.178128	-0.564643
21	6	0	3.987253	1.335620	-1.361942
22	6	0	5.055116	-0.065887	0.269743

23	6	0	5.093603	2.180172	-1.360035
24	1	0	3.120176	1.594829	-1.962701
25	6	0	6.158215	0.782698	0.273998
26	1	0	5.043847	-0.925259	0.932825
27	6	0	6.190995	1.907737	-0.547225
28	1	0	5.088681	3.065654	-1.989512
29	1	0	6.996609	0.562293	0.928538
30	1	0	7.053012	2.567265	-0.543739
31	46	0	-0.001926	-0.041842	-1.152877
32	1	0	2.052016	0.136689	0.376410
33	6	0	3.159597	2.888009	1.736658
34	6	0	2.163009	3.419238	0.701942
35	6	0	2.481686	1.591563	2.237669
36	6	0	1.404941	2.158360	0.303419
37	8	0	0.723450	2.068210	-0.752979
38	7	0	1.574688	1.163766	1.172152
39	1	0	1.910928	1.764481	3.160409
40	1	0	3.210289	0.800069	2.447396
41	1	0	3.366800	3.592481	2.546008
42	1	0	4.107140	2.641896	1.246118
43	1	0	1.447309	4.131145	1.131861
44	1	0	2.620040	3.889617	-0.171925
45	15	0	-2.331771	0.132102	-0.172944
46	6	0	-2.398067	-0.811967	1.401359
47	6	0	-3.426975	-1.698234	1.728507
48	6	0	-1.335886	-0.624432	2.296480
49	6	0	-3.393440	-2.393605	2.936015
50	1	0	-4.253171	-1.851971	1.039738
51	6	0	-1.308886	-1.320878	3.501226
52	1	0	-0.522987	0.057979	2.041344
53	6	0	-2.335742	-2.208442	3.821560
54	1	0	-4.195904	-3.082565	3.181831
55	1	0	-0.479174	-1.174969	4.186586
56	1	0	-2.309742	-2.755480	4.759086
57	6	0	-3.725932	-0.575175	-1.133924
58	6	0	-4.971520	0.040541	-1.275354
59	6	0	-3.502150	-1.811640	-1.753479
60	6	0	-5.977836	-0.575849	-2.017961
61	1	0	-5.157221	1.004030	-0.810291
62	6	0	-4.511439	-2.432393	-2.480342
63	1	0	-2.529344	-2.291651	-1.656092
64	6	0	-5.752831	-1.812189	-2.615359
65	1	0	-6.941137	-0.087072	-2.126899
66	1	0	-4.328457	-3.394751	-2.948205
67	1	0	-6.540155	-2.290958	-3.189266
68	6	0	-2.904979	1.793171	0.334710
69	6	0	-2.329152	2.910411	-0.276377
70	6	0	-3.887379	1.968824	1.317278
71	6	0	-2.751025	4.191134	0.078207
72	1	0	-1.528474	2.776879	-0.998628
73	6	0	-4.305465	3.248152	1.666510
74	1	0	-4.317435	1.100484	1.811218
75	6	0	-3.738722	4.360184	1.043828
76	1	0	-2.297064	5.056258	-0.394942
77	1	0	-5.067361	3.379560	2.428604
78	1	0	-4.061669	5.358922	1.321776

Zero-point correction= 0.639688 (Hartree/Particle)
Thermal correction to Energy= 0.677672
Thermal correction to Enthalpy= 0.678616
Thermal correction to Gibbs Free Energy= 0.565800
Sum of electronic and zero-point Energies= -2066.254387
Sum of electronic and thermal Energies= -2066.216403
Sum of electronic and thermal Enthalpies= -2066.215459
Sum of electronic and thermal Free Energies= -2066.328274
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -2066.869796
Frequencies

-1471.1438	16.8800	21.9491
25.6558	30.9578	35.2458
44.7188	46.4897	47.6617
54.7895	58.1145	59.5013
66.8708	72.6461	77.1733
86.7934	90.1639	97.5806
106.3845	113.7904	119.8826
136.7111	156.4902	163.1338

191.0175	202.6838	209.0199
214.9234	218.7386	223.7062
226.9549	235.2298	254.1548
255.6850	262.0086	268.3150
276.5393	308.2467	324.9351
377.7448	407.9893	413.3581
414.5667	417.5812	419.9155
428.7182	430.9746	438.6670
451.6150	495.8234	505.0466
508.0442	519.0839	527.8178
531.9348	579.0897	582.5512
625.6817	627.9083	629.1357
630.5748	633.2927	634.5957
658.7142	686.4369	702.5100
708.1050	713.7678	717.3088
718.5734	720.6092	722.2498
724.5481	727.7864	737.8987
769.0827	771.5354	772.4222
779.1523	785.0947	813.3221
843.3598	863.2695	879.9509
880.9351	885.6263	886.6220
888.8950	890.4232	913.4259
919.6609	924.4562	945.1534
947.5146	951.2895	953.4717
959.1426	964.9597	997.5164
1003.1060	1005.7240	1007.9272
1011.9730	1013.3555	1014.0182
1015.4359	1017.2890	1017.5031
1018.4945	1021.2597	1026.2839
1028.3424	1030.8311	1032.2941
1032.9080	1041.9654	1049.3956
1069.9757	1070.8632	1071.1554
1076.6329	1085.6916	1089.0429
1093.7212	1122.2117	1122.8290
1125.9489	1129.0449	1131.0847
1137.1521	1138.2130	1141.2277
1143.8897	1160.3319	1174.7968
1187.5362	1190.1070	1190.9750
1194.3379	1194.9116	1196.1698
1216.5750	1224.9488	1227.4190
1229.3702	1230.4715	1231.4938
1237.0635	1264.4996	1304.3898
1309.6560	1318.6413	1334.8602
1336.2677	1341.8142	1344.3259
1346.7756	1361.7448	1363.3423
1370.4989	1371.2414	1375.6282
1378.1861	1385.1665	1418.1925
1468.3995	1483.6885	1493.6092
1496.0953	1498.2521	1499.0953
1500.3408	1511.6859	1527.4494
1533.0909	1538.7889	1545.6868
1546.2295	1546.4050	1552.4821
1556.6468	1564.2019	1667.1807
1670.5159	1671.6204	1673.6354
1675.0792	1686.1733	1687.6432
1689.5128	1691.0021	1697.6831
1705.3513	3061.0126	3073.5438
3089.7775	3109.0848	3119.4343
3149.9460	3151.5902	3163.4890
3166.9125	3195.5799	3201.0329
3204.5193	3205.2673	3208.0800
3209.5171	3212.8181	3213.2147
3214.9555	3217.6481	3220.3904
3220.5184	3222.7057	3224.8952
3226.5482	3230.5133	3231.1421
3232.9289	3235.0901	3236.4440
3238.3826	3239.2989	3240.1765
3245.5079	3245.9117	3248.2542

INT10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.794695	-2.624269	-1.044084

2	6	0	2.419124	-1.833872	-2.186195
3	1	0	2.375801	-3.319374	-0.445557
4	1	0	1.805519	-1.708648	-3.074872
5	6	0	2.026869	-1.153033	-0.930632
6	6	0	2.978985	-0.486883	0.047959
7	1	0	0.759800	-2.963051	-1.235644
8	1	0	3.481085	-1.975638	-2.377872
9	6	0	4.169640	-1.393738	0.342010
10	6	0	5.321890	-1.373573	-0.448306
11	6	0	4.096411	-2.306228	1.397887
12	6	0	6.370010	-2.255139	-0.195168
13	1	0	5.402044	-0.647063	-1.253104
14	6	0	5.144312	-3.185395	1.656227
15	1	0	3.205058	-2.322082	2.021373
16	6	0	6.284454	-3.164169	0.856283
17	1	0	7.259572	-2.226348	-0.817181
18	1	0	5.072365	-3.883536	2.484789
19	1	0	7.104069	-3.847467	1.055789
20	6	0	3.422454	0.904121	-0.377534
21	6	0	3.384905	1.354333	-1.696861
22	6	0	3.911768	1.763593	0.609939
23	6	0	3.845255	2.628964	-2.023483
24	1	0	2.964057	0.720539	-2.470136
25	6	0	4.368889	3.037308	0.289034
26	1	0	3.927769	1.424354	1.643790
27	6	0	4.340571	3.473731	-1.034635
28	1	0	3.803187	2.965484	-3.055047
29	1	0	4.742314	3.691269	1.071814
30	1	0	4.694476	4.467805	-1.290604
31	46	0	0.112923	-0.742619	-0.743445
32	1	0	2.415472	-0.363966	0.982036
33	6	0	0.897665	3.605080	1.673324
34	6	0	0.607682	3.406027	0.183710
35	6	0	0.361008	2.296114	2.299373
36	6	0	0.465636	1.894291	0.093723
37	8	0	0.412391	1.321814	-1.059152
38	7	0	0.374938	1.290606	1.241277
39	1	0	-0.670164	2.431987	2.665637
40	1	0	0.962337	1.971399	3.157206
41	1	0	0.435567	4.500835	2.097394
42	1	0	1.978555	3.673863	1.830692
43	1	0	-0.340123	3.861094	-0.129941
44	1	0	1.396398	3.760741	-0.486193
45	15	0	-2.304508	-0.402991	-0.102032
46	6	0	-2.707041	-1.019598	1.577364
47	6	0	-3.922879	-1.631150	1.894771
48	6	0	-1.731264	-0.856333	2.570957
49	6	0	-4.162955	-2.074379	3.193572
50	1	0	-4.682414	-1.766223	1.130403
51	6	0	-1.984448	-1.291469	3.868822
52	1	0	-0.790949	-0.369321	2.313363
53	6	0	-3.196562	-1.903621	4.181445
54	1	0	-5.107661	-2.553547	3.431980
55	1	0	-1.228829	-1.155974	4.636673
56	1	0	-3.387316	-2.249285	5.193042
57	6	0	-3.631949	-1.110770	-1.151038
58	6	0	-4.875788	-0.493489	-1.321751
59	6	0	-3.385159	-2.333328	-1.783155
60	6	0	-5.854649	-1.095152	-2.108053
61	1	0	-5.074320	0.460519	-0.840642
62	6	0	-4.366525	-2.938272	-2.563089
63	1	0	-2.414525	-2.811322	-1.664333
64	6	0	-5.602346	-2.317410	-2.727384
65	1	0	-6.816296	-0.608429	-2.238291
66	1	0	-4.163981	-3.887578	-3.049077
67	1	0	-6.366734	-2.782864	-3.341983
68	6	0	-2.724401	1.376853	-0.050308
69	6	0	-2.546952	2.110843	-1.228927
70	6	0	-3.177115	2.021905	1.102005
71	6	0	-2.856240	3.466451	-1.261395
72	1	0	-2.148682	1.622652	-2.114354
73	6	0	-3.464719	3.386146	1.070756
74	1	0	-3.301679	1.463264	2.025452
75	6	0	-3.315272	4.106497	-0.110619
76	1	0	-2.720022	4.027148	-2.181006

77	1	0	-3.812176	3.882203	1.971950
78	1	0	-3.545879	5.167238	-0.133588

Zero-point correction= 0.644257 (Hartree/Particle)
Thermal correction to Energy= 0.682724
Thermal correction to Enthalpy= 0.683668
Thermal correction to Gibbs Free Energy= 0.568607
Sum of electronic and zero-point Energies= -2066.272949
Sum of electronic and thermal Energies= -2066.234482
Sum of electronic and thermal Enthalpies= -2066.233537
Sum of electronic and thermal Free Energies= -2066.348598
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -2066.893008
Frequencies

13.6726	19.7210	26.5358
33.5524	37.4739	39.4603
44.2841	46.0526	47.7678
50.4648	54.7169	60.2850
63.6972	65.0251	75.0178
81.7838	89.8353	94.4004
103.6189	118.9589	123.9486
131.7404	153.5498	169.6464
190.5171	198.1579	212.7452
223.1633	233.1969	241.2796
252.1228	253.5471	259.8755
265.5026	277.6579	280.5319
289.9048	298.9149	325.5681
391.4368	406.4045	410.5704
416.2346	417.2225	419.6637
430.8410	446.2632	451.9511
489.2756	494.3912	507.1322
514.2801	531.5473	559.4362
576.9452	591.0503	614.9586
628.2160	628.4047	629.3721
630.6001	633.1610	650.2531
669.4591	701.2413	706.3139
713.9444	716.9342	717.5352
718.7873	720.7754	723.1172
723.5201	760.1535	763.0111
769.9241	776.9563	778.1494
784.8361	820.6989	837.6138
862.2683	864.4401	868.1826
872.4914	880.7329	882.0711
894.9315	900.8567	908.1052
927.1747	936.2332	943.5774
944.7269	948.3493	950.4050
972.1439	985.9088	986.5863
990.7586	997.8231	1002.6807
1011.3623	1014.0910	1015.1932
1015.6439	1016.5164	1017.0258
1018.4998	1020.9199	1022.0930
1024.4865	1025.0304	1033.5433
1042.8303	1054.5112	1070.2359
1071.8223	1072.0133	1074.7731
1077.0033	1083.6127	1092.9898
1118.8659	1122.3438	1125.1905
1126.9411	1127.8412	1129.3179
1138.8936	1141.2084	1144.0336
1164.6362	1178.4920	1182.5951
1187.9700	1189.3547	1190.3936
1194.8174	1195.5698	1213.3435
1218.9431	1222.9609	1223.9147
1227.5634	1233.2901	1234.8622
1235.5556	1258.2809	1295.4244
1304.1239	1332.3880	1334.0206
1336.9890	1341.3447	1343.9691
1358.0552	1359.2431	1366.6132
1368.4351	1368.5769	1371.6724
1372.6635	1381.5381	1384.2670
1464.0208	1475.2314	1491.2882
1494.0605	1498.3094	1502.0002
1509.4204	1517.2044	1519.6635
1521.2040	1542.9304	1544.6584
1546.9768	1548.0889	1559.1412
1559.3049	1669.2783	1672.6717
1675.2003	1676.6285	1682.7666

1685.4684	1687.0251	1689.3642
1690.6009	1702.5725	1706.3656
2994.6744	3018.2887	3087.1013
3089.1951	3092.1501	3101.1600
3141.4094	3145.0396	3153.8770
3198.3312	3198.8843	3202.7815
3205.9630	3206.0694	3208.3473
3208.7688	3210.6627	3212.4840
3214.4305	3217.4527	3218.2985
3219.8505	3221.4581	3223.0017
3223.2743	3223.7984	3227.6045
3228.1609	3231.6970	3232.0511
3236.6713	3239.7549	3241.4098
3241.9560	3242.1494	3244.6733

TS8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.115260	0.914880	0.078664
2	6	0	4.639611	1.405264	1.429314
3	1	0	5.709070	0.003527	0.057800
4	1	0	4.631451	2.479370	1.611138
5	6	0	3.674698	0.832125	0.441381
6	6	0	2.907134	-0.369893	0.538985
7	1	0	5.406846	1.663795	-0.655396
8	1	0	4.920970	0.810432	2.296499
9	6	0	3.204109	-1.423315	-0.478217
10	6	0	3.586840	-2.713665	-0.093272
11	6	0	3.185963	-1.095682	-1.842253
12	6	0	3.930509	-3.664062	-1.051460
13	1	0	3.630481	-2.965640	0.963272
14	6	0	3.520236	-2.052168	-2.794360
15	1	0	2.879889	-0.094155	-2.136989
16	6	0	3.892442	-3.338147	-2.404296
17	1	0	4.235094	-4.658004	-0.737663
18	1	0	3.490450	-1.790858	-3.847813
19	1	0	4.157041	-4.080304	-3.151441
20	6	0	2.049757	-0.667859	1.676191
21	6	0	1.930416	0.223975	2.784751
22	6	0	1.094774	-1.724144	1.585726
23	6	0	0.977967	0.024009	3.755334
24	1	0	2.608962	1.066764	2.847077
25	6	0	0.133375	-1.917030	2.604392
26	1	0	1.217194	-2.497827	0.834711
27	6	0	0.068771	-1.053742	3.672023
28	1	0	0.917382	0.710512	4.594682
29	1	0	-0.564438	-2.745103	2.520168
30	1	0	-0.686492	-1.188220	4.440068
31	46	0	0.677954	-0.071788	-0.063386
32	1	0	3.090624	1.852566	-0.214341
33	6	0	1.170065	4.822673	-0.528280
34	6	0	0.304847	3.641025	-0.967253
35	6	0	2.443331	4.129507	-0.003657
36	6	0	1.341987	2.552320	-1.237338
37	8	0	1.070895	1.448064	-1.776825
38	7	0	2.542157	2.892216	-0.773881
39	1	0	2.347769	3.898463	1.069391
40	1	0	3.340571	4.743091	-0.130322
41	1	0	0.699295	5.466276	0.218651
42	1	0	1.424319	5.438879	-1.396137
43	1	0	-0.360313	3.283696	-0.167651
44	1	0	-0.319737	3.829147	-1.843310
45	15	0	-1.740900	-0.161289	-0.252234
46	6	0	-2.464761	-0.079059	1.433730
47	6	0	-3.248607	-1.085868	2.000130
48	6	0	-2.137915	1.042674	2.206769
49	6	0	-3.710871	-0.964309	3.311356
50	1	0	-3.502194	-1.968988	1.420867
51	6	0	-2.612917	1.171319	3.506397
52	1	0	-1.494493	1.813760	1.786898
53	6	0	-3.403439	0.165591	4.062703
54	1	0	-4.319685	-1.754318	3.740942
55	1	0	-2.356537	2.050261	4.090080

56	1	0	-3.771974	0.261163	5.079499
57	6	0	-2.421350	-1.719036	-0.943695
58	6	0	-3.771751	-1.867227	-1.280944
59	6	0	-1.550606	-2.796784	-1.125947
60	6	0	-4.242774	-3.079208	-1.774988
61	1	0	-4.453972	-1.029130	-1.162821
62	6	0	-2.023024	-4.010990	-1.620872
63	1	0	-0.494355	-2.673534	-0.896565
64	6	0	-3.369224	-4.153220	-1.942407
65	1	0	-5.291373	-3.185030	-2.035747
66	1	0	-1.335622	-4.838909	-1.763518
67	1	0	-3.738645	-5.096659	-2.332456
68	6	0	-2.675154	1.138776	-1.144930
69	6	0	-2.106695	1.649272	-2.317613
70	6	0	-3.920405	1.612541	-0.716007
71	6	0	-2.794662	2.604409	-3.063422
72	1	0	-1.109655	1.328221	-2.613413
73	6	0	-4.597844	2.573502	-1.460802
74	1	0	-4.356355	1.235262	0.205588
75	6	0	-4.037948	3.066276	-2.637698
76	1	0	-2.350036	2.998589	-3.972398
77	1	0	-5.561965	2.938907	-1.120524
78	1	0	-4.567103	3.817181	-3.216608

Zero-point correction= 0.639204 (Hartree/Particle)
Thermal correction to Energy= 0.677593
Thermal correction to Enthalpy= 0.678537
Thermal correction to Gibbs Free Energy= 0.564675
Sum of electronic and zero-point Energies= -2066.269844
Sum of electronic and thermal Energies= -2066.231455
Sum of electronic and thermal Enthalpies= -2066.230510
Sum of electronic and thermal Free Energies= -2066.344372
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -2066.885058
Frequencies

-1270.5308	11.0920	20.1191
27.3260	31.1169	39.6677
42.6413	50.6566	54.0952
55.5032	59.6889	65.8054
67.1944	73.0758	78.1504
87.1827	88.5524	92.8620
00.3107	118.6850	127.1066
135.5713	135.9719	141.5027
154.5592	170.6324	179.1497
189.6673	207.2812	218.8424
228.5765	235.5654	255.1391
259.1925	260.8422	267.1079
280.9824	305.9687	309.9119
352.2037	391.7855	403.8581
408.9526	417.0732	418.9985
427.1336	436.5085	438.9189
449.5947	478.8922	488.0419
506.6084	511.2453	521.7250
527.0294	553.1338	580.4717
624.5312	625.3298	628.6256
629.8793	630.5043	630.6145
653.3648	659.5903	702.0953
704.9480	710.8736	713.0898
717.8365	718.9841	720.1677
723.6122	724.5855	735.7918
767.1094	769.4312	773.1019
776.3902	791.0964	818.2284
851.6422	854.1879	872.6861
873.8471	888.1401	888.3847
905.5331	910.0731	915.9167
926.2083	943.1203	946.5835
948.7712	953.4720	955.2454
958.5749	959.1929	980.3804
995.8859	996.8336	1003.8610
1006.9964	1007.3193	1011.6323
1014.5188	1016.5767	1016.7232
1017.3056	1018.7830	1022.2339
1027.9039	1028.7941	1032.6407
1034.4127	1051.4690	1067.1485
1069.7787	1072.3049	1072.9095
1076.0239	1085.1903	1091.6454

1094.6462	1116.2648	1121.5025
1126.8944	1128.5549	1130.2459
1136.5832	1141.0545	1141.8243
1147.3243	1168.7490	1183.3738
1187.5840	1189.8050	1191.7350
1194.3591	1196.6540	1202.9477
1217.1406	1222.5787	1227.4837
1228.4578	1229.9996	1235.2327
1252.1008	1255.6217	1271.5020
1306.6221	1329.5857	1332.9202
1336.2929	1342.3668	1343.4003
1349.0177	1357.3594	1363.5233
1365.2328	1374.7608	1379.1941
1380.5950	1400.9900	1474.6097
1482.3813	1487.2239	1492.1389
1493.9704	1494.6137	1497.7972
1501.0902	1511.5391	1523.0141
1527.5743	1540.7424	1541.6342
1546.2691	1548.4017	1549.9278
1558.4055	1615.6915	1632.8779
1670.6312	1671.0521	1672.8032
1674.2670	1685.0906	1689.3587
1690.7977	1696.6584	1699.0626
1706.1074	3031.5707	3060.4923
3106.6115	3122.5430	3131.0984
3139.3718	3154.5661	3163.2614
3191.3703	3198.3250	3202.5136
3205.3851	3206.1835	3209.1946
3212.0350	3212.3302	3212.6099
3213.1900	3214.9681	3215.5634
3218.7169	3219.2047	3221.9598
3224.2400	3225.9215	3227.7788
3229.3127	3237.7356	3239.6231
3240.5541	3244.4003	3247.5189
3249.8428	3253.1735	3256.8263

INT11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.525465	1.036982	-0.776558
2	6	0	5.119860	0.645098	0.539302
3	1	0	4.545630	0.297450	-1.567749
4	1	0	5.652991	1.384538	1.127870
5	6	0	3.616899	0.806313	0.392530
6	6	0	2.714496	-0.377509	0.520425
7	1	0	4.583624	2.064710	-1.116097
8	1	0	5.494944	-0.370315	0.632380
9	6	0	2.892947	-1.505253	-0.448577
10	6	0	3.293804	-2.774055	-0.013882
11	6	0	2.638662	-1.301196	-1.815917
12	6	0	3.424988	-3.824523	-0.918903
13	1	0	3.502729	-2.934444	1.040905
14	6	0	2.765309	-2.356486	-2.713984
15	1	0	2.317444	-0.313358	-2.145164
16	6	0	3.155178	-3.619922	-2.269824
17	1	0	3.742074	-4.801631	-0.567523
18	1	0	2.555679	-2.188948	-3.766187
19	1	0	3.256718	-4.438722	-2.975701
20	6	0	2.109423	-0.644115	1.814660
21	6	0	2.354096	0.181275	2.951978
22	6	0	0.990023	-1.535892	1.865458
23	6	0	1.535852	0.122627	4.051984
24	1	0	3.214889	0.841628	2.937352
25	6	0	0.149592	-1.553965	3.006017
26	1	0	0.886321	-2.327166	1.127491
27	6	0	0.406776	-0.729071	4.074204
28	1	0	1.755516	0.742645	4.916030
29	1	0	-0.704410	-2.226185	3.023753
30	1	0	-0.245093	-0.742575	4.941860
31	46	0	0.661319	0.063810	0.186034
32	1	0	3.209357	1.720108	0.817847
33	6	0	1.089902	4.725449	0.146567
34	6	0	0.724771	3.249026	0.281527

35	6	0	2.386982	4.653429	-0.693080
36	6	0	1.434900	2.647137	-0.943472
37	8	0	1.123956	1.457644	-1.374628
38	7	0	2.339089	3.411368	-1.455071
39	1	0	3.274782	4.652755	-0.039181
40	1	0	2.495153	5.516388	-1.359861
41	1	0	1.216182	5.247872	1.098878
42	1	0	0.310000	5.243125	-0.422589
43	1	0	1.139524	2.796982	1.197246
44	1	0	-0.350476	3.041181	0.274500
45	15	0	-1.751356	-0.077021	-0.186213
46	6	0	-2.658588	-0.619360	1.306408
47	6	0	-3.253249	-1.877890	1.425077
48	6	0	-2.619811	0.227679	2.422360
49	6	0	-3.801776	-2.281793	2.642270
50	1	0	-3.284140	-2.547487	0.570488
51	6	0	-3.183235	-0.170414	3.629093
52	1	0	-2.133335	1.198707	2.344137
53	6	0	-3.770003	-1.430899	3.743330
54	1	0	-4.258373	-3.263269	2.726648
55	1	0	-3.152468	0.496509	4.485351
56	1	0	-4.199601	-1.748072	4.688571
57	6	0	-2.097978	-1.372124	-1.434197
58	6	0	-3.365727	-1.528217	-2.007105
59	6	0	-1.062484	-2.230296	-1.814823
60	6	0	-3.593499	-2.538738	-2.935311
61	1	0	-4.170862	-0.852015	-1.729361
62	6	0	-1.291782	-3.240256	-2.747050
63	1	0	-0.065007	-2.099522	-1.399837
64	6	0	-2.556991	-3.396146	-3.304668
65	1	0	-4.578107	-2.653817	-3.377780
66	1	0	-0.474380	-3.892177	-3.039625
67	1	0	-2.736211	-4.178756	-4.035481
68	6	0	-2.667356	1.382926	-0.789191
69	6	0	-2.004326	2.197667	-1.716455
70	6	0	-3.969818	1.695775	-0.388312
71	6	0	-2.651471	3.312308	-2.242029
72	1	0	-0.977407	1.965317	-1.997596
73	6	0	-4.607570	2.815670	-0.916791
74	1	0	-4.482358	1.070927	0.338688
75	6	0	-3.950311	3.621747	-1.843372
76	1	0	-2.132928	3.944530	-2.956054
77	1	0	-5.618267	3.058777	-0.603353
78	1	0	-4.449443	4.495734	-2.250850

Zero-point correction= 0.644995 (Hartree/Particle)
Thermal correction to Energy= 0.683320
Thermal correction to Enthalpy= 0.684264
Thermal correction to Gibbs Free Energy= 0.570982
Sum of electronic and zero-point Energies= -2066.290345
Sum of electronic and thermal Energies= -2066.252019
Sum of electronic and thermal Enthalpies= -2066.251075
Sum of electronic and thermal Free Energies= -2066.364357
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -2066.910616
Frequencies

17.1776	21.1859	28.0393
32.2894	38.4401	43.0361
48.0577	49.7798	54.0984
59.4343	64.1090	67.6146
75.8585	76.3702	82.0776
86.7686	93.6846	108.4778
111.6054	127.6931	134.6884
139.5824	147.7378	161.5840
182.3666	190.4195	195.0027
214.1193	222.5801	224.7048
246.0811	251.5426	259.6107
269.7974	271.0412	280.6484
301.0829	315.2292	325.7595
375.6643	406.5742	412.4132
416.7186	430.0648	432.0033
443.2426	448.3129	451.7663
468.7866	504.7096	508.1729
515.7454	523.7750	529.2254
551.3822	578.8128	618.8826
624.7543	625.6446	626.8783

628.8727	630.3749	652.4022
662.0051	700.7163	705.5444
713.0615	715.7589	720.6063
723.1411	724.6869	725.9765
731.8489	732.3177	769.2032
772.1835	778.6283	779.7780
788.9524	800.5378	831.9938
852.4892	871.5272	884.5088
886.5802	890.2631	895.5202
903.7740	911.6582	919.1007
921.6720	932.2006	946.4552
948.9021	959.0788	961.8308
965.9301	968.0511	992.4601
1003.9814	1006.9090	1009.6497
1012.9478	1013.0985	1014.7002
1015.3188	1015.9931	1018.2621
1025.6937	1027.8728	1030.6409
1033.1909	1041.7739	1052.4051
1060.7170	1064.4764	1068.2012
1069.3000	1069.3459	1069.7464
1075.7195	1088.3739	1091.9650
1104.5840	1116.7539	1121.8534
1124.0358	1126.3856	1127.0603
1137.1797	1140.0302	1140.4380
1144.1170	1162.5945	1183.0473
1187.3709	1189.2214	1190.6594
1193.2853	1196.8101	1201.9402
1218.3129	1219.3309	1221.0429
1223.0517	1223.8662	1225.0262
1250.8731	1255.9239	1300.6638
1306.3685	1322.5423	1331.9944
1333.8543	1339.8582	1342.0599
1343.6091	1353.3767	1365.8460
1367.7981	1369.1861	1374.3937
1374.7310	1394.5229	1423.3189
1441.1889	1486.2432	1491.4672
1492.4199	1495.1653	1496.0173
1497.8287	1505.0897	1520.6989
1533.5091	1540.4743	1542.4083
1543.6586	1544.3263	1546.8193
1555.0608	1621.7702	1668.8523
1669.0667	1671.3044	1672.4567
1685.8286	1686.2774	1687.6746
1695.7918	1700.1812	1712.4529
3016.7849	3031.9223	3087.6923
3101.8985	3126.3279	3142.8636
3163.6995	3196.1049	3196.9129
3198.7360	3201.7936	3202.8389
3204.2300	3206.7318	3208.5205
3210.7399	3212.1225	3213.9409
3214.7091	3217.1533	3221.9684
3222.6431	3225.1901	3225.3265
3225.4912	3226.4580	3232.7620
3233.1306	3233.8052	3234.8783
3241.8118	3242.5454	3247.8252
3248.6828	3249.6120	3285.4002

TS9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.132096	-2.237216	0.485637
2	1	0	0.164354	-2.766320	-0.472227
3	1	0	-0.662282	-2.646455	1.114720
4	6	0	1.515062	-2.139166	1.150113
5	1	0	1.393313	-2.085385	2.240092
6	6	0	2.052795	-0.819621	0.623324
7	6	0	3.262096	-0.660560	0.034574
8	46	0	-0.106082	-0.280738	0.111410
9	1	0	2.154201	-3.003839	0.928295
10	1	0	1.678331	0.397498	1.134409
11	6	0	4.323357	-1.709281	0.040645
12	6	0	5.027916	-2.016305	-1.130754
13	6	0	4.655075	-2.392585	1.216395

14	6	0	6.012357	-2.998527	-1.132601
15	1	0	4.793278	-1.476394	-2.044214
16	6	0	5.645681	-3.370189	1.218414
17	1	0	4.133961	-2.138769	2.135519
18	6	0	6.324179	-3.679782	0.042498
19	1	0	6.541211	-3.230536	-2.052176
20	1	0	5.892025	-3.886609	2.141339
21	1	0	7.097231	-4.442356	0.042737
22	6	0	3.629459	0.625585	-0.626904
23	6	0	2.714892	1.299289	-1.443861
24	6	0	4.902811	1.187441	-0.450152
25	6	0	3.047009	2.511365	-2.043015
26	1	0	1.735123	0.860949	-1.610422
27	6	0	5.237957	2.397502	-1.049001
28	1	0	5.629376	0.666754	0.168258
29	6	0	4.310409	3.065037	-1.848959
30	1	0	2.317654	3.015624	-2.670515
31	1	0	6.225976	2.820749	-0.893620
32	1	0	4.574938	4.005705	-2.322826
33	6	0	2.583340	3.820538	1.433460
34	6	0	1.210178	3.885381	0.756086
35	6	0	2.517451	2.499062	2.232321
36	6	0	0.813469	2.417189	0.705041
37	8	0	-0.069023	1.964457	-0.080271
38	7	0	1.511957	1.690402	1.555945
39	1	0	2.227576	2.670776	3.278031
40	1	0	3.478791	1.972252	2.239350
41	1	0	2.806414	4.685954	2.062321
42	1	0	3.363837	3.740571	0.670411
43	1	0	0.468141	4.432062	1.350962
44	1	0	1.219255	4.314102	-0.248836
45	15	0	-2.406489	-0.313135	-0.095976
46	6	0	-3.159531	0.807423	1.136461
47	6	0	-2.373810	1.287094	2.187359
48	6	0	-4.500040	1.197094	1.037206
49	6	0	-2.932034	2.135580	3.141552
50	1	0	-1.323249	1.010525	2.248140
51	6	0	-5.053057	2.043588	1.991776
52	1	0	-5.106790	0.842005	0.207249
53	6	0	-4.268248	2.511667	3.045201
54	1	0	-2.316965	2.506946	3.955119
55	1	0	-6.092934	2.344490	1.910979
56	1	0	-4.699420	3.177527	3.786557
57	6	0	-3.245496	-1.920297	0.127587
58	6	0	-4.129385	-2.177580	1.176853
59	6	0	-2.932876	-2.945558	-0.775062
60	6	0	-4.703032	-3.441466	1.313474
61	1	0	-4.372491	-1.394670	1.888881
62	6	0	-3.514082	-4.200658	-0.641632
63	1	0	-2.233946	-2.753852	-1.586791
64	6	0	-4.401002	-4.450459	0.405544
65	1	0	-5.389551	-3.633064	2.132249
66	1	0	-3.270594	-4.986404	-1.349865
67	1	0	-4.850742	-5.432463	0.513907
68	6	0	-3.045503	0.303650	-1.696545
69	6	0	-2.384469	1.390088	-2.283887
70	6	0	-4.172864	-0.243522	-2.315668
71	6	0	-2.858592	1.918721	-3.481352
72	1	0	-1.513306	1.820877	-1.793064
73	6	0	-4.635996	0.288319	-3.516714
74	1	0	-4.687743	-1.086921	-1.864562
75	6	0	-3.979602	1.368277	-4.099932
76	1	0	-2.346681	2.761375	-3.935626
77	1	0	-5.509755	-0.143306	-3.995089
78	1	0	-4.340758	1.780396	-5.037241

Zero-point correction= 0.639855 (Hartree/Particle)
Thermal correction to Energy= 0.677899
Thermal correction to Enthalpy= 0.678843
Thermal correction to Gibbs Free Energy= 0.564462
Sum of electronic and zero-point Energies= -2066.281712
Sum of electronic and thermal Energies= -2066.243669
Sum of electronic and thermal Enthalpies= -2066.242725
Sum of electronic and thermal Free Energies= -2066.357106
M06-2x/6-311++G(d,p) /SMD// M06-2x /6-31G(d) energy= -2066.897823

Frequencies

-1353.9195	8.5693	14.1165
22.3246	30.8488	37.9635
39.0397	41.3525	49.2506
52.7959	57.7290	62.8086
66.6636	69.7445	76.5931
80.2582	88.5876	97.9278
103.7975	114.1382	129.5356
139.2937	144.6084	156.7016
174.9223	188.5772	199.4660
206.5413	220.1359	224.4184
241.8066	245.3277	254.6603
257.7070	263.1187	284.5702
292.1139	303.9918	339.8973
373.0270	404.8546	409.0707
411.1883	422.6535	428.3835
438.7380	443.4217	460.0942
463.9412	481.6119	507.3035
510.2251	525.2634	536.9018
548.3529	566.0103	595.0497
620.4863	628.0098	628.3355
630.0709	630.6112	634.2525
649.0257	660.5207	685.7433
706.6752	710.0127	715.5138
717.3767	719.7604	721.8704
725.4763	726.4359	727.8379
730.7170	766.6292	767.7272
769.1914	775.4003	796.7901
803.2825	846.8408	871.8858
873.6691	878.8735	886.1047
888.9678	900.5263	909.5284
926.3665	931.4441	946.9661
952.2677	954.3533	954.7082
960.7749	965.6994	995.3242
998.9579	1000.6661	1004.6616
1011.0178	1013.1954	1013.8965
1014.9359	1015.3945	1016.3348
1020.1616	1021.0185	1022.2975
1024.4912	1026.5745	1032.0121
1036.4844	1055.3914	1070.4932
1072.1445	1072.8834	1073.9699
1074.2275	1094.7203	1117.6061
1119.1953	1125.2409	1127.5227
1129.5784	1130.6013	1142.7895
1145.8590	1146.9403	1147.2241
1166.9889	1177.2879	1180.9348
1192.0315	1193.1067	1196.6386
1197.6038	1208.4490	1210.7106
1214.7898	1220.1329	1229.0402
1232.7178	1234.0240	1259.1357
1269.2560	1303.7272	1307.9305
1323.5163	1335.4937	1336.7242
1338.9675	1344.3536	1345.9545
1348.4721	1360.4272	1360.4662
1363.9130	1367.6721	1374.3707
1378.4632	1380.2781	1475.3257
1480.8472	1495.6257	1496.0296
1498.0286	1499.1262	1500.7813
1501.6243	1504.6121	1512.8295
1529.8427	1542.7367	1543.5406
1548.8557	1550.5364	1550.7258
1556.1382	1659.8701	1671.0975
1674.3528	1675.0775	1678.0102
1681.5949	1686.9093	1687.9484
1689.3504	1697.5371	1699.4276
1702.7318	3055.4944	3058.5556
3084.1726	3090.6347	3103.7430
3104.4126	3114.3981	3149.6807
3163.8049	3165.8115	3198.4971
3201.4631	3201.8722	3203.5652
3206.6009	3207.8125	3208.5694
3209.3417	3212.0049	3215.0783
3215.2299	3217.7374	3218.9586
3222.2265	3223.6186	3225.3484
3225.9306	3229.2005	3229.6817

3230.6567 3236.1393 3238.3918
3240.8343 3244.1400 3247.1980

INT12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.031883	-0.114811	-2.256808
2	1	0	0.232225	-1.106867	-1.890196
3	1	0	0.730007	0.201886	-2.979524
4	6	0	-1.427504	-0.116704	-2.873622
5	1	0	-1.589318	0.831790	-3.396270
6	6	0	-2.550896	-0.273395	-1.872877
7	6	0	-2.688640	-1.142058	-0.855325
8	46	0	-0.014931	1.215699	-0.740849
9	1	0	-1.475413	-0.900432	-3.646061
10	1	0	-3.326494	0.485912	-1.944605
11	6	0	-1.813021	-2.320537	-0.606813
12	6	0	-1.393443	-2.622113	0.696461
13	6	0	-1.440650	-3.187696	-1.640717
14	6	0	-0.617826	-3.747547	0.958711
15	1	0	-1.687453	-1.967704	1.511542
16	6	0	-0.673274	-4.320827	-1.380917
17	1	0	-1.780680	-2.982106	-2.651748
18	6	0	-0.261634	-4.607467	-0.080274
19	1	0	-0.294903	-3.948463	1.976317
20	1	0	-0.409352	-4.988541	-2.196057
21	1	0	0.330221	-5.495186	0.123544
22	6	0	-3.791602	-0.911690	0.121730
23	6	0	-4.079960	0.387887	0.558322
24	6	0	-4.558153	-1.972384	0.619342
25	6	0	-5.127520	0.621824	1.444815
26	1	0	-3.456328	1.208387	0.207507
27	6	0	-5.606774	-1.737015	1.502163
28	1	0	-4.332838	-2.986710	0.300728
29	6	0	-5.897574	-0.438317	1.915978
30	1	0	-5.333820	1.635144	1.777620
31	1	0	-6.200725	-2.569903	1.866772
32	1	0	-6.712798	-0.256166	2.609592
33	6	0	-3.335770	4.296036	-1.019170
34	6	0	-2.255231	4.555853	0.039008
35	6	0	-2.648874	3.305882	-1.991322
36	6	0	-1.401691	3.303271	-0.084549
37	8	0	-0.502750	2.933851	0.733982
38	7	0	-1.659678	2.620902	-1.179487
39	1	0	-2.165758	3.837487	-2.824301
40	1	0	-3.365411	2.602638	-2.432244
41	1	0	-3.692203	5.200386	-1.517995
42	1	0	-4.197482	3.805603	-0.553562
43	1	0	-1.634698	5.427053	-0.203203
44	1	0	-2.631890	4.687509	1.055634
45	15	0	1.847207	0.200056	0.126050
46	6	0	3.121500	1.417580	0.622475
47	6	0	2.765154	2.765182	0.725679
48	6	0	4.416046	1.010851	0.969311
49	6	0	3.707138	3.697160	1.160447
50	1	0	1.748998	3.080546	0.496744
51	6	0	5.351120	1.946589	1.394600
52	1	0	4.695085	-0.037559	0.898357
53	6	0	4.996574	3.292211	1.488650
54	1	0	3.426070	4.742331	1.242563
55	1	0	6.354935	1.627269	1.656996
56	1	0	5.727253	4.021901	1.824375
57	6	0	2.726815	-1.018369	-0.907467
58	6	0	3.778458	-0.635402	-1.745483
59	6	0	2.233154	-2.325829	-0.978887
60	6	0	4.347316	-1.559116	-2.619116
61	1	0	4.158237	0.382053	-1.712303
62	6	0	2.803163	-3.244669	-1.853759
63	1	0	1.395610	-2.626143	-0.353521
64	6	0	3.864293	-2.864331	-2.672146
65	1	0	5.169416	-1.255880	-3.259798
66	1	0	2.406567	-4.254764	-1.896547
67	1	0	4.309097	-3.580908	-3.355706

68	6	0	1.470640	-0.681564	1.685867
69	6	0	0.367753	-0.249950	2.429976
70	6	0	2.270876	-1.720492	2.170507
71	6	0	0.062781	-0.867454	3.641344
72	1	0	-0.248525	0.568661	2.059861
73	6	0	1.959094	-2.337457	3.377533
74	1	0	3.129131	-2.060163	1.597189
75	6	0	0.851900	-1.914558	4.111532
76	1	0	-0.797494	-0.533009	4.212753
77	1	0	2.580008	-3.148879	3.744828
78	1	0	0.608067	-2.398723	5.052363

Zero-point correction= 0.646295 (Hartree/Particle)
Thermal correction to Energy= 0.684299
Thermal correction to Enthalpy= 0.685243
Thermal correction to Gibbs Free Energy= 0.572726
Sum of electronic and zero-point Energies= -2066.323023
Sum of electronic and thermal Energies= -2066.285019
Sum of electronic and thermal Enthalpies= -2066.284074
Sum of electronic and thermal Free Energies= -2066.396591
M06-2x/6-311++G(d,p) /SMD// M06-2x /6-31G(d) energy= -2066.93577
Frequencies

8.7791	24.4096	29.3183
30.3134	38.5833	47.2075
52.3369	54.5865	58.4805
61.9907	64.5537	67.8312
74.1763	82.0264	86.8434
95.3313	100.2664	106.4042
117.0426	123.1455	133.9603
154.2360	161.7822	179.8980
189.4444	214.1990	224.7141
226.6681	235.1971	238.3566
250.6934	253.5086	260.8595
266.7748	274.9463	285.5508
296.5121	308.3108	350.8661
404.7123	413.6737	417.7935
422.0656	427.4912	429.7437
440.9312	453.1313	468.7389
471.2764	494.1854	500.7464
513.8047	528.1770	535.2625
556.4797	561.8886	576.6870
625.0431	625.1902	628.5324
630.5935	631.1569	651.2351
657.6216	661.9871	701.7992
711.8535	715.7980	718.8378
720.8449	721.2941	723.5250
727.2942	728.0301	734.7092
754.9389	764.5965	768.4642
777.4606	784.5245	801.5209
851.2504	878.4597	879.2335
881.8449	885.7212	888.6614
897.7969	914.2866	927.6148
930.0505	933.0351	943.0920
953.6597	958.3155	959.4514
963.8159	967.9682	977.2733
1000.5271	1001.9903	1003.8828
1006.0044	1008.7982	1013.9686
1015.8409	1016.8028	1018.7146
1020.2996	1023.8739	1025.0054
1027.0771	1027.4301	1028.9449
1033.5691	1070.1919	1070.7157
1070.8750	1072.1902	1076.5788
1093.2705	1100.5413	1121.4549
1124.4316	1125.6752	1127.4976
1128.8445	1140.2899	1143.3457
1146.9696	1161.2855	1163.1986
1178.5490	1184.9100	1187.3957
1187.9924	1188.1380	1191.6631
1193.3333	1212.6350	1214.6679
1219.1981	1226.0105	1227.3179
1227.7327	1230.1579	1255.4222
1277.1743	1306.9694	1311.5647
1330.7469	1336.5672	1340.6058
1343.9577	1344.8340	1350.7786
1360.6107	1363.3838	1367.8364

1371.7152	1375.1211	1376.5521
1390.4045	1428.1555	1487.2419
1492.8873	1497.3988	1500.4586
1500.8234	1502.0544	1504.8683
1506.1060	1513.6379	1533.6218
1543.8719	1546.0807	1547.4757
1552.5527	1554.2696	1561.6556
1665.9308	1669.4281	1669.8572
1673.6250	1674.2276	1676.0885
1686.4976	1688.5843	1690.3586
1698.0784	1702.2221	1735.6631
3037.9885	3049.2703	3091.6338
3092.8484	3094.8480	3107.5045
3113.8048	3149.7125	3160.5239
3190.2953	3193.8799	3196.1471
3203.2235	3204.2593	3207.7511
3208.2817	3208.7051	3211.7087
3211.8701	3214.2360	3214.8488
3216.9943	3219.6457	3219.8546
3221.4211	3223.0872	3227.3148
3228.3063	3228.3466	3229.4888
3229.9096	3234.3927	3235.5187
3237.5294	3239.2155	3243.1592

TS10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.119151	0.906307	-0.778756
2	6	0	-2.362769	2.096775	-0.257126
3	1	0	-4.105905	0.786836	-0.309085
4	1	0	-3.261351	1.009912	-1.863107
5	1	0	-2.208524	2.136487	0.818678
6	1	0	-1.499584	2.432826	-0.832463
7	6	0	-2.087053	-0.116815	-0.403920
8	6	0	-2.390343	-1.409884	-0.147922
9	6	0	-3.745463	-2.003963	-0.344091
10	6	0	-4.525591	-1.702351	-1.467992
11	6	0	-4.283192	-2.885726	0.606574
12	6	0	-5.802304	-2.235162	-1.625700
13	1	0	-4.109478	-1.062374	-2.240072
14	6	0	-5.558586	-3.417930	0.453608
15	1	0	-3.683948	-3.151762	1.473276
16	6	0	-6.327418	-3.092067	-0.662844
17	1	0	-6.382862	-1.987971	-2.509854
18	1	0	-5.954170	-4.093607	1.206602
19	1	0	-7.321278	-3.511772	-0.785353
20	6	0	-1.340037	-2.348739	0.361930
21	6	0	-1.164888	-3.610828	-0.220268
22	6	0	-0.482550	-1.985452	1.410810
23	6	0	-0.139910	-4.458476	0.196963
24	1	0	-1.832259	-3.918642	-1.021463
25	6	0	0.542626	-2.828616	1.831706
26	1	0	-0.618851	-1.016532	1.883575
27	6	0	0.723591	-4.067264	1.218108
28	1	0	-0.012515	-5.425560	-0.282104
29	1	0	1.204769	-2.511090	2.634052
30	1	0	1.529016	-4.722686	1.535623
31	46	0	-0.041851	0.507705	-0.327061
32	1	0	-3.397208	3.731536	-1.479825
33	6	0	-3.361212	4.504795	1.719129
34	6	0	-4.779963	3.985174	1.449975
35	6	0	-2.758390	4.698742	0.316832
36	6	0	-4.749893	3.457149	0.028410
37	8	0	-5.635975	3.013206	-0.642214
38	7	0	-3.396198	3.616195	-0.466118
39	1	0	-1.672866	4.586171	0.290018
40	1	0	-3.032556	5.669793	-0.107316
41	1	0	-2.777598	3.770061	2.278926
42	1	0	-3.349918	5.437157	2.284681
43	1	0	-5.105518	3.195539	2.131605
44	1	0	-5.535349	4.776979	1.485798
45	15	0	2.283597	0.455384	-0.177466
46	6	0	2.953102	-0.924430	-1.199263

47	6	0	2.141404	-2.058777	-1.331090
48	6	0	4.213702	-0.912378	-1.802728
49	6	0	2.594792	-3.168200	-2.037021
50	1	0	1.149572	-2.068818	-0.881814
51	6	0	4.658507	-2.020771	-2.521884
52	1	0	4.851375	-0.036609	-1.713613
53	6	0	3.852684	-3.150699	-2.636071
54	1	0	1.955504	-4.042304	-2.119350
55	1	0	5.637328	-1.999558	-2.992262
56	1	0	4.202193	-4.013576	-3.195472
57	6	0	2.807560	-0.074267	1.510354
58	6	0	3.860198	-0.964312	1.746260
59	6	0	2.061572	0.393766	2.597810
60	6	0	4.161320	-1.374079	3.043487
61	1	0	4.434933	-1.355171	0.910502
62	6	0	2.366215	-0.009058	3.895091
63	1	0	1.217760	1.054301	2.407830
64	6	0	3.415951	-0.897894	4.119546
65	1	0	4.973867	-2.074451	3.212349
66	1	0	1.774588	0.356028	4.729443
67	1	0	3.646488	-1.225163	5.129003
68	6	0	3.454793	1.820517	-0.573206
69	6	0	3.145020	2.597464	-1.696005
70	6	0	4.611108	2.113748	0.154936
71	6	0	3.982673	3.632772	-2.096251
72	1	0	2.234379	2.380986	-2.251287
73	6	0	5.442510	3.162222	-0.237048
74	1	0	4.863633	1.523228	1.031400
75	6	0	5.133396	3.919539	-1.363693
76	1	0	3.734484	4.221587	-2.974296
77	1	0	6.335892	3.385337	0.338706
78	1	0	5.784264	4.733695	-1.667903

Zero-point correction= 0.643741 (Hartree/Particle)
Thermal correction to Energy= 0.682641
Thermal correction to Enthalpy= 0.683585
Thermal correction to Gibbs Free Energy= 0.565528
Sum of electronic and zero-point Energies= -2066.204949
Sum of electronic and thermal Energies= -2066.166049
Sum of electronic and thermal Enthalpies= -2066.165105
Sum of electronic and thermal Free Energies= -2066.283162
M06-2x/6-311++G(d,p) /SMD// M06-2x /6-31G(d) energy= -2066.850861
Frequencies

-549.6852	11.8018	17.0172
19.4812	24.6137	29.2204
35.3199	40.0941	41.4437
44.0287	50.9211	52.6835
55.3613	63.3358	64.9225
70.0490	71.5068	82.0975
94.7754	98.4958	104.7280
107.1142	130.1477	132.7743
141.1333	170.8869	189.5645
196.5535	213.8750	216.7594
225.3261	229.6791	248.7307
256.3571	265.9743	268.5462
271.9461	299.2979	317.4039
372.0975	409.1205	409.7743
413.9596	421.4502	424.0384
427.9037	434.8320	435.8050
449.4453	473.7665	481.7685
506.6041	513.1428	517.4405
520.9786	552.3850	605.5688
609.5662	626.0738	629.2473
629.9903	633.2624	633.3394
648.7279	664.0028	669.4508
700.2027	710.2249	713.5842
714.7423	716.4373	716.7123
717.7002	726.0541	750.2725
758.5702	765.3977	769.3402
770.1100	791.8816	798.0623
824.5580	841.3808	868.7560
873.8791	877.8774	883.8520
884.3205	904.3789	926.7839
933.1998	937.3666	947.6116
948.8707	950.4097	956.0723

982.8014	989.1131	996.5564
998.6488	999.2318	1003.9250
1006.8304	1011.7794	1013.4207
1014.6326	1016.5131	1016.9513
1017.6836	1018.1438	1019.1851
1019.9807	1021.0679	1028.9350
1052.8834	1067.6261	1070.5744
1073.6679	1074.2347	1076.9266
1079.2583	1082.5538	1104.4814
1118.7428	1120.2793	1121.3364
1127.1599	1128.9628	1130.8407
1131.8353	1137.1083	1140.5185
1142.6102	1183.1287	1187.5075
1191.1609	1193.1421	1196.5477
1202.6917	1209.6042	1214.4047
1215.6687	1220.0193	1221.7686
1222.5614	1230.5774	1239.9863
1270.5785	1276.5495	1285.0703
1314.3771	1321.2125	1328.0679
1335.6600	1338.4450	1339.7898
1346.8116	1348.0503	1361.2861
1364.9860	1365.4016	1370.2143
1372.5822	1375.4963	1417.5238
1468.3774	1481.8293	1488.7941
1489.1294	1493.9378	1501.9504
1502.1863	1505.8570	1527.8258
1535.6002	1541.4298	1541.9018
1550.5941	1554.0585	1558.8734
1647.8241	1666.6801	1668.9557
1670.9169	1673.1647	1676.9501
1684.0895	1686.9132	1693.1910
1694.9778	1698.9940	1933.4160
3046.8287	3101.1375	3112.2171
3113.3474	3127.4203	3162.7463
3165.0361	3177.8448	3186.2617
3194.9211	3197.9775	3198.0279
3199.1743	3202.4763	3205.7191
3210.4900	3211.4462	3212.1554
3213.2942	3214.4387	3215.7970
3217.3985	3220.6320	3220.9170
3226.6212	3227.2533	3228.8585
3230.9771	3231.1556	3231.2357
3235.4497	3238.4640	3242.4614
3244.0600	3276.6457	3526.2864

INT13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.225754	-1.042570	1.004805
2	6	0	-2.249144	-1.614883	-0.395719
3	1	0	-3.234998	-1.110067	1.438252
4	1	0	-1.547371	-1.620943	1.640376
5	1	0	-2.945244	-1.048672	-1.019700
6	1	0	-1.248375	-1.583126	-0.842504
7	6	0	-1.710816	0.383756	0.780948
8	6	0	-2.659573	1.311132	0.490868
9	6	0	-4.128103	0.995280	0.436640
10	6	0	-4.884847	0.689751	1.577394
11	6	0	-4.788201	0.976118	-0.803554
12	6	0	-6.238615	0.366381	1.483502
13	1	0	-4.395568	0.721121	2.547692
14	6	0	-6.140309	0.652898	-0.904860
15	1	0	-4.223736	1.250003	-1.692946
16	6	0	-6.872967	0.343373	0.242114
17	1	0	-6.802110	0.142375	2.384849
18	1	0	-6.628039	0.660349	-1.876336
19	1	0	-7.929449	0.102617	0.170649
20	6	0	-2.330997	2.717796	0.113183
21	6	0	-3.231487	3.756334	0.391981
22	6	0	-1.132005	3.052230	-0.532169
23	6	0	-2.936930	5.077508	0.066771
24	1	0	-4.172873	3.526730	0.884763
25	6	0	-0.836570	4.370766	-0.859547

26	1	0	-0.428005	2.257605	-0.769686
27	6	0	-1.735438	5.393410	-0.560491
28	1	0	-3.649663	5.861858	0.306392
29	1	0	0.100928	4.598416	-1.359907
30	1	0	-1.503992	6.422832	-0.818086
31	46	0	0.446775	0.296273	0.472450
32	1	0	-1.961077	-3.689175	-0.166057
33	6	0	-4.706313	-2.795540	-1.770996
34	6	0	-5.107645	-2.770710	-0.281481
35	6	0	-3.284980	-3.401219	-1.812278
36	6	0	-3.910991	-3.290575	0.463150
37	8	0	-3.769093	-3.852804	1.496249
38	7	0	-2.723028	-3.072896	-0.466782
39	1	0	-2.639567	-2.976883	-2.582277
40	1	0	-3.309336	-4.489327	-1.910502
41	1	0	-4.714305	-1.783035	-2.179253
42	1	0	-5.386085	-3.403707	-2.368876
43	1	0	-5.312062	-1.749328	0.070347
44	1	0	-5.972284	-3.387933	-0.031463
45	15	0	2.635847	-0.116726	0.066566
46	6	0	3.809625	0.302946	1.427454
47	6	0	3.498264	1.431581	2.194362
48	6	0	4.966408	-0.423571	1.727960
49	6	0	4.338748	1.840968	3.224839
50	1	0	2.579140	1.974089	1.982466
51	6	0	5.801852	-0.019431	2.767551
52	1	0	5.213230	-1.312816	1.152914
53	6	0	5.492242	1.115021	3.513820
54	1	0	4.085317	2.719011	3.811038
55	1	0	6.695022	-0.593448	2.996329
56	1	0	6.143351	1.426820	4.325043
57	6	0	3.425812	0.726481	-1.373657
58	6	0	4.796092	0.993550	-1.466308
59	6	0	2.589961	1.109068	-2.428081
60	6	0	5.319175	1.617063	-2.596147
61	1	0	5.456794	0.719706	-0.647814
62	6	0	3.113219	1.727222	-3.561098
63	1	0	1.520536	0.927752	-2.338226
64	6	0	4.479488	1.981535	-3.646790
65	1	0	6.383842	1.823451	-2.654339
66	1	0	2.452585	2.021581	-4.371212
67	1	0	4.889165	2.471135	-4.525334
68	6	0	3.083683	-1.883791	-0.243070
69	6	0	2.540119	-2.830757	0.636715
70	6	0	3.907450	-2.327631	-1.280090
71	6	0	2.829396	-4.183013	0.495495
72	1	0	1.883509	-2.488233	1.434653
73	6	0	4.183220	-3.687214	-1.433176
74	1	0	4.335701	-1.612030	-1.975908
75	6	0	3.650513	-4.616599	-0.545770
76	1	0	2.414063	-4.901727	1.196444
77	1	0	4.821551	-4.016749	-2.247894
78	1	0	3.872480	-5.673193	-0.663228

Zero-point correction= 0.647312 (Hartree/Particle)
Thermal correction to Energy= 0.685827
Thermal correction to Enthalpy= 0.686771
Thermal correction to Gibbs Free Energy= 0.569066
Sum of electronic and zero-point Energies= -2066.211624
Sum of electronic and thermal Energies= -2066.173109
Sum of electronic and thermal Enthalpies= -2066.172165
Sum of electronic and thermal Free Energies= -2066.289870
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -2066.864684
Frequencies

9.1264	10.3459	18.4603
27.5682	29.8497	32.8721
33.9093	41.6866	45.9595
49.2274	51.6471	60.6866
62.9097	69.4581	71.6127
83.0438	89.2053	93.7236
102.0112	110.4474	119.1381
120.9823	137.6172	148.2161
180.1827	196.1158	214.7635
221.4961	225.6993	229.3004
245.0063	257.1735	259.2891

275.9391	282.9148	302.1612
304.9657	337.8845	407.9224
410.0586	411.2382	415.5898
417.9067	422.3388	434.7572
440.9981	446.0391	463.8204
478.2288	503.0172	511.5756
512.3420	519.6854	524.7441
566.4331	597.1237	625.0904
629.8541	630.4004	631.2305
632.8074	650.4676	653.4522
662.4064	672.2633	702.1139
713.0280	714.1698	715.2577
716.6115	717.8580	719.2315
728.8578	736.7937	746.6987
766.6545	772.2614	774.1098
792.1677	794.3816	804.7664
837.2932	840.1669	869.0477
880.4724	882.9368	886.4992
887.4127	916.3302	926.1970
933.5299	943.8666	948.9589
950.1122	954.9559	958.8527
988.2466	989.5630	998.9302
1001.1316	1002.9929	1004.7279
1008.0940	1011.3838	1014.1205
1014.8061	1015.2283	1015.7563
1018.0479	1021.4422	1021.6922
1021.8794	1022.3070	1059.2980
1070.0260	1071.2544	1071.4333
1072.6568	1073.7015	1078.3629
1086.5055	1108.1752	1118.5236
1119.1850	1121.1526	1124.8683
1128.8025	1130.0074	1136.7706
1138.2340	1142.8083	1181.3194
1183.3924	1187.1629	1188.7205
1189.4780	1197.0682	1204.9605
1208.3728	1216.3013	1218.0075
1223.3694	1230.0726	1238.3256
1241.9754	1256.0329	1285.4960
1306.3020	1310.6906	1322.1796
1323.7723	1331.5440	1334.0310
1336.4904	1339.4044	1340.5193
1357.4764	1358.4887	1362.6311
1366.4117	1367.3103	1369.4010
1373.9752	1395.6988	1418.4212
1470.0736	1492.9500	1493.6974
1495.1925	1496.9100	1498.8846
1502.7589	1523.4538	1526.6568
1540.1973	1542.0315	1544.4729
1545.0114	1549.9279	1555.1274
1617.5524	1660.5535	1667.9698
1672.4005	1673.5220	1674.2666
1685.7444	1688.6633	1689.5578
1693.0308	1696.0396	1997.3765
3044.3365	3100.3086	3108.3198
3119.0711	3132.9801	3136.8545
3178.8780	3182.5760	3184.5498
3189.6492	3190.4723	3192.3924
3194.2077	3194.3985	3199.7412
3202.4463	3202.9903	3203.7959
3204.7233	3204.8847	3209.2797
3210.5966	3210.6802	3212.6639
3217.3836	3218.3101	3218.7632
3219.6000	3227.3694	3230.9492
3232.9031	3233.9928	3235.5690
3243.2082	3243.6207	3467.6574

INT14

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.707725	-3.490450	0.256544
2	1	0	3.536808	-4.061073	-0.158474
3	1	0	1.760147	-4.021466	0.270696
4	6	0	3.003899	-2.554363	1.432488

5	1	0	2.243194	-2.468720	2.203325
6	6	0	2.717677	-2.026660	0.089141
7	6	0	2.935054	-1.011639	-0.791057
8	46	0	0.671986	-1.072540	-0.111139
9	1	0	4.024419	-2.510781	1.810337
10	6	0	3.486311	0.309077	-0.341809
11	6	0	4.810454	0.389480	0.133664
12	6	0	5.315323	1.631978	0.540547
13	6	0	3.244446	2.715574	-0.054134
14	6	0	4.540374	2.779951	0.453010
15	1	0	6.335071	1.688358	0.913647
16	1	0	2.631656	3.607522	-0.136319
17	1	0	4.955964	3.729423	0.777669
18	6	0	2.934994	-1.254776	-2.284112
19	15	0	-1.446893	-0.085907	0.000168
20	6	0	-2.579952	-0.279013	-1.434404
21	6	0	-1.996780	-0.408285	-2.699588
22	6	0	-3.973921	-0.281626	-1.322505
23	6	0	-2.792474	-0.516397	-3.836236
24	1	0	-0.911820	-0.433896	-2.782034
25	6	0	-4.769116	-0.399372	-2.459955
26	1	0	-4.439815	-0.195085	-0.344350
27	6	0	-4.180256	-0.512385	-3.717235
28	1	0	-2.329363	-0.615251	-4.813154
29	1	0	-5.850561	-0.404231	-2.362986
30	1	0	-4.802353	-0.604030	-4.602423
31	6	0	-1.345088	1.740757	0.196417
32	6	0	-2.241736	2.636028	-0.394969
33	6	0	-0.308656	2.240496	0.994256
34	6	0	-2.108083	4.006724	-0.182087
35	1	0	-3.043838	2.264777	-1.026957
36	6	0	-0.182607	3.609050	1.213131
37	1	0	0.411746	1.548858	1.427172
38	6	0	-1.082604	4.494803	0.623536
39	1	0	-2.807166	4.694347	-0.648476
40	1	0	0.627539	3.980604	1.833499
41	1	0	-0.980204	5.563530	0.785666
42	6	0	-2.511084	-0.578701	1.416044
43	6	0	-2.512311	-1.929504	1.782059
44	6	0	-3.318954	0.318537	2.120586
45	6	0	-3.321185	-2.379605	2.820691
46	1	0	-1.866798	-2.624849	1.249227
47	6	0	-4.121177	-0.131846	3.167032
48	1	0	-3.318743	1.372118	1.854416
49	6	0	-4.126372	-1.479796	3.515789
50	1	0	-3.315373	-3.430281	3.094232
51	1	0	-4.741836	0.573165	3.711763
52	1	0	-4.751320	-1.827242	4.332785
53	1	0	3.968411	-1.233738	-2.655906
54	1	0	2.488014	-2.222777	-2.525560
55	1	0	2.385713	-0.466738	-2.808609
56	6	0	2.737645	1.482970	-0.450996
57	1	0	1.722732	1.409409	-0.836265
58	7	0	5.647170	-0.729048	0.126417
59	1	0	6.399544	-0.693968	0.801598
60	1	0	5.160773	-1.615236	0.145383

Zero-point correction= 0.492993 (Hartree/Particle)
Thermal correction to Energy= 0.524172
Thermal correction to Enthalpy= 0.525117
Thermal correction to Gibbs Free Energy= 0.425559
Sum of electronic and zero-point Energies= -1643.613045
Sum of electronic and thermal Energies= -1643.581866
Sum of electronic and thermal Enthalpies= -1643.580922
Sum of electronic and thermal Free Energies= -1643.680480
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1644.096829
Frequencies

11.3894	16.4558	23.3994
27.6695	32.9567	41.7151
45.4786	52.6544	60.0371
65.4730	71.6041	75.4594
84.9399	102.4673	107.8877
120.8509	124.7250	162.9020
181.3113	193.5312	217.4032
219.9654	220.7639	223.2946

247.7694	257.2186	266.9203
268.6108	290.1120	313.5503
330.3801	362.9826	410.0096
410.9626	416.5252	435.8111
439.1185	441.7123	442.0326
479.4820	513.2817	515.6252
520.4553	524.5007	562.8268
591.3910	598.4615	628.5772
628.7254	629.0311	630.1283
674.2075	702.3226	713.7701
714.3229	717.1695	717.7341
718.7982	763.1885	767.9694
769.4069	772.1685	772.6995
780.6421	821.7872	866.4663
879.7818	881.2208	884.3149
887.2053	902.5475	951.5956
953.9458	956.2030	971.4911
994.1729	996.9881	1002.8337
1003.5742	1006.4927	1014.8938
1015.2421	1015.7119	1023.8965
1024.2620	1025.3006	1027.9903
1055.2876	1064.3685	1068.9890
1070.2604	1070.6843	1070.8107
1084.7443	1097.1326	1100.5664
1118.0018	1122.2719	1123.3025
1124.9848	1136.1520	1137.5456
1141.8596	1169.4417	1176.2019
1188.0319	1188.8676	1189.1687
1189.1993	1203.4222	1219.6787
1221.9647	1223.0401	1298.1024
1323.0624	1331.1881	1334.5823
1336.0751	1343.8633	1364.6341
1365.6070	1365.7982	1366.7903
1425.5388	1481.0227	1494.1241
1495.6335	1495.8368	1501.9444
1503.7705	1515.4386	1522.6414
1541.7429	1542.6211	1543.5008
1561.1297	1668.5344	1670.7213
1671.1385	1671.5616	1682.6843
1686.3454	1688.0641	1689.1142
1707.4302	1775.4623	3057.4957
3131.4064	3139.7036	3143.7468
3167.9854	3194.0531	3195.0051
3197.9492	3199.9102	3206.7715
3209.8461	3211.4762	3212.2785
3218.2449	3219.0113	3221.8026
3222.8249	3224.1656	3225.9307
3232.5910	3234.2116	3234.2589
3237.1042	3237.2161	3241.5093
3242.9050	3590.3680	3694.5795

TS11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.086248	-3.288970	-0.499626
2	1	0	2.272233	-3.238784	-1.569592
3	1	0	1.258334	-3.953173	-0.232163
4	6	0	3.314537	-3.330902	0.390355
5	1	0	3.139575	-3.858173	1.330338
6	6	0	2.903333	-1.922711	0.363417
7	6	0	3.622005	-0.784285	0.437534
8	46	0	0.823983	-1.649964	0.135652
9	1	0	4.272960	-3.605607	-0.057354
10	6	0	3.107781	0.584268	0.138070
11	6	0	2.461460	0.905136	-1.078651
12	6	0	1.962467	2.201279	-1.271797
13	6	0	2.851498	2.909366	0.852551
14	6	0	2.153710	3.193073	-0.319556
15	1	0	1.421655	2.419651	-2.190584
16	1	0	3.021878	3.680209	1.597298
17	1	0	1.756904	4.188007	-0.498414
18	6	0	5.053845	-0.848551	0.930906
19	15	0	-1.194101	-0.249948	0.103605

20	6	0	-2.846822	-1.045220	0.037445
21	6	0	-3.950784	-0.456787	-0.588347
22	6	0	-2.999929	-2.281027	0.674078
23	6	0	-5.188895	-1.092806	-0.569386
24	1	0	-3.839502	0.500155	-1.091664
25	6	0	-4.240426	-2.912374	0.698801
26	1	0	-2.136789	-2.746889	1.145019
27	6	0	-5.335757	-2.319023	0.076023
28	1	0	-6.040098	-0.630422	-1.059796
29	1	0	-4.349404	-3.871561	1.195498
30	1	0	-6.301935	-2.814287	0.088476
31	6	0	-1.218767	0.867000	-1.357553
32	6	0	-1.573009	2.217468	-1.286460
33	6	0	-0.839855	0.324376	-2.590212
34	6	0	-1.555700	3.010299	-2.432658
35	1	0	-1.851771	2.655432	-0.331912
36	6	0	-0.833923	1.114456	-3.736484
37	1	0	-0.525163	-0.715027	-2.639426
38	6	0	-1.188837	2.460513	-3.658565
39	1	0	-1.829015	4.059100	-2.366280
40	1	0	-0.544704	0.681583	-4.689942
41	1	0	-1.177302	3.079047	-4.550982
42	6	0	-1.347149	0.934614	1.492156
43	6	0	-0.168586	1.587214	1.870056
44	6	0	-2.543824	1.237284	2.145218
45	6	0	-0.190105	2.545425	2.877003
46	1	0	0.765296	1.344005	1.367786
47	6	0	-2.558195	2.187148	3.165401
48	1	0	-3.463422	0.733794	1.860612
49	6	0	-1.385527	2.844250	3.528984
50	1	0	0.730886	3.050688	3.152310
51	1	0	-3.489621	2.414834	3.674995
52	1	0	-1.403150	3.585333	4.322632
53	1	0	5.164925	-0.359098	1.904874
54	1	0	5.389936	-1.881807	1.042921
55	1	0	5.726601	-0.330707	0.237202
56	6	0	3.311964	1.613840	1.065277
57	1	0	3.827345	1.380792	1.992751
58	7	0	2.274584	-0.045768	-2.077841
59	1	0	2.244841	0.336061	-3.014365
60	1	0	2.868163	-0.861343	-1.993311

Zero-point correction= 0.491377 (Hartree/Particle)
Thermal correction to Energy= 0.521822
Thermal correction to Enthalpy= 0.522766
Thermal correction to Gibbs Free Energy= 0.426607
Sum of electronic and zero-point Energies= -1643.579753
Sum of electronic and thermal Energies= -1643.549309
Sum of electronic and thermal Enthalpies= -1643.548365
Sum of electronic and thermal Free Energies= -1643.644523
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1644.058035
Frequencies

-293.2650	21.1662	22.4176
30.9909	33.0418	37.4583
46.6726	54.0689	57.7773
61.8786	65.8715	71.2605
88.0513	89.8841	92.4797
112.7282	129.1817	144.7831
164.1256	174.6223	193.0145
212.8755	223.2288	246.8191
257.2990	263.9911	275.5508
300.3359	314.2321	348.8834
354.0304	369.7952	407.3334
409.7587	414.2012	428.8713
436.1531	438.8175	445.8836
458.3546	498.7679	509.5975
515.4291	524.1547	534.0500
558.4869	589.0142	600.8848
626.9939	628.4963	629.4570
640.5492	701.3869	711.6365
713.5456	716.1186	717.8460
719.0720	722.9375	764.2009
769.9391	771.0266	774.6849
775.4259	780.6507	837.3493
859.6609	870.1553	882.4686

887.8548	888.8028	945.7699
950.1461	955.8017	956.6862
960.0355	989.1042	990.3606
992.9944	1003.3128	1008.8434
1014.8156	1015.3929	1015.9668
1016.2113	1019.3400	1022.6133
1027.7200	1050.6993	1068.5266
1068.7300	1069.4921	1070.1993
1080.4694	1105.5681	1108.0203
1119.2584	1122.7112	1123.4741
1136.7736	1139.2504	1142.3439
1166.1049	1178.3203	1186.1521
1188.4862	1191.1294	1191.4859
1212.6034	1215.7099	1221.1564
1222.1690	1223.3775	1304.7429
1312.7162	1332.2202	1335.1749
1337.8373	1348.6824	1361.6668
1366.7279	1367.4030	1369.1682
1435.0537	1454.0655	1491.5372
1493.7120	1495.9785	1497.4271
1506.2108	1516.4503	1527.6554
1539.4561	1542.5805	1542.7508
1561.2537	1654.0173	1670.0799
1670.8645	1672.2499	1675.0828
1683.7606	1686.8665	1689.3532
1695.6289	1705.8353	3070.0643
3086.3182	3094.6380	3131.0692
3159.1805	3166.6450	3195.2914
3199.9516	3203.8172	3205.4277
3208.7304	3210.7955	3210.9258
3212.7474	3213.9785	3217.8272
3218.7057	3221.7155	3223.0333
3224.1715	3225.9485	3230.3132
3230.9484	3236.6314	3241.3582
3244.0346	3572.4189	3682.9671

INT15

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.653060	-3.072240	-0.453118
2	1	0	0.139635	-3.583253	0.098998
3	1	0	-0.496349	-3.165364	-1.530357
4	6	0	-2.092110	-3.429122	-0.017404
5	1	0	-2.669822	-4.037882	-0.729876
6	6	0	-2.553838	-2.013448	0.135594
7	6	0	-3.790475	-1.488526	0.172165
8	46	0	-0.808101	-1.091782	0.095450
9	1	0	-2.092950	-3.957332	0.946589
10	6	0	-4.061655	-0.027345	0.066125
11	6	0	-3.158999	0.990915	0.454330
12	6	0	-3.450678	2.332968	0.226976
13	6	0	-5.567696	1.743012	-0.722926
14	6	0	-4.644737	2.719315	-0.374273
15	1	0	-2.732443	3.086744	0.543792
16	1	0	-6.514158	2.017179	-1.178232
17	1	0	-4.851172	3.770662	-0.546683
18	6	0	-4.995906	-2.410296	0.163892
19	15	0	1.448565	-0.036986	-0.028314
20	6	0	2.978630	-1.039363	-0.013061
21	6	0	4.152356	-0.650558	0.639031
22	6	0	2.944654	-2.253926	-0.707458
23	6	0	5.281730	-1.464021	0.588054
24	1	0	4.181759	0.285658	1.190313
25	6	0	4.077965	-3.059891	-0.763609
26	1	0	2.023111	-2.566170	-1.193881
27	6	0	5.246229	-2.666243	-0.114678
28	1	0	6.189389	-1.159171	1.099982
29	1	0	4.045044	-4.000164	-1.305011
30	1	0	6.127466	-3.299345	-0.150004
31	6	0	1.675228	1.131268	1.371959
32	6	0	2.249485	2.399866	1.245427
33	6	0	1.210246	0.716109	2.627120
34	6	0	2.363702	3.233269	2.356591

35	1	0	2.603534	2.738727	0.275471
36	6	0	1.331301	1.546656	3.737092
37	1	0	0.749317	-0.265573	2.726385
38	6	0	1.907345	2.808833	3.601929
39	1	0	2.808734	4.217525	2.246885
40	1	0	0.971364	1.211787	4.705054
41	1	0	1.994675	3.461797	4.464842
42	6	0	1.647285	1.044884	-1.495279
43	6	0	0.495478	1.672530	-1.984922
44	6	0	2.873585	1.272748	-2.125870
45	6	0	0.573999	2.530092	-3.077884
46	1	0	-0.467232	1.478354	-1.514037
47	6	0	2.947510	2.125402	-3.225171
48	1	0	3.770306	0.778870	-1.760849
49	6	0	1.800267	2.756138	-3.699855
50	1	0	-0.325211	3.009531	-3.451943
51	1	0	3.902964	2.293214	-3.712764
52	1	0	1.859295	3.416790	-4.559340
53	1	0	-5.456962	-2.483714	-0.829600
54	1	0	-4.700235	-3.419119	0.461082
55	1	0	-5.771053	-2.065403	0.857760
56	6	0	-5.273221	0.402014	-0.495195
57	1	0	-6.001790	-0.345565	-0.789844
58	7	0	-1.917331	0.663823	1.094992
59	1	0	-1.416647	1.502910	1.381324
60	1	0	-2.092795	0.102067	1.929512

Zero-point correction= 0.494504 (Hartree/Particle)
Thermal correction to Energy= 0.524453
Thermal correction to Enthalpy= 0.525397
Thermal correction to Gibbs Free Energy= 0.429565
Sum of electronic and zero-point Energies= -1643.601236
Sum of electronic and thermal Energies= -1643.571288
Sum of electronic and thermal Enthalpies= -1643.570343
Sum of electronic and thermal Free Energies= -1643.666176
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1644.080589
Frequencies

12.1011	18.3401	24.1539
32.5744	39.2687	44.9338
50.7018	53.2685	56.4277
63.6252	73.4145	83.8980
104.8032	118.6155	132.7508
150.2914	190.8514	193.9310
197.1164	216.8289	219.1365
235.6206	254.1187	267.3867
268.6808	289.2983	297.7416
306.6121	336.3268	397.2370
407.1495	410.2040	414.5944
417.0928	433.7666	440.1205
450.3328	464.7117	477.8673
515.0243	516.8130	524.3611
525.9437	557.5303	577.2855
579.6460	594.9505	628.3136
628.6161	629.7838	652.1525
683.6092	701.7914	713.4483
716.1728	716.8186	722.2251
725.7986	757.9616	769.5225
770.1267	772.7913	779.8631
786.2589	827.0342	852.7287
875.7270	876.3444	884.6177
899.1331	947.4628	954.2211
954.8096	963.9856	986.0047
992.5429	998.2508	999.3661
1006.0554	1014.5396	1014.9782
1015.6440	1016.4706	1024.3097
1026.5614	1027.7272	1035.2501
1048.0517	1064.5935	1070.2069
1070.5476	1073.2742	1077.7722
1097.0255	1109.5953	1115.6052
1121.9926	1125.4756	1126.2640
1137.2193	1141.3865	1149.4286
1156.7574	1187.8851	1188.4415
1191.5309	1193.9402	1194.1664
1222.8424	1226.4560	1227.4331
1246.2125	1272.6726	1296.4753

1315.4086	1331.5019	1331.7751
1335.2508	1338.7322	1368.0714
1368.4208	1369.7299	1373.0397
1426.8949	1466.3307	1486.9659
1493.4838	1496.3938	1497.4302
1507.3282	1522.0863	1527.2961
1544.1232	1544.8884	1550.0086
1558.6297	1666.4705	1666.9400
1670.1522	1672.3994	1674.4754
1688.0157	1688.5285	1690.0165
1703.0518	1716.2246	3022.0887
3059.2582	3071.5724	3101.6931
3119.4853	3163.2038	3170.4219
3185.6531	3196.4045	3201.8521
3206.0688	3209.7405	3210.6298
3210.9413	3217.7912	3218.1490
3221.6616	3225.1487	3225.3146
3228.3488	3229.0410	3236.6682
3236.9268	3239.6999	3243.5830
3245.3931	3478.7298	3576.8760

INT16

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.047506	-0.526575	0.134835
2	6	0	2.330225	-1.735258	-0.071706
3	6	0	2.616531	-0.249887	0.358807
4	1	0	1.866047	-1.911517	-1.043461
5	1	0	2.041930	-2.443172	0.702988
6	1	0	2.525033	-0.002672	1.414617
7	6	0	3.676130	-1.165015	-0.036848
8	6	0	4.979374	-1.377906	-0.193610
9	1	0	2.356078	0.563109	-0.320391
10	6	0	5.977841	-0.299704	0.039899
11	6	0	7.112880	-0.566601	0.813900
12	6	0	5.834884	0.987291	-0.524112
13	6	0	8.076558	0.399800	1.069636
14	1	0	7.229335	-1.559045	1.240456
15	6	0	6.812873	1.957651	-0.264563
16	6	0	7.916946	1.671992	0.523885
17	1	0	8.938465	0.164077	1.684462
18	1	0	6.692153	2.947932	-0.696755
19	1	0	8.658321	2.444183	0.705493
20	6	0	5.491489	-2.741271	-0.589094
21	15	0	-2.152200	-0.021448	0.053131
22	6	0	-2.541823	1.762172	-0.196240
23	6	0	-1.749851	2.693094	0.485476
24	6	0	-3.587535	2.222412	-1.001841
25	6	0	-2.009613	4.055578	0.381196
26	1	0	-0.920337	2.338153	1.093597
27	6	0	-3.839360	3.588621	-1.115533
28	1	0	-4.207099	1.514061	-1.545150
29	6	0	-3.055049	4.506248	-0.422452
30	1	0	-1.389471	4.766268	0.919013
31	1	0	-4.651424	3.934477	-1.748086
32	1	0	-3.253153	5.569957	-0.512926
33	6	0	-3.170845	-0.421646	1.534164
34	6	0	-4.265954	0.348365	1.938968
35	6	0	-2.837308	-1.566482	2.265776
36	6	0	-5.018967	-0.027075	3.048944
37	1	0	-4.530744	1.246029	1.387092
38	6	0	-3.595679	-1.946098	3.369737
39	1	0	-1.970248	-2.151026	1.965733
40	6	0	-4.687702	-1.175770	3.763340
41	1	0	-5.865313	0.579863	3.355994
42	1	0	-3.327765	-2.837259	3.928968
43	1	0	-5.274525	-1.465800	4.629540
44	6	0	-3.117300	-0.808775	-1.304855
45	6	0	-2.481914	-0.949039	-2.544238
46	6	0	-4.438274	-1.244839	-1.167270
47	6	0	-3.158686	-1.494963	-3.629818
48	1	0	-1.445906	-0.631688	-2.645227
49	6	0	-5.111374	-1.804194	-2.252020

50	1	0	-4.944085	-1.152542	-0.210232
51	6	0	-4.475827	-1.926374	-3.484367
52	1	0	-2.655600	-1.594898	-4.586841
53	1	0	-6.134972	-2.146097	-2.131603
54	1	0	-5.001919	-2.363664	-4.327551
55	7	0	4.736430	1.325701	-1.317703
56	1	0	4.936076	2.054026	-1.992000
57	1	0	4.287396	0.527143	-1.750692
58	1	0	4.660650	-3.415434	-0.810402
59	1	0	6.141786	-2.674002	-1.467615
60	1	0	6.086002	-3.190174	0.214550

Zero-point correction= 0.493231 (Hartree/Particle)
Thermal correction to Energy= 0.524602
Thermal correction to Enthalpy= 0.525546
Thermal correction to Gibbs Free Energy= 0.422660
Sum of electronic and zero-point Energies= -1643.598772
Sum of electronic and thermal Energies= -1643.567401
Sum of electronic and thermal Enthalpies= -1643.566457
Sum of electronic and thermal Free Energies= -1643.669343
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1644.08928
Frequencies

7.8066	14.1246	15.6907
23.6656	27.1029	28.4867
33.6921	45.0889	50.0913
55.1868	60.0273	61.5045
77.9459	84.0628	92.0570
105.8091	144.2455	157.7275
175.9253	201.2613	204.5383
219.4719	220.1837	224.8289
249.5844	259.2138	267.4121
272.4790	288.6067	331.5013
372.8222	392.1806	407.0008
408.7087	413.6345	438.9938
439.7714	444.4996	447.1915
472.0139	513.5754	515.8487
524.3659	528.4586	566.2882
590.6575	600.1952	629.0848
629.5892	632.6503	673.4921
685.5164	703.2432	712.2601
713.6959	716.8661	717.3016
720.5876	736.4107	764.9904
767.3768	770.4299	775.4716
783.0268	803.9257	859.7381
876.6467	881.1595	884.8703
887.7754	900.4414	949.8436
951.6130	957.7762	958.5314
966.5219	997.4046	999.2072
1002.2874	1005.0285	1015.5277
1016.1349	1016.7755	1020.9934
1022.3972	1028.0753	1041.2595
1046.7886	1058.8132	1066.5272
1071.2759	1071.4529	1074.1906
1076.2105	1105.5716	1109.3859
1122.2999	1123.0932	1123.5908
1129.3385	1136.5190	1138.7991
1146.0227	1149.2828	1182.4718
1187.8053	1188.4325	1197.3250
1197.3490	1212.5686	1219.1103
1219.9194	1229.0768	1306.6837
1332.4663	1332.5509	1335.5676
1338.2389	1352.3772	1363.7948
1364.1777	1371.7064	1372.2373
1435.5951	1461.8851	1483.3644
1495.1871	1496.5739	1501.7530
1510.9217	1517.8049	1523.6429
1541.3297	1542.0270	1550.6994
1568.2873	1665.8906	1673.0596
1673.5472	1674.5100	1684.6524
1687.5558	1688.9062	1690.1093
1711.9551	1887.1210	3074.1516
3125.3148	3127.4109	3137.2492
3169.7649	3193.0373	3197.0996
3206.4878	3207.4117	3210.2504
3212.7002	3214.6471	3214.7401

3215.5677	3219.5839	3221.8239
3222.0514	3224.0251	3228.1131
3231.5303	3231.6189	3232.7445
3234.5710	3237.8697	3249.0071
3250.4624	3570.0430	3673.1738

TS12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.223015	0.875445	-0.011869
2	6	0	-2.022362	2.045638	-0.287666
3	6	0	-2.287354	0.204604	0.254228
4	1	0	-1.776099	2.339498	-1.311995
5	1	0	-1.802669	2.802319	0.469449
6	1	0	-2.209083	-0.038080	1.315583
7	6	0	-3.243773	1.252351	-0.095092
8	6	0	-4.563815	1.420321	-0.188235
9	1	0	-2.209213	-0.652233	-0.418505
10	6	0	-5.507095	0.300297	0.081487
11	6	0	-6.527926	0.461395	1.024137
12	6	0	-5.426288	-0.920333	-0.622041
13	6	0	-7.440307	-0.548200	1.303126
14	1	0	-6.591983	1.404282	1.561308
15	6	0	-6.350103	-1.935589	-0.338663
16	6	0	-7.343754	-1.754222	0.611816
17	1	0	-8.213401	-0.398099	2.049080
18	1	0	-6.276482	-2.876108	-0.879230
19	1	0	-8.047274	-2.557383	0.809724
20	6	0	-5.152201	2.759258	-0.554541
21	15	0	2.041017	0.049776	0.057602
22	6	0	2.151741	-1.783938	-0.032654
23	6	0	1.172796	-2.522610	0.641098
24	6	0	3.163131	-2.460451	-0.721726
25	6	0	1.215741	-3.913290	0.644566
26	1	0	0.369206	-1.998724	1.154455
27	6	0	3.199520	-3.853183	-0.724356
28	1	0	3.921798	-1.899317	-1.260889
29	6	0	2.229843	-4.580678	-0.039285
30	1	0	0.450901	-4.475001	1.171788
31	1	0	3.987237	-4.369896	-1.264196
32	1	0	2.259688	-5.665944	-0.044464
33	6	0	3.059875	0.441213	1.535409
34	6	0	4.066654	-0.401749	2.016682
35	6	0	2.812198	1.652111	2.189698
36	6	0	4.822657	-0.030544	3.125522
37	1	0	4.254808	-1.353563	1.527004
38	6	0	3.572964	2.025261	3.294539
39	1	0	2.010554	2.295191	1.832487
40	6	0	4.578983	1.183968	3.763125
41	1	0	5.599445	-0.693208	3.494702
42	1	0	3.373146	2.967671	3.794969
43	1	0	5.167095	1.469824	4.629769
44	6	0	3.114356	0.576255	-1.339061
45	6	0	2.511161	0.677851	-2.598439
46	6	0	4.478672	0.852182	-1.212939
47	6	0	3.262899	1.026828	-3.715554
48	1	0	1.444088	0.486704	-2.693216
49	6	0	5.227889	1.212585	-2.331609
50	1	0	4.958506	0.788620	-0.240227
51	6	0	4.623748	1.295669	-3.583046
52	1	0	2.785013	1.100059	-4.687655
53	1	0	6.286344	1.428861	-2.222644
54	1	0	5.210095	1.576649	-4.452446
55	7	0	-4.432338	-1.147319	-1.578332
56	1	0	-4.710875	-1.788638	-2.310226
57	1	0	-4.032642	-0.294916	-1.954630
58	1	0	-4.364399	3.497874	-0.725727
59	1	0	-5.767701	2.683777	-1.458041
60	1	0	-5.805398	3.135915	0.240885

Zero-point correction= 0.491016 (Hartree/Particle)
Thermal correction to Energy= 0.521680
Thermal correction to Enthalpy= 0.522624

Thermal correction to Gibbs Free Energy= 0.421919
Sum of electronic and zero-point Energies= -1643.581232
Sum of electronic and thermal Energies= -1643.550568
Sum of electronic and thermal Enthalpies= -1643.549624
Sum of electronic and thermal Free Energies= -1643.650329
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1644.067699
Frequencies

-214.5768	7.0015	11.8311
18.6187	19.7068	29.6701
33.8433	40.7645	46.2651
51.7472	55.5229	63.6193
66.2634	74.9642	86.5273
126.9155	128.6613	164.2755
169.9280	191.3885	215.9965
216.3940	223.7469	233.3505
258.1643	267.2561	271.9570
298.0335	325.1963	353.7805
388.3301	397.0827	406.4598
409.1747	414.5313	436.8125
438.8076	445.1310	453.9821
477.0628	511.3804	512.6306
517.1825	527.7114	529.7822
568.3206	573.3183	597.7560
605.7482	628.8835	629.3954
631.8515	687.3346	691.0732
703.6416	713.8162	716.7648
717.1783	720.5254	722.9584
753.0531	767.9497	769.9303
775.4386	777.3534	778.0062
846.0505	875.8591	877.5376
881.8905	891.6242	903.5015
938.5125	951.3899	953.3085
954.8500	958.5342	961.0557
979.4902	990.6838	998.3677
1003.2905	1011.1854	1014.6834
1015.3933	1016.7848	1025.6375
1029.6152	1030.5154	1064.4567
1068.0665	1070.8204	1071.7774
1074.8215	1100.2765	1110.9008
1124.0693	1124.7856	1129.9831
1132.6553	1137.3991	1141.9457
1149.6503	1166.5362	1190.4854
1190.8721	1190.9006	1197.7059
1198.6563	1214.8692	1221.1838
1226.9282	1230.6414	1306.2805
1332.6532	1336.0313	1339.3402
1340.5103	1352.9618	1365.9163
1369.7259	1372.3184	1375.5442
1419.0796	1433.8611	1445.0124
1495.9390	1496.5389	1501.8039
1512.1932	1515.9146	1522.3953
1543.0339	1546.4613	1552.5330
1568.8031	1666.5571	1669.6183
1673.5316	1677.1015	1685.8846
1687.5409	1689.9788	1691.4932
1712.3817	1843.3240	3067.5564
3090.1807	3107.5039	3126.9735
3164.6608	3183.7252	3195.3812
3195.5502	3197.3734	3201.0402
3204.5052	3211.0838	3213.3807
3213.4361	3218.1562	3219.3772
3220.3110	3223.5160	3226.5069
3228.1305	3229.4855	3235.6598
3243.4997	3248.1800	3248.5483
3248.8290	3567.1802	3671.3815

INT17

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.006504	-2.012753	0.403165
2	6	0	-1.524987	-1.161111	1.479186
3	6	0	-1.701557	-3.221295	0.570090
4	1	0	-1.520681	-0.079189	1.362276

5	1	0	-1.332950	-1.494977	2.501821
6	1	0	-1.600370	-3.832963	1.470423
7	6	0	-2.504784	-1.979419	0.738395
8	6	0	-3.614208	-1.569592	0.087898
9	1	0	-1.876675	-3.815511	-0.329834
10	6	0	-4.054996	-0.145894	0.123999
11	6	0	-5.290716	0.203313	0.676730
12	6	0	-3.272830	0.879166	-0.451759
13	6	0	-5.752213	1.515112	0.692174
14	1	0	-5.896265	-0.587754	1.113012
15	6	0	-3.731616	2.202366	-0.425918
16	6	0	-4.961148	2.518107	0.136702
17	1	0	-6.713474	1.752348	1.136389
18	1	0	-3.110836	2.981721	-0.863263
19	1	0	-5.300674	3.549743	0.139125
20	6	0	-4.439017	-2.513419	-0.750433
21	15	0	1.564880	-0.106714	0.029522
22	6	0	1.406301	1.289230	1.206313
23	6	0	0.194234	1.993469	1.250028
24	6	0	2.422706	1.610827	2.108574
25	6	0	0.012662	3.008393	2.183918
26	1	0	-0.598551	1.744814	0.544883
27	6	0	2.231315	2.625481	3.044787
28	1	0	3.365904	1.072764	2.083137
29	6	0	1.028936	3.324612	3.084310
30	1	0	-0.929415	3.547644	2.209794
31	1	0	3.027102	2.868420	3.742248
32	1	0	0.882481	4.113117	3.815947
33	6	0	1.185498	0.661165	-1.594858
34	6	0	1.280739	2.034486	-1.839852
35	6	0	0.740682	-0.182999	-2.618361
36	6	0	0.930747	2.551889	-3.085120
37	1	0	1.607563	2.703625	-1.048525
38	6	0	0.396953	0.332735	-3.864658
39	1	0	0.642059	-1.250282	-2.427682
40	6	0	0.486378	1.703802	-4.097492
41	1	0	1.000626	3.620640	-3.262915
42	1	0	0.047594	-0.332880	-4.647767
43	1	0	0.206732	2.110580	-5.064399
44	6	0	3.373582	-0.400989	-0.034072
45	6	0	3.876918	-1.509377	0.653009
46	6	0	4.259186	0.450887	-0.702535
47	6	0	5.247660	-1.758855	0.681557
48	1	0	3.189703	-2.176046	1.170365
49	6	0	5.626431	0.196943	-0.679756
50	1	0	3.876866	1.311141	-1.245805
51	6	0	6.121876	-0.906466	0.013997
52	1	0	5.629044	-2.621229	1.219405
53	1	0	6.307423	0.860098	-1.204330
54	1	0	7.189546	-1.102378	0.029834
55	7	0	-2.012064	0.602175	-1.004467
56	1	0	-1.866617	-0.385173	-1.194943
57	1	0	-1.771994	1.172762	-1.808529
58	1	0	-4.187006	-3.556065	-0.535500
59	1	0	-5.508996	-2.373542	-0.556504
60	1	0	-4.294464	-2.344672	-1.826933

Zero-point correction= 0.492663 (Hartree/Particle)
Thermal correction to Energy= 0.522858
Thermal correction to Enthalpy= 0.523802
Thermal correction to Gibbs Free Energy= 0.428315
Sum of electronic and zero-point Energies= -1643.594812
Sum of electronic and thermal Energies= -1643.564616
Sum of electronic and thermal Enthalpies= -1643.563672
Sum of electronic and thermal Free Energies= -1643.659159
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1644.075931
Frequencies

15.8184	20.0147	25.1324
34.0132	41.5779	49.5973
53.7110	60.7040	66.1866
71.9853	82.2550	89.1849
91.7835	108.0023	121.9756
140.1519	167.1068	187.3457
195.2516	207.0950	231.2821
234.0675	250.6592	256.4776

258.2567	283.9958	294.6527
323.4879	372.3795	394.5330
407.9354	408.4237	415.5210
419.6385	426.3018	438.3875
453.1497	456.9830	479.7878
497.0481	500.1950	520.0418
530.9386	535.1910	555.4727
580.1971	600.9228	626.2722
628.1893	629.5445	630.9809
690.0623	699.7585	702.0301
712.7839	714.4103	717.6771
719.4650	722.4857	723.5879
764.2168	766.1149	769.5723
774.7003	775.1795	779.8310
846.6730	874.0792	879.9529
885.5996	887.2481	898.1062
951.4404	955.1828	955.9301
958.0494	962.6569	988.3367
989.6775	997.5734	1008.4957
1010.5531	1014.2287	1015.3533
1016.5551	1024.4946	1025.1502
1026.3102	1043.2536	1061.4967
1064.5737	1068.7967	1069.3285
1070.1589	1072.8164	1093.1766
1105.3224	1120.4309	1123.9950
1130.3515	1138.3138	1138.5286
1141.8568	1169.6889	1182.5870
1185.4966	1188.5484	1189.9583
1196.9775	1216.5062	1223.8194
1233.1869	1240.6391	1298.3682
1330.0101	1331.2779	1333.3982
1341.8583	1343.7547	1361.9389
1363.4381	1367.1338	1379.6558
1434.6487	1453.8814	1475.1031
1493.1797	1495.7031	1499.3825
1509.8097	1515.1243	1525.4774
1541.2817	1543.6659	1548.3651
1559.0157	1657.3390	1669.7933
1673.1987	1674.4652	1677.5997
1687.8395	1688.3413	1689.6513
1704.2103	1747.9965	3046.1957
3095.8921	3105.3990	3124.3327
3157.3465	3173.6401	3185.1785
3191.2708	3193.5596	3193.6540
3196.2938	3207.6161	3208.8319
3209.1943	3215.3772	3216.7430
3217.2461	3218.3644	3223.7461
3223.9367	3226.1905	3231.2270
3234.1258	3234.4660	3234.7649
3241.0270	3541.8490	3647.3650

TS13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.041765	-1.844110	-0.614990
2	6	0	1.692391	-3.040818	-1.110314
3	6	0	1.885805	-0.725729	-1.653723
4	1	0	1.452771	-3.254653	-2.152584
5	1	0	1.835081	-3.914929	-0.481150
6	1	0	1.536231	-0.927933	-2.662849
7	6	0	2.416293	-1.839624	-0.837432
8	6	0	3.335154	-1.574066	0.177475
9	1	0	1.557929	0.201852	-1.194088
10	6	0	3.907877	-0.255355	0.327571
11	6	0	4.048616	0.620236	-0.781339
12	6	0	4.425082	0.235306	1.550577
13	6	0	4.562356	1.905013	-0.667393
14	6	0	4.976159	1.503992	1.661529
15	1	0	4.364706	-0.396072	2.431665
16	6	0	5.029152	2.363702	0.560368
17	1	0	4.625089	2.535710	-1.552148
18	1	0	5.351615	1.838459	2.624505
19	1	0	5.444795	3.361239	0.651175

20	6	0	3.619594	-2.632074	1.209462
21	15	0	-1.556250	-0.117452	-0.010104
22	1	0	2.871057	-2.653357	2.016974
23	1	0	3.618396	-3.627756	0.753028
24	1	0	4.601588	-2.490668	1.672170
25	7	0	3.629239	0.096919	-2.043787
26	1	0	3.690413	0.775882	-2.799599
27	1	0	4.151111	-0.751209	-2.277246
28	6	0	-2.564840	-0.383204	1.501094
29	6	0	-3.150204	-1.643897	1.665296
30	6	0	-2.780276	0.601650	2.469202
31	6	0	-3.954469	-1.909724	2.768537
32	1	0	-2.967560	-2.419077	0.923819
33	6	0	-3.578580	0.330691	3.578682
34	1	0	-2.319689	1.579415	2.357016
35	6	0	-4.168842	-0.921664	3.727638
36	1	0	-4.405143	-2.890371	2.885773
37	1	0	-3.736634	1.099389	4.328933
38	1	0	-4.788553	-1.131595	4.594023
39	6	0	-0.619916	1.420501	0.360823
40	6	0	-1.101496	2.703402	0.080994
41	6	0	0.658465	1.277261	0.917471
42	6	0	-0.317101	3.821738	0.355162
43	1	0	-2.085496	2.829946	-0.362383
44	6	0	1.443750	2.394872	1.184924
45	1	0	1.054092	0.280302	1.115377
46	6	0	0.954810	3.668629	0.902651
47	1	0	-0.698686	4.813651	0.131571
48	1	0	2.440881	2.262406	1.593700
49	1	0	1.570000	4.541028	1.102229
50	6	0	-2.810031	0.448117	-1.229182
51	6	0	-2.485546	0.326863	-2.584445
52	6	0	-4.046019	0.995244	-0.870683
53	6	0	-3.371151	0.762698	-3.565423
54	1	0	-1.535130	-0.125032	-2.862428
55	6	0	-4.934921	1.424476	-1.853459
56	1	0	-4.316252	1.081102	0.178701
57	6	0	-4.597955	1.312051	-3.200185
58	1	0	-3.109199	0.663208	-4.614363
59	1	0	-5.894003	1.844466	-1.565606
60	1	0	-5.294109	1.645292	-3.963851

Zero-point correction= 0.493706 (Hartree/Particle)
Thermal correction to Energy= 0.523178
Thermal correction to Enthalpy= 0.524122
Thermal correction to Gibbs Free Energy= 0.429718
Sum of electronic and zero-point Energies= -1643.565558
Sum of electronic and thermal Energies= -1643.536087
Sum of electronic and thermal Enthalpies= -1643.535143
Sum of electronic and thermal Free Energies= -1643.629547
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1644.045206
Frequencies

-481.6793	12.1020	19.0222
26.4715	32.5920	35.0525
45.7915	55.0114	61.0449
65.2041	69.0070	92.4801
98.7198	103.4469	114.8824
145.8879	149.0527	170.9029
189.8798	207.0414	217.1487
225.0030	237.0293	255.7855
267.2434	268.6052	306.6119
333.6766	351.4572	377.4062
407.5500	410.0041	412.6336
417.9306	429.2946	438.0282
441.2693	445.8049	480.4372
485.5335	513.6080	517.0563
523.2784	541.8414	580.7465
588.3027	600.8586	627.7723
629.1918	630.0479	683.1992
697.1670	701.8593	713.9987
714.5571	716.1880	718.4890
719.2147	724.8459	750.4877
769.4053	771.0344	776.4981
777.7779	813.6076	828.7252
875.6027	877.1434	890.8403

902.1519	908.9589	929.7295
939.0028	953.6552	955.6415
969.0595	988.3174	992.7158
998.2951	1009.6677	1012.4453
1013.4666	1014.8315	1015.9444
1023.8051	1028.7305	1030.5169
1031.7042	1043.2367	1060.4289
1070.4546	1071.1313	1071.6526
1076.6849	1094.5241	1120.4592
1125.6120	1126.3106	1129.6426
1138.1890	1139.6669	1143.3825
1154.0751	1171.9937	1185.8238
1186.7943	1191.2175	1194.3149
1199.4457	1218.6198	1228.8556
1230.3899	1255.1837	1311.9028
1331.5969	1333.9543	1336.4082
1339.1382	1364.1966	1370.6253
1372.0557	1381.4128	1395.1224
1438.7386	1473.0795	1489.5188
1492.3435	1494.5029	1498.6566
1518.6922	1522.6336	1527.3493
1541.8776	1543.1698	1543.8240
1548.9320	1585.5176	1630.5125
1640.7687	1665.9506	1670.6903
1672.0823	1685.4244	1687.9929
1689.9791	1701.2217	3028.5563
3103.3460	3140.8118	3145.3415
3186.4825	3188.6623	3191.1925
3194.8042	3206.4995	3206.6097
3209.0085	3214.5798	3215.9881
3221.4154	3221.4925	3225.6608
3230.4506	3231.8842	3233.3289
3233.9925	3238.9190	3243.1114
3244.4883	3248.9301	3252.5772
3292.0543	3455.0852	3584.7202

INT18

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.118542	-1.811834	0.733589
2	6	0	1.791629	-3.071097	1.032104
3	6	0	2.478228	-1.830416	-1.001767
4	1	0	1.532377	-3.906208	0.386038
5	1	0	1.804678	-3.267102	2.099036
6	1	0	2.261646	-2.767998	-1.517660
7	6	0	2.462814	-1.972474	0.505465
8	6	0	3.117675	-0.934380	1.219870
9	1	0	1.816059	-1.034929	-1.356068
10	6	0	3.776697	0.109091	0.516171
11	6	0	4.157016	-0.047952	-0.841488
12	6	0	4.159478	1.374249	1.056305
13	6	0	4.820432	0.888019	-1.612272
14	6	0	4.823093	2.323625	0.302643
15	1	0	3.903430	1.602249	2.084958
16	6	0	5.159912	2.110105	-1.044407
17	1	0	5.072409	0.664447	-2.647872
18	1	0	5.078507	3.271644	0.768118
19	1	0	5.671765	2.868777	-1.623680
20	6	0	2.935878	-0.898630	2.709285
21	15	0	-1.571069	-0.173886	0.093855
22	1	0	1.887876	-0.687501	2.978966
23	1	0	3.183549	-1.869516	3.157229
24	1	0	3.573946	-0.154625	3.191643
25	7	0	3.875144	-1.385189	-1.384639
26	1	0	4.011248	-1.394548	-2.398875
27	1	0	4.525908	-2.062150	-0.957521
28	6	0	-2.235611	0.969810	1.375006
29	6	0	-2.636800	0.406911	2.591264
30	6	0	-2.364153	2.350326	1.190880
31	6	0	-3.178032	1.203684	3.595839
32	1	0	-2.508749	-0.662065	2.747521
33	6	0	-2.897464	3.148882	2.200033
34	1	0	-2.040999	2.803631	0.257137

35	6	0	-3.308716	2.576890	3.401380
36	1	0	-3.487631	0.754447	4.534683
37	1	0	-2.989394	4.220228	2.047703
38	1	0	-3.722041	3.201566	4.187529
39	6	0	-0.650636	0.995055	-1.001599
40	6	0	-1.164498	1.540804	-2.180941
41	6	0	0.655688	1.326322	-0.612625
42	6	0	-0.385443	2.400664	-2.955934
43	1	0	-2.172399	1.291425	-2.500770
44	6	0	1.428217	2.193340	-1.379160
45	1	0	1.073454	0.882121	0.291503
46	6	0	0.906442	2.730123	-2.556562
47	1	0	-0.793357	2.813135	-3.874244
48	1	0	2.437249	2.439678	-1.059373
49	1	0	1.509876	3.399711	-3.162489
50	6	0	-3.073747	-0.537717	-0.908959
51	6	0	-3.059085	-1.702481	-1.683653
52	6	0	-4.200324	0.290371	-0.951484
53	6	0	-4.138279	-2.023317	-2.502560
54	1	0	-2.193721	-2.359823	-1.626525
55	6	0	-5.283924	-0.035254	-1.763655
56	1	0	-4.232895	1.191065	-0.344673
57	6	0	-5.253077	-1.189237	-2.543312
58	1	0	-4.114548	-2.929944	-3.099646
59	1	0	-6.155439	0.612162	-1.784976
60	1	0	-6.100313	-1.442813	-3.173325

Zero-point correction= 0.496599 (Hartree/Particle)
Thermal correction to Energy= 0.526416
Thermal correction to Enthalpy= 0.527360
Thermal correction to Gibbs Free Energy= 0.431418
Sum of electronic and zero-point Energies= -1643.586504
Sum of electronic and thermal Energies= -1643.556687
Sum of electronic and thermal Enthalpies= -1643.555743
Sum of electronic and thermal Free Energies= -1643.651684
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1644.084682
Frequencies

10.6971	15.0946	27.1291
29.4056	40.7953	46.8707
55.7768	57.6595	60.3880
65.2140	74.7439	91.2810
93.5493	100.0577	113.6710
142.3443	163.5707	185.3375
194.9535	213.6081	220.1565
221.4081	258.3009	264.5173
272.4988	278.8387	316.9348
332.5555	362.8264	401.1043
409.1183	411.6410	417.7487
434.4334	435.8360	441.6004
445.4262	463.4562	486.2543
513.0060	518.3167	523.3812
529.2157	568.6751	585.9428
628.9262	630.7935	632.0916
654.7221	688.5271	693.7383
701.7223	712.6479	715.5582
717.8801	718.2901	721.2014
726.4475	744.9260	759.4971
768.8421	776.7554	778.3682
794.0401	853.2483	858.1337
880.3814	887.0744	894.5047
920.1500	927.1623	948.7162
950.8939	954.6101	956.8869
992.5282	998.7642	1001.0534
1005.9300	1007.4742	1013.5161
1015.2996	1015.9142	1022.1205
1026.5311	1030.9796	1044.1421
1059.5380	1068.5999	1069.9207
1071.0599	1071.8921	1079.2312
1118.3935	1124.2662	1125.2158
1128.8680	1133.9307	1137.3218
1139.9895	1167.1469	1184.4060
1184.8847	1193.6946	1196.1144
1200.7374	1217.3597	1222.7735
1225.3087	1241.2452	1253.7998
1304.1099	1329.5955	1334.9003

1335.2986	1357.1840	1361.0896
1365.6572	1366.8974	1382.9581
1396.4918	1419.8422	1429.3289
1446.9461	1468.6055	1492.7273
1494.4270	1498.8124	1499.7252
1505.7406	1521.6995	1539.0615
1540.8179	1540.9911	1543.5528
1556.2161	1585.8637	1614.9161
1625.8865	1668.1466	1669.3576
1672.7080	1683.6149	1687.7407
1688.9223	1709.2226	3024.3031
3083.6806	3124.0374	3154.7984
3172.4912	3183.6636	3191.5084
3196.3808	3201.2374	3202.0451
3205.3408	3207.8151	3213.4770
3214.9917	3218.5252	3222.7311
3224.6410	3227.6524	3230.9436
3232.0138	3235.8770	3239.6355
3244.1923	3249.0480	3253.4329
3262.9326	3352.0786	3491.2331

TS14

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.753079	-0.697252	-0.953426
2	6	0	-3.491360	-3.383948	-0.776116
3	6	0	-3.072771	-1.964225	1.191318
4	1	0	-3.588873	-4.229491	-0.100859
5	1	0	-3.652626	-3.578936	-1.829439
6	1	0	-4.066899	-2.032981	1.649467
7	6	0	-3.175933	-2.162890	-0.314214
8	6	0	-2.957436	-0.944920	-1.128871
9	1	0	-2.421625	-2.718530	1.642947
10	6	0	-3.430220	0.288425	-0.481618
11	6	0	-3.213979	0.435473	0.908780
12	6	0	-4.040515	1.378939	-1.132262
13	6	0	-3.518726	1.602366	1.600825
14	6	0	-4.364047	2.540721	-0.445323
15	1	0	-4.255437	1.310971	-2.193827
16	6	0	-4.101360	2.666832	0.922362
17	1	0	-3.301102	1.671009	2.665005
18	1	0	-4.833826	3.361623	-0.979143
19	1	0	-4.362029	3.575609	1.454530
20	6	0	-3.254854	-1.097791	-2.606654
21	15	0	1.368798	-0.059634	-0.170887
22	1	0	-2.959432	-0.206411	-3.169288
23	1	0	-2.702725	-1.945231	-3.027005
24	1	0	-4.324660	-1.280412	-2.800012
25	7	0	-2.495362	-0.636913	1.490998
26	1	0	-1.303839	-0.702885	0.585854
27	1	0	-2.294097	-0.504770	2.479047
28	6	0	2.896624	-0.100318	-1.189861
29	6	0	4.037280	-0.829682	-0.847520
30	6	0	2.880727	0.617331	-2.393238
31	6	0	5.146144	-0.835742	-1.693618
32	1	0	4.064147	-1.395630	0.078874
33	6	0	3.990707	0.618679	-3.228958
34	1	0	1.993717	1.183730	-2.670118
35	6	0	5.127243	-0.111259	-2.880544
36	1	0	6.026647	-1.408589	-1.419215
37	1	0	3.968604	1.184734	-4.154980
38	1	0	5.992959	-0.116100	-3.535356
39	6	0	1.844106	-0.987258	1.342393
40	6	0	2.698421	-0.463145	2.318035
41	6	0	1.334894	-2.279893	1.503268
42	6	0	3.041223	-1.222732	3.432892
43	1	0	3.090995	0.544344	2.209995
44	6	0	1.682943	-3.041491	2.617000
45	1	0	0.655583	-2.679284	0.752602
46	6	0	2.535169	-2.512884	3.582789
47	1	0	3.702841	-0.806553	4.186400
48	1	0	1.283382	-4.044452	2.731353
49	1	0	2.802699	-3.102744	4.454103

50	6	0	1.325143	1.692149	0.387946
51	6	0	2.474544	2.484713	0.488700
52	6	0	0.085389	2.243131	0.731229
53	6	0	2.384470	3.797285	0.944344
54	1	0	3.440382	2.078142	0.197962
55	6	0	-0.001989	3.554622	1.189355
56	1	0	-0.820989	1.650934	0.622241
57	6	0	1.147639	4.332559	1.298858
58	1	0	3.281488	4.405064	1.014860
59	1	0	-0.975496	3.964521	1.442226
60	1	0	1.080543	5.358525	1.647918

Zero-point correction= 0.490890 (Hartree/Particle)
Thermal correction to Energy= 0.519844
Thermal correction to Enthalpy= 0.520788
Thermal correction to Gibbs Free Energy= 0.427146
Sum of electronic and zero-point Energies= -1643.590664
Sum of electronic and thermal Energies= -1643.561710
Sum of electronic and thermal Enthalpies= -1643.560766
Sum of electronic and thermal Free Energies= -1643.654408
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1644.071714
Frequencies

-307.6984	15.9393	18.5128
23.1664	24.1947	40.1005
47.3770	49.5904	56.4998
61.2713	67.9473	74.0721
89.5553	110.6101	127.8307
150.0459	165.6397	187.4107
197.4474	213.2484	228.8025
230.5583	251.0349	254.2313
264.4747	283.7383	307.6804
366.8237	378.4905	405.7880
410.0872	412.5776	432.9388
435.8378	444.4516	450.6604
455.5111	476.1002	488.9211
507.3276	521.6383	525.8204
534.7292	564.3385	583.9546
624.1909	629.5083	630.8078
631.6170	695.6032	704.8459
713.8589	715.7258	717.9542
720.9063	722.2654	723.7805
752.2012	767.6971	768.6721
772.2829	778.7368	805.4765
817.9532	830.2531	864.3429
871.9648	876.1730	882.0595
885.6127	895.0532	936.0396
950.7782	952.1891	963.0960
972.2478	990.4649	992.1071
998.6705	1002.0949	1007.7687
1013.5926	1015.4628	1016.4912
1025.1270	1028.1389	1031.4464
1042.6202	1066.4332	1070.3200
1071.5991	1073.1373	1073.7692
1079.0230	1095.1377	1124.9778
1129.1100	1129.9936	1135.7898
1138.4000	1146.0223	1147.7407
1171.2371	1188.9287	1192.4601
1196.5588	1197.8097	1220.8012
1229.4174	1232.1386	1252.8150
1263.3332	1282.3283	1297.6073
1322.5450	1330.2760	1337.0641
1340.0250	1347.2166	1364.3455
1367.6467	1373.9800	1376.7228
1398.6509	1428.5563	1452.3611
1473.2336	1493.6655	1498.3944
1500.0262	1505.4991	1524.2632
1533.8666	1540.7481	1543.2981
1546.2600	1550.0956	1552.0311
1654.1771	1668.5564	1673.3182
1674.7192	1687.6571	1688.8762
1692.4411	1701.0037	1711.8959
3020.1909	3085.0337	3106.4646
3140.7085	3145.1600	3183.0249
3187.5112	3202.6051	3206.0592
3206.2943	3207.2234	3214.2961

3215.2329	3216.9453	3222.1393
3222.6495	3226.8522	3227.2586
3228.7375	3232.5227	3234.2271
3236.4275	3238.6703	3248.6840
3250.2305	3276.4714	3558.9899

INT19

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.750744	0.106310	0.468876
2	6	0	-1.226524	2.363158	0.799421
3	6	0	-2.863701	1.898020	-1.035140
4	1	0	-0.815931	3.140765	0.162913
5	1	0	-0.926377	2.396375	1.842490
6	1	0	-2.631134	2.920396	-1.342812
7	6	0	-2.360387	1.669801	0.381336
8	6	0	-2.880127	0.525672	1.064725
9	1	0	-2.353102	1.206363	-1.729815
10	6	0	-4.029403	-0.172829	0.428462
11	6	0	-4.738740	0.461496	-0.612067
12	6	0	-4.496263	-1.409426	0.882629
13	6	0	-5.879750	-0.136002	-1.153297
14	6	0	-5.627776	-2.008159	0.340662
15	1	0	-3.944900	-1.919761	1.666965
16	6	0	-6.325789	-1.362456	-0.677925
17	1	0	-6.416946	0.373851	-1.949790
18	1	0	-5.961607	-2.972530	0.709165
19	1	0	-7.212330	-1.816220	-1.110164
20	6	0	-2.831417	0.439666	2.582371
21	15	0	1.500803	-0.129857	-0.028481
22	1	0	-2.727652	-0.591800	2.925003
23	1	0	-1.997148	1.004719	3.004037
24	1	0	-3.762787	0.839426	3.005260
25	7	0	-4.304151	1.717903	-1.048622
26	1	0	-0.873538	-1.484563	0.476053
27	1	0	-4.731036	1.997297	-1.923855
28	6	0	1.855059	-1.396205	-1.301278
29	6	0	0.834709	-1.743222	-2.189856
30	6	0	3.115914	-1.987885	-1.431924
31	6	0	1.076656	-2.659449	-3.210465
32	1	0	-0.153456	-1.308281	-2.060762
33	6	0	3.353073	-2.908182	-2.448600
34	1	0	3.910047	-1.732762	-0.734557
35	6	0	2.334707	-3.241448	-3.339924
36	1	0	0.278015	-2.926840	-3.895176
37	1	0	4.331629	-3.368727	-2.542910
38	1	0	2.520378	-3.962954	-4.129688
39	6	0	2.537259	-0.620992	1.401032
40	6	0	3.858185	-0.186895	1.554613
41	6	0	1.977868	-1.476405	2.357012
42	6	0	4.611108	-0.608871	2.647279
43	1	0	4.296676	0.488119	0.824424
44	6	0	2.736131	-1.899316	3.444929
45	1	0	0.946243	-1.800725	2.242368
46	6	0	4.051627	-1.465253	3.592253
47	1	0	5.634086	-0.263756	2.761566
48	1	0	2.295928	-2.562889	4.182680
49	1	0	4.638765	-1.788695	4.446262
50	6	0	2.361969	1.366600	-0.657895
51	6	0	2.291676	2.526234	0.125431
52	6	0	3.053014	1.404803	-1.870196
53	6	0	2.914681	3.696568	-0.288824
54	1	0	1.739970	2.505620	1.063005
55	6	0	3.665208	2.585757	-2.291474
56	1	0	3.113160	0.516785	-2.491954
57	6	0	3.600970	3.729179	-1.503240
58	1	0	2.859958	4.586752	0.330188
59	1	0	4.194947	2.606487	-3.238938
60	1	0	4.079741	4.646068	-1.832968

Zero-point correction= 0.492280 (Hartree/Particle)
Thermal correction to Energy= 0.521771
Thermal correction to Enthalpy= 0.522716

Thermal correction to Gibbs Free Energy= 0.428601
Sum of electronic and zero-point Energies= -1643.616393
Sum of electronic and thermal Energies= -1643.586902
Sum of electronic and thermal Enthalpies= -1643.585958
Sum of electronic and thermal Free Energies= -1643.680072
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1644.094331
Frequencies

17.7594	19.8794	23.3738
31.9986	37.7975	46.5727
51.7180	58.5696	61.7327
68.7191	71.7035	101.4203
112.2015	137.5080	155.9481
179.4312	186.0374	191.7638
204.5792	215.3184	228.2513
251.2280	256.4701	263.0785
265.0317	280.1177	306.1305
350.6912	367.7567	407.0097
410.1862	413.2810	428.1186
441.2188	446.0058	457.5631
466.3336	499.1403	501.6652
509.8686	525.0377	532.8078
552.0200	558.5633	567.6727
585.4295	629.1302	629.7924
631.0516	650.1611	660.1753
702.9086	705.1062	712.1949
714.6161	715.6059	721.6353
727.1378	747.4818	763.9763
767.5085	769.1502	770.2711
773.8506	776.4519	849.0845
865.1712	876.3585	879.1233
880.3728	882.3296	888.9715
946.9425	952.0376	957.6260
959.7282	978.8684	985.6572
999.3211	1004.8313	1006.3156
1015.3533	1015.5266	1016.3284
1021.7678	1027.7923	1028.2079
1030.3560	1065.5656	1071.0633
1071.5910	1072.5555	1074.8473
1092.9560	1124.8817	1126.8463
1128.3032	1132.1477	1136.7200
1146.1092	1147.6735	1150.7548
1184.4225	1192.9429	1193.4900
1195.5238	1197.6901	1222.9967
1224.7881	1225.6279	1261.3460
1301.3641	1304.2946	1329.9504
1333.9952	1337.1922	1341.2394
1349.6475	1366.2264	1369.1768
1369.8343	1370.3003	1409.5923
1441.9071	1470.6585	1489.3414
1496.2715	1498.4776	1500.1814
1516.6438	1518.7222	1531.5523
1544.5230	1545.6045	1546.1449
1557.1107	1569.7325	1585.9286
1672.2701	1674.2517	1675.3117
1679.0016	1688.2161	1689.0186
1690.2464	1708.5412	1869.1333
2998.2538	3067.5694	3145.8158
3145.8417	3169.3980	3185.9385
3198.2868	3204.3299	3205.8982
3206.4978	3210.4163	3213.0547
3213.1636	3219.3930	3224.1574
3226.5549	3227.4678	3227.7429
3231.4598	3232.4591	3237.5017
3240.8035	3242.7044	3243.2875
3243.3483	3266.9887	3594.1819

TS15

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.686859	0.566688	-0.245652
2	6	0	1.772795	2.841505	-0.713822
3	6	0	3.187714	1.966227	1.142071
4	1	0	1.627743	3.743862	-0.129555

5	1	0	1.394273	2.852098	-1.730366
6	1	0	3.084131	2.991224	1.504927
7	6	0	2.579397	1.841837	-0.239247
8	6	0	2.819531	0.554975	-0.913709
9	1	0	2.661144	1.292822	1.842534
10	6	0	3.964462	-0.241591	-0.349223
11	6	0	4.854211	0.340930	0.573463
12	6	0	4.237284	-1.537724	-0.794774
13	6	0	5.992041	-0.362390	0.989244
14	6	0	5.361853	-2.238476	-0.381317
15	1	0	3.531685	-2.010458	-1.473830
16	6	0	6.249738	-1.637885	0.510895
17	1	0	6.673094	0.107623	1.695016
18	1	0	5.541170	-3.244880	-0.744555
19	1	0	7.135242	-2.169230	0.846146
20	6	0	2.797120	0.585077	-2.438676
21	15	0	-1.540500	-0.030735	0.065387
22	1	0	2.851652	-0.423026	-2.853413
23	1	0	1.885509	1.045719	-2.826919
24	1	0	3.660151	1.154681	-2.806992
25	7	0	4.601458	1.632767	1.044955
26	1	0	1.583840	-0.722711	-0.627092
27	1	0	5.122937	1.851340	1.885574
28	6	0	-1.804574	-1.341222	1.322462
29	6	0	-0.893929	-1.431204	2.379076
30	6	0	-2.876863	-2.237229	1.264171
31	6	0	-1.064004	-2.389344	3.375072
32	1	0	-0.041522	-0.755589	2.404709
33	6	0	-3.043135	-3.197884	2.257963
34	1	0	-3.578838	-2.188339	0.435494
35	6	0	-2.139040	-3.272560	3.315323
36	1	0	-0.350115	-2.453686	4.190298
37	1	0	-3.875855	-3.892335	2.203225
38	1	0	-2.267456	-4.025440	4.086877
39	6	0	-2.322708	-0.747075	-1.436663
40	6	0	-3.660694	-0.528886	-1.778522
41	6	0	-1.534451	-1.569968	-2.249869
42	6	0	-4.202748	-1.131325	-2.912048
43	1	0	-4.281605	0.114572	-1.161276
44	6	0	-2.080811	-2.175992	-3.376789
45	1	0	-0.488726	-1.725083	-1.993875
46	6	0	-3.415773	-1.956878	-3.710387
47	1	0	-5.241907	-0.952214	-3.170861
48	1	0	-1.460967	-2.813517	-3.999665
49	1	0	-3.840012	-2.423431	-4.594166
50	6	0	-2.742142	1.276093	0.549610
51	6	0	-2.586168	2.534787	-0.042450
52	6	0	-3.795855	1.070588	1.444244
53	6	0	-3.481781	3.562040	0.235117
54	1	0	-1.748309	2.707053	-0.715527
55	6	0	-4.684455	2.104968	1.732037
56	1	0	-3.922251	0.103549	1.922097
57	6	0	-4.533162	3.348224	1.124492
58	1	0	-3.353004	4.532721	-0.233754
59	1	0	-5.495544	1.937078	2.434035
60	1	0	-5.227779	4.151879	1.348946

Zero-point correction= 0.490534 (Hartree/Particle)
Thermal correction to Energy= 0.519983
Thermal correction to Enthalpy= 0.520927
Thermal correction to Gibbs Free Energy= 0.425562
Sum of electronic and zero-point Energies= -1643.602098
Sum of electronic and thermal Energies= -1643.572649
Sum of electronic and thermal Enthalpies= -1643.571704
Sum of electronic and thermal Free Energies= -1643.667070
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1644.080844
Frequencies

-736.2470	7.8521	18.0992
24.5997	25.3993	32.2378
45.8781	49.7133	54.4510
64.7251	69.9251	73.7156
96.5068	111.9930	128.8651
153.3332	168.6831	178.6100
194.4274	205.2582	216.1057
226.3953	228.6876	259.2050

266.9132	274.9529	275.5090
307.5675	347.9339	378.6070
407.9953	410.6419	413.6898
421.9335	438.9520	446.2541
451.0928	471.3424	494.0937
513.2083	516.3212	521.7596
527.1936	553.7575	560.0993
582.0481	629.7636	630.6044
632.4900	638.4153	654.6324
702.7481	704.2834	712.6880
714.8632	716.6044	717.2726
722.6737	725.2841	754.3090
767.9803	771.9417	772.5312
773.7308	777.1545	846.3929
868.2881	873.5604	878.0761
881.9901	886.3670	890.2624
952.2390	956.1595	957.5356
961.6558	981.2955	990.4938
997.1754	1004.9951	1009.1611
1014.4502	1015.3227	1016.7239
1019.9388	1025.2375	1026.0582
1028.1688	1071.7760	1072.7658
1074.3961	1076.5637	1078.2532
1087.5026	1121.7525	1125.2148
1127.1872	1129.9821	1137.9607
1140.1291	1144.5584	1152.0690
1176.3977	1183.2750	1193.9856
1195.2366	1198.7732	1225.7874
1226.7304	1228.8735	1256.6691
1292.8163	1296.8469	1312.9540
1333.9548	1337.5978	1342.1479
1349.7684	1370.0940	1370.4964
1370.9957	1372.6117	1383.9377
1431.5169	1459.6626	1482.5562
1498.2425	1499.3904	1502.9737
1512.2974	1515.5248	1533.5342
1545.4656	1547.7203	1549.2030
1551.1155	1563.7730	1639.3067
1670.3379	1672.9091	1677.1082
1678.2012	1690.4655	1691.0076
1692.0267	1705.5994	1806.7238
3001.9058	3071.1221	3144.4659
3151.1087	3175.7675	3191.2072
3193.4324	3198.2575	3199.6333
3204.6290	3205.8558	3208.4854
3210.8910	3212.3491	3220.0191
3221.9834	3224.9914	3225.8350
3227.1714	3235.0200	3240.5735
3242.6007	3244.0099	3246.9682
3248.5153	3274.3746	3603.4953

MCP 4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.405621	-1.160698	-0.956671
2	6	0	3.416045	-0.155643	-0.394713
3	1	0	2.336020	-2.139351	-0.487186
4	1	0	2.238831	-1.173164	-2.031008
5	1	0	3.933504	0.496030	-1.094845
6	6	0	1.971085	0.013395	-0.205220
7	6	0	0.977716	0.776758	0.240639
8	1	0	4.025053	-0.476494	0.447580
9	6	0	1.270541	2.086711	0.932057
10	6	0	-0.448517	0.393186	0.052863
11	6	0	-1.365761	1.346662	-0.404114
12	6	0	-0.921859	-0.903412	0.352241
13	6	0	-2.707324	1.047706	-0.602393
14	1	0	-1.006463	2.348088	-0.625043
15	6	0	-2.277658	-1.198552	0.151887
16	6	0	-3.159600	-0.239534	-0.321831
17	1	0	-3.389160	1.806570	-0.971381
18	1	0	-2.631179	-2.202054	0.376612
19	1	0	-4.204303	-0.497930	-0.467494

20	7	0	-0.074361	-1.908207	0.826009
21	1	0	0.772051	-1.551499	1.253773
22	1	0	-0.543664	-2.577394	1.423603
23	1	0	2.345510	2.203407	1.088766
24	1	0	0.923061	2.938899	0.337005
25	1	0	0.759529	2.142875	1.899081

Zero-point correction= 0.214610 (Hartree/Particle)
Thermal correction to Energy= 0.225862
Thermal correction to Enthalpy= 0.226806
Thermal correction to Gibbs Free Energy= 0.177885
Sum of electronic and zero-point Energies= -481.258908
Sum of electronic and thermal Energies= -481.247656
Sum of electronic and thermal Enthalpies= -481.246712
Sum of electronic and thermal Free Energies= -481.295633
M06-2x/6-311++G(d,p) // M06-2x /6-31G(d) energy= -481.460555
Frequencies

52.1253	93.7528	132.8191
171.7547	191.0068	226.2012
249.4206	279.0808	330.3861
360.7645	392.1640	437.9227
466.0988	520.3999	564.6996
588.6331	598.2871	672.9683
687.6985	758.4854	763.8735
777.2620	824.8477	868.5701
876.1635	886.2196	954.0950
989.9287	998.6717	1037.4110
1060.6494	1064.7799	1073.3678
1092.5788	1103.3455	1105.2771
1128.4837	1172.4408	1183.3439
1190.0744	1216.2277	1304.7871
1332.7042	1346.4765	1369.3435
1432.9541	1479.3450	1501.3813
1511.3276	1518.1013	1526.4663
1562.2506	1665.1663	1685.7155
1708.6639	1883.5748	3074.4723
3136.3320	3147.5308	3152.5135
3172.6013	3194.4387	3208.7678
3216.3744	3222.7597	3234.5347
3238.8123	3564.1400	3669.2903

Product 5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.872931	0.034183	-1.059677
2	6	0	-1.524287	-1.735198	0.034588
3	1	0	-3.383173	-0.724883	-1.646663
4	1	0	-3.191940	1.060045	-1.208304
5	1	0	-2.212351	-2.180756	0.764367
6	6	0	-1.912347	-0.291145	-0.198463
7	6	0	-1.099387	0.702345	0.609196
8	1	0	-1.636687	-2.292005	-0.906332
9	1	0	-1.202137	0.400466	1.665428
10	6	0	0.353927	0.466264	0.235746
11	6	0	0.773286	-0.876721	0.224471
12	6	0	1.270380	1.462390	-0.077219
13	6	0	2.103179	-1.190659	-0.060723
14	6	0	2.599965	1.151118	-0.365246
15	1	0	0.952145	2.500726	-0.085332
16	6	0	3.012632	-0.176527	-0.345247
17	1	0	2.420085	-2.231018	-0.062762
18	1	0	3.304938	1.942442	-0.598001
19	1	0	4.045362	-0.430616	-0.564900
20	6	0	-1.556427	2.146442	0.469238
21	1	0	-1.436032	2.499753	-0.560279
22	1	0	-2.610335	2.242623	0.744616
23	1	0	-0.974450	2.800069	1.124570
24	7	0	-0.165862	-1.849802	0.573758
25	1	0	0.197666	-2.793182	0.517294

Zero-point correction= 0.217689 (Hartree/Particle)
Thermal correction to Energy= 0.227715
Thermal correction to Enthalpy= 0.228659

Thermal correction to Gibbs Free Energy= 0.182463
Sum of electronic and zero-point Energies= -481.296343
Sum of electronic and thermal Energies= -481.286317
Sum of electronic and thermal Enthalpies= -481.285373
Sum of electronic and thermal Free Energies= -481.331570
M06-2x/6-311++G(d,p) // M06-2x /6-31G(d) energy= -481.4917335
Frequencies

68.8189	88.1823	154.3451
224.6327	290.3833	311.7948
326.1880	362.4523	421.3420
456.8887	469.6329	494.1521
519.4879	557.9600	584.8599
625.0319	709.5806	726.8486
756.0888	775.4448	796.0416
829.3747	868.8028	881.4950
931.3113	953.4533	970.4543
990.9053	1014.8737	1034.2851
1082.5085	1096.3180	1108.4809
1119.0282	1166.7301	1189.2760
1215.8124	1254.4144	1271.0929
1302.9496	1318.8105	1321.8283
1348.3013	1378.5166	1390.7470
1432.3413	1475.8893	1491.4851
1528.2227	1530.1437	1536.7558
1554.8172	1568.2740	1684.4770
1707.1439	1769.0207	3020.5597
3049.7704	3080.1735	3089.2393
3155.6805	3167.3094	3183.6205
3205.0819	3215.6524	3232.2796
3239.9032	3266.9755	3609.7250

TS16

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.585888	-0.332546	-1.311673
2	6	0	0.987959	-2.463380	-0.833706
3	6	0	2.410982	-1.134570	-2.102004
4	1	0	0.688552	-3.020277	-1.718480
5	1	0	0.543575	-2.790140	0.103604
6	1	0	3.204681	-0.407107	-2.243232
7	6	0	2.245315	-1.778662	-0.839643
8	6	0	2.922738	-1.311912	0.371266
9	1	0	2.025513	-1.625033	-2.994284
10	1	0	2.093682	-0.165695	0.585376
11	6	0	4.016900	-0.325891	0.121894
12	6	0	3.502850	0.994168	-0.068321
13	6	0	5.391358	-0.529424	0.138847
14	6	0	4.389719	2.057527	-0.265833
15	6	0	6.269829	0.538415	-0.054586
16	1	0	5.781563	-1.531505	0.304265
17	6	0	5.762555	1.821175	-0.259044
18	1	0	4.004492	3.063586	-0.411909
19	1	0	7.342295	0.370465	-0.050045
20	1	0	6.446262	2.651833	-0.412426
21	6	0	3.114747	-2.317095	1.492423
22	15	0	-1.463698	0.096741	-0.140931
23	6	0	-3.057692	-0.084889	-1.020878
24	6	0	-4.179351	0.699016	-0.733684
25	6	0	-3.145243	-1.075960	-2.004833
26	6	0	-5.373701	0.486926	-1.417214
27	1	0	-4.117395	1.479690	0.019332
28	6	0	-4.342377	-1.290469	-2.681371
29	1	0	-2.267598	-1.674206	-2.240789
30	6	0	-5.457219	-0.508192	-2.388185
31	1	0	-6.239509	1.101520	-1.191241
32	1	0	-4.402949	-2.061610	-3.442942
33	1	0	-6.389496	-0.670130	-2.920259
34	6	0	-1.517792	1.785250	0.568451
35	6	0	-2.147851	2.073184	1.783457
36	6	0	-0.892450	2.815522	-0.142118
37	6	0	-2.162313	3.376628	2.272592
38	1	0	-2.619245	1.274505	2.350725
39	6	0	-0.909835	4.118496	0.348120

40	1	0	-0.371863	2.589838	-1.070982
41	6	0	-1.545435	4.399330	1.555315
42	1	0	-2.649996	3.591917	3.218220
43	1	0	-0.418069	4.911116	-0.206920
44	1	0	-1.552010	5.413683	1.941913
45	6	0	-1.641726	-0.974506	1.336744
46	6	0	-0.495519	-1.184311	2.114794
47	6	0	-2.846423	-1.573420	1.710778
48	6	0	-0.558950	-1.976316	3.255981
49	1	0	0.452482	-0.734545	1.820287
50	6	0	-2.903733	-2.371747	2.853207
51	1	0	-3.740266	-1.421556	1.111718
52	6	0	-1.764124	-2.572640	3.625608
53	1	0	0.336516	-2.134043	3.849415
54	1	0	-3.842700	-2.837493	3.136424
55	1	0	-1.811119	-3.196812	4.512528
56	1	0	3.378225	-1.802900	2.422729
57	1	0	2.197907	-2.889139	1.680948
58	1	0	3.912006	-3.046527	1.287778
59	7	0	2.116723	1.047542	0.024660
60	1	0	1.762713	1.920255	0.408234

Zero-point correction= 0.487888 (Hartree/Particle)
Thermal correction to Energy= 0.517564
Thermal correction to Enthalpy= 0.518508
Thermal correction to Gibbs Free Energy= 0.424050
Sum of electronic and zero-point Energies= -1643.544692
Sum of electronic and thermal Energies= -1643.515016
Sum of electronic and thermal Enthalpies= -1643.514072
Sum of electronic and thermal Free Energies= -1643.608531
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1644.023917
Frequencies

-1598.1247	16.2253	22.2273
25.2493	28.2623	43.4332
49.7488	54.1536	57.6522
60.2095	70.6663	76.2966
87.5945	112.3255	127.4372
146.4764	159.3469	171.7566
189.7942	193.7142	212.7347
220.7567	228.5462	255.2370
261.1564	271.6342	273.6057
298.5236	341.9776	355.1308
367.7218	407.1231	408.5702
412.3022	439.8872	442.1786
449.6110	475.3081	494.3077
507.9190	512.5389	517.4582
526.4496	547.5012	580.5737
597.2296	616.0374	626.1930
626.6117	629.8655	680.5176
693.6889	701.3535	713.7742
715.0660	717.6597	719.1027
721.2780	730.9040	758.3252
769.4414	770.9825	772.7357
773.4574	775.6239	792.7449
856.5588	877.0557	878.5267
882.2446	885.2343	888.6971
947.2338	949.4435	951.2670
954.5962	958.1267	961.5796
982.1180	997.8154	1001.1364
1002.1097	1007.2247	1014.0103
1015.2979	1015.8773	1027.6169
1028.1634	1030.8733	1037.3269
1061.9537	1069.2861	1070.1030
1071.3462	1073.9767	1081.5625
1122.7087	1125.3034	1126.3996
1128.0859	1136.6514	1141.0275
1142.6132	1176.4861	1180.1864
1184.7838	1186.1450	1188.7163
1192.2301	1221.9863	1223.1082
1225.5386	1278.7598	1307.5940
1325.8064	1331.4834	1333.4686
1338.5886	1348.3996	1365.7955
1366.9125	1369.1859	1369.7579
1413.4931	1439.2786	1484.5409
1492.6316	1494.5850	1497.8070

1513.6745	1517.5388	1521.4670
1533.8965	1535.5614	1542.1104
1542.9843	1545.0091	1552.1570
1650.2114	1669.6536	1671.4514
1672.5137	1682.9263	1687.6750
1689.8559	1700.3532	1839.7287
3037.1220	3098.3053	3130.8613
3158.9142	3175.5421	3190.7901
3192.9911	3197.3466	3201.9216
3208.6930	3208.9475	3209.0278
3212.4327	3216.5738	3218.9234
3221.4247	3222.7988	3223.1882
3223.6722	3232.4051	3233.9892
3242.0918	3242.4497	3244.1446
3264.3074	3269.6861	3568.5728

INT20

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.652007	-0.533647	-1.177341
2	6	0	1.013914	-2.747878	-0.934866
3	6	0	2.465440	-1.280070	-2.135963
4	1	0	0.728997	-3.280921	-1.837914
5	1	0	0.647861	-3.162444	0.001258
6	1	0	3.271074	-0.556386	-2.189560
7	6	0	2.198961	-1.962108	-0.937591
8	6	0	2.884277	-1.513459	0.360986
9	1	0	2.079845	-1.671365	-3.075224
10	1	0	2.065433	-1.316763	1.071940
11	6	0	3.683156	-0.218938	0.203953
12	6	0	3.055045	1.021596	-0.168126
13	6	0	5.062007	-0.230505	0.424861
14	6	0	3.900028	2.153228	-0.292110
15	6	0	5.862550	0.901683	0.311746
16	1	0	5.540263	-1.164323	0.701948
17	6	0	5.260874	2.104298	-0.049583
18	1	0	3.438735	3.094827	-0.583351
19	1	0	6.929144	0.840992	0.499205
20	1	0	5.854714	3.009114	-0.150161
21	6	0	3.681184	-2.698839	0.917895
22	15	0	-1.393156	0.050378	-0.104043
23	6	0	-2.964554	-0.743857	-0.605539
24	6	0	-4.208349	-0.123521	-0.446715
25	6	0	-2.904139	-2.038659	-1.130485
26	6	0	-5.374523	-0.795526	-0.801591
27	1	0	-4.264829	0.886135	-0.049227
28	6	0	-4.072753	-2.711048	-1.477840
29	1	0	-1.934088	-2.511251	-1.268646
30	6	0	-5.308173	-2.089555	-1.314260
31	1	0	-6.336568	-0.307748	-0.679053
32	1	0	-4.016840	-3.716230	-1.883867
33	1	0	-6.219166	-2.610893	-1.591528
34	6	0	-1.737695	1.845074	-0.184261
35	6	0	-2.315416	2.547611	0.877477
36	6	0	-1.409804	2.524995	-1.361590
37	6	0	-2.575771	3.910095	0.754935
38	1	0	-2.551996	2.028884	1.803032
39	6	0	-1.672994	3.886367	-1.482656
40	1	0	-0.932725	1.985665	-2.177743
41	6	0	-2.257286	4.579006	-0.424543
42	1	0	-3.022704	4.450024	1.583973
43	1	0	-1.413547	4.408062	-2.398462
44	1	0	-2.456228	5.642311	-0.516111
45	6	0	-1.272801	-0.280746	1.692577
46	6	0	-0.119181	0.175336	2.347109
47	6	0	-2.256035	-0.965163	2.410000
48	6	0	0.036300	-0.052492	3.710357
49	1	0	0.648139	0.698099	1.774165
50	6	0	-2.087927	-1.194068	3.775282
51	1	0	-3.150601	-1.323454	1.908284
52	6	0	-0.945286	-0.738497	4.425465
53	1	0	0.930043	0.302423	4.214448
54	1	0	-2.853785	-1.729636	4.327884

55	1	0	-0.816949	-0.919109	5.488403
56	1	0	4.137475	-2.448546	1.879367
57	1	0	3.013887	-3.553157	1.065046
58	1	0	4.472114	-3.007490	0.226799
59	7	0	1.702117	1.148550	-0.366785
60	1	0	1.476216	2.099234	-0.648621

Zero-point correction= 0.493985 (Hartree/Particle)
Thermal correction to Energy= 0.523435
Thermal correction to Enthalpy= 0.524379
Thermal correction to Gibbs Free Energy= 0.431037
Sum of electronic and zero-point Energies= -1643.601164
Sum of electronic and thermal Energies= -1643.571714
Sum of electronic and thermal Enthalpies= -1643.570770
Sum of electronic and thermal Free Energies= -1643.664113
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1644.076665
Frequencies

16.3718	21.1389	26.9664
37.5680	44.7073	49.0685
56.3901	57.7791	62.4559
76.8898	80.6550	96.2703
108.2628	125.6379	139.0607
167.1125	192.1917	213.8242
220.2830	224.3111	243.2265
255.1635	260.0669	276.6896
280.6823	296.3088	311.9588
334.7564	352.3481	358.5683
410.4440	411.5948	414.7813
415.3830	438.7205	441.4861
454.2202	470.4412	493.6432
511.4943	518.8018	529.4593
542.7863	571.1841	590.8004
626.3718	627.9217	629.6767
632.7021	664.9708	687.6479
702.0065	715.0107	717.2649
719.3808	720.9338	722.4103
724.3367	743.2131	763.9782
770.2131	774.9045	778.3966
781.2697	817.1090	821.8246
860.3359	873.4119	882.6377
889.2816	894.1774	899.0434
944.0841	957.6536	964.0899
967.1019	974.9876	975.6963
998.0385	1004.2440	1010.4794
1012.9658	1015.5316	1015.9825
1019.9107	1027.9324	1032.2996
1033.3734	1050.2449	1054.2794
1070.2292	1071.2432	1072.0663
1079.6594	1088.9053	1112.1543
1122.6130	1123.8862	1125.1803
1138.0532	1141.3872	1145.0078
1152.7331	1188.3905	1189.6352
1190.9298	1191.6257	1217.8692
1224.0893	1224.8279	1226.3797
1230.1552	1289.8159	1320.8475
1332.8148	1335.9094	1340.0789
1348.2272	1360.4497	1369.9533
1370.8710	1373.1813	1376.8742
1385.0729	1413.2717	1426.1579
1493.7095	1496.4412	1497.2081
1497.5716	1525.4285	1530.8669
1539.1228	1543.4526	1545.0588
1546.3783	1547.2793	1562.6400
1641.0902	1669.2073	1671.0326
1673.4792	1687.1604	1689.2124
1690.3435	1693.7220	3036.2279
3075.5117	3152.4180	3162.8273
3176.5613	3179.4904	3182.4977
3186.5451	3202.5183	3205.7465
3208.1790	3212.0920	3212.2118
3216.7766	3217.7855	3217.8427
3218.2722	3223.0741	3227.2959
3228.6939	3232.3668	3232.7888
3237.4880	3238.3038	3242.3188
3266.4139	3287.6315	3542.3359

INT21

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.800559	0.967537	2.607404
2	46	0	0.604288	1.036748	0.973815
3	15	0	-1.341764	0.308430	0.130585
4	6	0	-2.119996	-1.110584	1.011376
5	6	0	-1.265563	-1.978119	1.701644
6	6	0	-3.491371	-1.382064	0.993584
7	6	0	-1.767266	-3.108430	2.340767
8	1	0	-0.200642	-1.752403	1.729897
9	6	0	-3.995240	-2.505011	1.646394
10	1	0	-4.170425	-0.712669	0.472502
11	6	0	-3.135079	-3.372067	2.315736
12	1	0	-1.092020	-3.776106	2.867825
13	1	0	-5.062884	-2.702719	1.631455
14	1	0	-3.530890	-4.247405	2.821918
15	6	0	-1.141560	-0.375335	-1.570471
16	6	0	-1.560017	-1.650104	-1.961110
17	6	0	-0.494303	0.442078	-2.508008
18	6	0	-1.327931	-2.100917	-3.261250
19	1	0	-2.060743	-2.300697	-1.249151
20	6	0	-0.285246	0.001449	-3.809406
21	1	0	-0.140515	1.423584	-2.199469
22	6	0	-0.696213	-1.277628	-4.187478
23	1	0	-1.644452	-3.099316	-3.547748
24	1	0	0.213982	0.647866	-4.524853
25	1	0	-0.518209	-1.631048	-5.198545
26	6	0	-2.764835	1.453919	-0.101702
27	6	0	-2.925547	2.476566	0.838551
28	6	0	-3.682698	1.344845	-1.151782
29	6	0	-3.995136	3.362192	0.744875
30	1	0	-2.193244	2.577423	1.636568
31	6	0	-4.747854	2.236975	-1.250425
32	1	0	-3.560261	0.564041	-1.898378
33	6	0	-4.907393	3.243938	-0.301037
34	1	0	-4.110468	4.151045	1.481892
35	1	0	-5.453085	2.146756	-2.071210
36	1	0	-5.736628	3.940268	-0.381401
37	6	0	2.046153	-2.230137	-1.589995
38	6	0	1.466908	-3.095233	-0.467227
39	1	0	1.366523	-1.555394	-2.107220
40	1	0	2.811857	-2.675837	-2.221053
41	1	0	1.856672	-4.104799	-0.353546
42	6	0	2.352220	-1.961614	-0.185723
43	6	0	2.952459	-1.204332	0.726011
44	1	0	0.403482	-2.993307	-0.259113
45	6	0	2.778933	-1.501368	2.199288
46	6	0	3.822953	-0.079779	0.279972
47	6	0	4.773759	-0.306537	-0.719843
48	6	0	3.708007	1.226156	0.791627
49	6	0	5.576954	0.712845	-1.219777
50	1	0	4.869989	-1.315643	-1.108565
51	6	0	4.515979	2.248368	0.295376
52	6	0	5.442825	1.999902	-0.710583
53	1	0	6.301910	0.502270	-1.999255
54	1	0	4.404912	3.252788	0.697465
55	1	0	6.060440	2.809932	-1.085419
56	7	0	2.708851	1.536639	1.769374
57	1	0	2.768061	2.512562	2.047240
58	1	0	2.526974	-2.556387	2.339498
59	1	0	3.695769	-1.291377	2.762848
60	1	0	1.957192	-0.914138	2.632232

Zero-point correction= 0.494690 (Hartree/Particle)
Thermal correction to Energy= 0.525110
Thermal correction to Enthalpy= 0.526054
Thermal correction to Gibbs Free Energy= 0.430118
Sum of electronic and zero-point Energies= -1643.615401
Sum of electronic and thermal Energies= -1643.584980
Sum of electronic and thermal Enthalpies= -1643.584036
Sum of electronic and thermal Free Energies= -1643.679973

M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1644.095498
Frequencies --

17.9887	20.4329	25.4448
40.5555	44.7089	50.3746
57.0331	60.1394	66.3393
68.4762	75.0711	88.0331
92.2603	97.2143	114.4079
140.8643	156.4473	179.4731
194.1513	205.9411	216.3731
226.1291	229.3652	236.9283
258.6858	262.9033	277.9579
288.7026	306.1251	316.4310
366.8508	406.7547	412.4099
417.2647	421.4580	437.2889
444.1598	447.5844	486.5825
507.1601	512.8427	518.0765
526.4744	528.9434	549.1974
595.1397	598.5741	628.7168
629.7249	633.7318	677.8227
703.0829	713.0681	714.2611
716.1359	718.2355	719.1880
756.3292	760.3370	764.5230
767.7078	770.6700	777.2775
814.5743	864.3258	875.5708
877.6275	880.3618	882.9045
888.1815	948.1682	952.5026
955.8641	960.8481	978.0082
997.9670	1001.5825	1002.6037
1005.1878	1009.4503	1015.3326
1015.6934	1016.2862	1018.2996
1020.7654	1021.9403	1036.6483
1057.5869	1062.2126	1070.9921
1071.3250	1073.8828	1080.2871
1095.2487	1099.4018	1110.4185
1119.6216	1121.5117	1130.4677
1133.4327	1136.8751	1139.8468
1143.7896	1178.4200	1179.8324
1185.4193	1186.4777	1186.6120
1199.0994	1212.9640	1218.6776
1224.5031	1230.6983	1272.3400
1330.0239	1332.8541	1334.0093
1336.9409	1342.2919	1362.7337
1363.6827	1367.1744	1375.0590
1420.6028	1463.9422	1491.0782
1492.0711	1494.0233	1504.0326
1510.8481	1514.1918	1539.3801
1541.7450	1543.1048	1551.2339
1560.2611	1668.6248	1670.7478
1675.2811	1676.1618	1683.3890
1687.2663	1689.0085	1694.0154
1711.4030	1880.8176	3050.1409
3116.1671	3144.9008	3147.4468
3151.6321	3197.2948	3198.2642
3201.2936	3205.4893	3205.6467
3207.3710	3209.8911	3212.1910
3215.3945	3217.1088	3219.9019
3221.0150	3222.9317	3224.0233
3226.1007	3229.4047	3230.3800
3232.1568	3234.0666	3238.8463
3239.0408	3524.6256	3607.8004

TS17

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.382464	1.921777	-0.424752
2	46	0	0.807551	0.491421	-0.653878
3	15	0	-1.430827	0.236773	-0.023395
4	6	0	-1.721793	-0.449656	1.651120
5	6	0	-0.944844	-1.554167	2.019817
6	6	0	-2.662425	0.057820	2.549665
7	6	0	-1.114190	-2.150668	3.263718
8	1	0	-0.199753	-1.940901	1.326598
9	6	0	-2.824409	-0.537285	3.800425

10	1	0	-3.265984	0.918937	2.278473
11	6	0	-2.055329	-1.640695	4.157495
12	1	0	-0.506497	-3.007188	3.539368
13	1	0	-3.553519	-0.134398	4.496559
14	1	0	-2.184124	-2.100316	5.132481
15	6	0	-2.274133	-0.988520	-1.102119
16	6	0	-3.265128	-1.861820	-0.641421
17	6	0	-1.881192	-1.046059	-2.444543
18	6	0	-3.861443	-2.767853	-1.514914
19	1	0	-3.563384	-1.839151	0.403720
20	6	0	-2.481043	-1.949835	-3.316188
21	1	0	-1.096217	-0.381194	-2.800597
22	6	0	-3.471765	-2.811903	-2.851576
23	1	0	-4.626862	-3.444961	-1.148501
24	1	0	-2.167948	-1.987132	-4.354853
25	1	0	-3.933521	-3.523408	-3.529134
26	6	0	-2.519973	1.708117	-0.088139
27	6	0	-1.948854	2.965654	0.126686
28	6	0	-3.897823	1.607763	-0.308526
29	6	0	-2.746927	4.107034	0.135290
30	1	0	-0.875052	3.044284	0.277291
31	6	0	-4.692328	2.750559	-0.305582
32	1	0	-4.349878	0.635928	-0.488243
33	6	0	-4.118018	4.000308	-0.081424
34	1	0	-2.294818	5.079729	0.301873
35	1	0	-5.760123	2.665293	-0.481990
36	1	0	-4.738811	4.890878	-0.082574
37	6	0	2.572566	-2.256449	-1.712367
38	6	0	1.630446	-2.947917	-0.718915
39	1	0	2.139772	-1.581335	-2.448755
40	1	0	3.429729	-2.823068	-2.068263
41	1	0	1.858425	-3.971913	-0.431335
42	6	0	2.534551	-1.863729	-0.307756
43	6	0	2.989648	-1.059328	0.648921
44	1	0	0.564020	-2.741074	-0.821152
45	6	0	2.515129	-1.178097	2.076716
46	6	0	4.033839	-0.029750	0.356797
47	6	0	5.254692	-0.119520	1.028365
48	6	0	3.836745	1.017594	-0.578896
49	6	0	6.300576	0.767090	0.794180
50	1	0	5.393810	-0.929256	1.741020
51	6	0	4.903038	1.912582	-0.797336
52	6	0	6.114049	1.788054	-0.134506
53	1	0	7.240777	0.661823	1.324991
54	1	0	4.757714	2.723417	-1.508193
55	1	0	6.910051	2.499256	-0.335970
56	7	0	2.660956	1.149430	-1.302522
57	1	0	2.717961	1.948464	-1.924088
58	1	0	1.926400	-2.087973	2.221109
59	1	0	3.364039	-1.201149	2.768443
60	1	0	1.897705	-0.314282	2.353534

Zero-point correction= 0.488165 (Hartree/Particle)
Thermal correction to Energy= 0.518628
Thermal correction to Enthalpy= 0.519572
Thermal correction to Gibbs Free Energy= 0.422649
Sum of electronic and zero-point Energies= -1643.553348
Sum of electronic and thermal Energies= -1643.522886
Sum of electronic and thermal Enthalpies= -1643.521942
Sum of electronic and thermal Free Energies= -1643.618864
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1644.037445
Frequencies

-695.0007	15.7378	21.7461
25.4233	32.7623	35.8664
47.0773	50.0196	52.3704
58.7017	69.0448	72.9376
84.2478	90.1518	101.2164
111.8105	128.8520	153.6400
193.4510	195.0487	208.2861
215.8714	217.9243	225.4841
249.7522	255.9449	262.5525
266.4661	279.4990	292.9517
337.0540	384.6767	407.9473
409.2183	414.6003	417.7019
438.1590	448.3334	453.5890

464.6618	511.8698	520.2667
526.4506	530.7623	551.3512
584.6960	596.9656	622.6578
628.4831	630.0538	630.9272
669.7531	704.9542	715.9656
717.6414	719.5856	721.6497
725.6211	754.2721	763.5838
767.0375	771.9020	778.6220
779.5346	822.9772	850.1111
867.7760	880.6862	882.1941
885.6575	886.9322	893.2385
950.5754	958.1109	962.8105
964.9156	980.1343	996.1834
1003.7551	1007.3651	1011.7918
1014.4878	1015.1230	1015.5958
1029.0502	1030.3895	1033.9900
1034.7246	1057.8825	1066.0031
1070.9893	1071.3635	1073.6148
1080.6136	1097.0100	1103.4776
1107.1317	1124.4744	1125.9443
1134.7001	1139.5728	1145.4499
1149.0153	1159.8030	1173.0778
1192.2818	1193.2868	1194.7816
1199.6866	1210.6890	1224.5342
1226.4964	1236.6208	1247.6655
1305.5125	1328.2280	1334.0964
1336.8217	1341.6410	1354.2985
1369.3478	1369.5214	1381.3170
1398.4024	1426.7540	1477.7272
1496.4566	1497.3495	1501.0119
1501.8036	1502.4080	1508.3681
1519.6353	1544.8948	1546.0203
1553.5681	1559.9011	1662.1856
1669.6365	1673.0425	1674.6278
1687.2796	1688.2865	1689.5382
1693.5383	1881.9923	1965.9661
3066.1655	3122.1232	3130.2861
3146.7613	3160.2854	3186.2160
3192.4779	3196.8716	3208.8314
3211.3698	3212.7810	3214.1403
3217.6871	3217.8907	3228.0040
3229.3133	3230.8736	3231.3879
3233.3704	3234.9592	3237.9007
3239.0627	3244.4354	3247.0561
3252.0666	3255.2003	3590.8826

INT22

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.223969	0.715293	-2.218503
2	46	0	0.845087	0.025543	-0.998194
3	15	0	-1.337244	0.140942	-0.154404
4	6	0	-1.485511	-0.038622	1.665826
5	6	0	-1.533008	-1.308141	2.254186
6	6	0	-1.400828	1.089497	2.487372
7	6	0	-1.490141	-1.444818	3.638237
8	1	0	-1.607374	-2.194535	1.631152
9	6	0	-1.353207	0.949292	3.871718
10	1	0	-1.364729	2.082006	2.046557
11	6	0	-1.393152	-0.316492	4.449920
12	1	0	-1.530704	-2.434960	4.081615
13	1	0	-1.285803	1.832850	4.498632
14	1	0	-1.353249	-0.424434	5.529254
15	6	0	-2.496718	-1.109714	-0.815920
16	6	0	-3.680658	-1.459758	-0.153406
17	6	0	-2.184148	-1.726016	-2.031888
18	6	0	-4.544107	-2.397949	-0.708784
19	1	0	-3.917315	-1.010551	0.807796
20	6	0	-3.052249	-2.664642	-2.586087
21	1	0	-1.255645	-1.469889	-2.536810
22	6	0	-4.231833	-2.998646	-1.927007
23	1	0	-5.458335	-2.664062	-0.187634
24	1	0	-2.801635	-3.138637	-3.529737

25	1	0	-4.905808	-3.732898	-2.357200
26	6	0	-2.127560	1.768363	-0.455824
27	6	0	-1.298019	2.874265	-0.665482
28	6	0	-3.513446	1.947685	-0.414788
29	6	0	-1.847802	4.145575	-0.817273
30	1	0	-0.221040	2.732981	-0.718557
31	6	0	-4.060215	3.216034	-0.581272
32	1	0	-4.171538	1.096872	-0.266848
33	6	0	-3.228386	4.316599	-0.777522
34	1	0	-1.195050	4.997939	-0.977296
35	1	0	-5.137751	3.345236	-0.557835
36	1	0	-3.657993	5.305375	-0.904998
37	6	0	2.170521	-2.862148	-0.436579
38	6	0	1.029947	-2.862409	0.588063
39	1	0	1.906335	-2.777253	-1.488011
40	1	0	3.046788	-3.473516	-0.234558
41	1	0	1.112741	-3.490024	1.472749
42	6	0	1.937686	-1.716006	0.437799
43	6	0	2.470170	-0.583127	0.930839
44	1	0	0.024615	-2.793613	0.175269
45	6	0	1.925646	0.068537	2.179230
46	6	0	3.710013	-0.014064	0.318774
47	6	0	4.824694	0.207938	1.125965
48	6	0	3.764604	0.285138	-1.073985
49	6	0	6.020142	0.704712	0.615415
50	1	0	4.760614	-0.031218	2.185236
51	6	0	4.988201	0.795799	-1.568751
52	6	0	6.084983	0.996234	-0.746788
53	1	0	6.874481	0.863872	1.264189
54	1	0	5.051282	1.038833	-2.627152
55	1	0	7.001785	1.393973	-1.174299
56	7	0	2.685784	0.076548	-1.886783
57	1	0	2.809239	0.501971	-2.797119
58	1	0	1.065660	-0.478578	2.573736
59	1	0	2.701707	0.095457	2.952376
60	1	0	1.635200	1.107872	1.986492

Zero-point correction= 0.489994 (Hartree/Particle)
Thermal correction to Energy= 0.520042
Thermal correction to Enthalpy= 0.520986
Thermal correction to Gibbs Free Energy= 0.427023
Sum of electronic and zero-point Energies= -1643.575955
Sum of electronic and thermal Energies= -1643.545907
Sum of electronic and thermal Enthalpies= -1643.544963
Sum of electronic and thermal Free Energies= -1643.638926
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1644.058963
Frequencies

13.2093	29.5624	35.8859
40.2624	49.2776	52.6530
58.2644	65.1065	73.4277
79.1198	86.9138	93.5957
108.7559	129.6950	142.5244
147.4062	164.5768	190.3128
196.5080	198.7630	218.1937
223.8958	234.3021	250.3626
260.4964	263.3690	275.1806
285.9542	308.2766	355.7338
390.7990	406.6749	407.8511
415.6333	433.0529	441.4420
459.5972	463.7327	503.9504
523.1291	530.7733	539.2423
541.6408	551.8983	578.8601
586.2161	616.6259	627.3298
629.0200	630.3056	657.6756
670.8359	702.1742	711.0142
714.5010	719.0711	722.2920
727.9168	752.1966	757.1489
765.3676	769.5954	770.6851
778.5238	813.4802	821.2723
854.9596	872.3511	873.6194
881.2292	882.5413	894.4473
939.7694	946.7644	956.7939
965.5973	980.9622	990.5964
996.4588	1000.3938	1007.5341
1015.2134	1015.4188	1016.8726

1024.2922	1030.5505	1033.1222
1038.7050	1055.4010	1059.9932
1070.9816	1071.2284	1072.3940
1076.5185	1094.7442	1101.3807
1109.0868	1120.9818	1124.9944
1126.8357	1142.9869	1143.8137
1146.6772	1153.2504	1174.2595
1187.3508	1190.2171	1191.4032
1193.6989	1210.1655	1218.0769
1222.2085	1225.6672	1234.4001
1320.0085	1324.4900	1329.8451
1336.4356	1340.4695	1364.3718
1366.6118	1368.0443	1369.8873
1385.1181	1425.8215	1471.4973
1492.1591	1494.1415	1496.7294
1498.8914	1504.9424	1510.4585
1517.9011	1542.5145	1544.0599
1545.2935	1550.0485	1646.3736
1669.6924	1673.6182	1675.4779
1685.8079	1687.1090	1690.2121
1691.8945	1828.1482	2093.6546
3072.5257	3131.5810	3137.7689
3151.9769	3178.5850	3188.1305
3193.9960	3205.5290	3208.5890
3209.0078	3211.5916	3212.2158
3215.6861	3216.7595	3218.6844
3222.2800	3224.0280	3227.4570
3228.5234	3228.8206	3230.6825
3234.1928	3236.8593	3242.6890
3243.7712	3248.7430	3620.0571

TS18

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.571942	-0.529558	-1.644704
2	6	0	1.717628	-0.536260	-0.106822
3	6	0	1.383247	0.351669	-2.290357
4	1	0	1.224606	-0.702966	0.848602
5	1	0	1.852491	-1.446324	-0.688175
6	1	0	1.340968	1.134628	-3.037110
7	6	0	1.398783	0.672571	-0.895356
8	6	0	1.210263	1.888151	-0.203852
9	1	0	1.941960	-0.533631	-2.594196
10	6	0	1.535394	1.912402	1.254547
11	6	0	0.722846	1.286126	2.213162
12	6	0	2.718757	2.526317	1.710108
13	6	0	1.090911	1.239631	3.557293
14	1	0	-0.210564	0.825526	1.894726
15	6	0	3.079817	2.498157	3.057127
16	1	0	3.359507	3.013042	0.978697
17	6	0	2.270438	1.843890	3.984888
18	1	0	0.445245	0.732148	4.267823
19	1	0	3.997985	2.981258	3.379697
20	1	0	2.555081	1.811239	5.032070
21	6	0	0.683445	3.110689	-0.795098
22	6	0	-0.026797	3.122950	-2.019887
23	6	0	0.741252	4.345420	-0.101816
24	6	0	-0.598492	4.286948	-2.522858
25	1	0	-0.204572	2.194806	-2.549731
26	6	0	0.180362	5.504671	-0.617079
27	1	0	1.227928	4.393112	0.866389
28	6	0	-0.490334	5.495027	-1.840690
29	1	0	-1.148612	4.238568	-3.458869
30	1	0	0.262448	6.428505	-0.050233
31	1	0	-0.926921	6.403684	-2.242771
32	15	0	-2.432281	-0.938939	-0.279475
33	6	0	-3.302819	0.663704	-0.044091
34	6	0	-2.493980	1.807453	-0.027743
35	6	0	-4.685530	0.800990	0.099373
36	6	0	-3.053200	3.071233	0.127555
37	1	0	-1.417655	1.708625	-0.153090
38	6	0	-5.245671	2.068498	0.256846
39	1	0	-5.326691	-0.076131	0.079807

40	6	0	-4.433962	3.200818	0.269901
41	1	0	-2.404322	3.943516	0.114332
42	1	0	-6.321904	2.170402	0.362002
43	1	0	-4.879842	4.184594	0.382343
44	6	0	-1.902174	-1.333743	1.443472
45	6	0	-2.449908	-0.720300	2.574701
46	6	0	-0.845667	-2.237866	1.609706
47	6	0	-1.946869	-1.004582	3.843951
48	1	0	-3.257566	-0.001896	2.461172
49	6	0	-0.338181	-2.517597	2.875087
50	1	0	-0.407094	-2.703816	0.728758
51	6	0	-0.888979	-1.897686	3.995708
52	1	0	-2.377276	-0.517661	4.714227
53	1	0	0.494474	-3.205601	2.985295
54	1	0	-0.488137	-2.104531	4.983618
55	6	0	-3.802622	-2.129447	-0.564009
56	6	0	-4.110554	-2.444739	-1.891500
57	6	0	-4.551176	-2.709161	0.465406
58	6	0	-5.160378	-3.309815	-2.187152
59	1	0	-3.514473	-2.010855	-2.691627
60	6	0	-5.595498	-3.581340	0.169390
61	1	0	-4.314685	-2.481445	1.501582
62	6	0	-5.903456	-3.879661	-1.156391
63	1	0	-5.392025	-3.545268	-3.221401
64	1	0	-6.168520	-4.030176	0.975257
65	1	0	-6.717810	-4.560604	-1.384734
66	6	0	4.928229	-1.177260	-0.985113
67	6	0	4.655375	-2.207567	-0.085151
68	6	0	5.186200	-3.479690	-0.252712
69	6	0	6.002703	-3.687154	-1.361990
70	6	0	6.277008	-2.651291	-2.266024
71	6	0	5.747010	-1.374622	-2.087885
72	6	0	4.277541	0.064871	-0.513516
73	6	0	3.761653	-1.708766	0.981485
74	1	0	4.968334	-4.271312	0.456341
75	1	0	6.437134	-4.666806	-1.531308
76	1	0	6.917287	-2.850389	-3.119114
77	1	0	5.954732	-0.563470	-2.777496
78	8	0	4.417873	1.204071	-0.834292
79	8	0	3.336459	-2.238133	1.967164
80	7	0	3.366198	-0.364929	0.561575
81	1	0	3.238331	0.338136	1.305913

Zero-point correction= 0.648793 (Hartree/Particle)
Thermal correction to Energy= 0.689671
Thermal correction to Enthalpy= 0.690615
Thermal correction to Gibbs Free Energy= 0.570175
Sum of electronic and zero-point Energies= -2292.593644
Sum of electronic and thermal Energies= -2292.552766
Sum of electronic and thermal Enthalpies= -2292.551822
Sum of electronic and thermal Free Energies= -2292.672261
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -2293.281516
Frequencies

-510.9888	12.3305	17.7977
21.1346	23.4470	31.6235
32.2027	37.2601	43.8005
49.8031	53.7829	58.6932
60.1765	67.8507	71.4855
80.6648	81.5647	88.6846
95.7815	98.9816	104.4133
111.3342	131.7531	140.2862
142.3264	156.6475	177.3986
193.9747	197.5901	219.8180
225.6210	238.3261	246.8881
255.8137	265.1831	274.4059
274.9365	286.4622	297.1139
309.7325	349.9643	361.6392
402.5550	410.3067	413.2748
417.2819	423.2568	425.9542
433.1032	435.9288	437.5493
448.5104	450.5794	463.8120
505.8391	510.6345	519.2415
524.2613	529.9365	537.6003
553.2271	583.1740	619.4241
622.9663	628.8255	628.9013

629.8225	631.6189	638.1709
651.8234	664.8243	670.1867
686.2276	700.4172	712.7352
713.1419	715.7767	716.7752
718.2610	720.6071	721.9037
737.9370	741.9408	754.4721
768.0525	772.8860	780.5739
781.3705	785.9088	788.3612
796.6913	814.3001	832.3689
870.2305	883.1733	885.8145
890.0277	896.0078	916.8224
923.2295	925.1006	936.2270
953.3631	954.5573	958.4123
963.6309	973.0881	986.3315
986.9222	997.6879	1002.4093
1003.5048	1007.0241	1007.4384
1009.9348	1011.8931	1013.1999
1014.7673	1015.3470	1017.8805
1021.4820	1022.9576	1024.7071
1037.3503	1038.1637	1038.6550
1056.1584	1068.7221	1069.5343
1070.2842	1070.6503	1077.2048
1090.4245	1112.4940	1118.8116
1120.6702	1123.1563	1129.0143
1135.4001	1137.7370	1138.9286
1141.6840	1146.6901	1181.7265
1184.0624	1187.9470	1189.9263
1190.6621	1193.4886	1195.1728
1211.4753	1213.3017	1220.2821
1223.1021	1226.4401	1229.6748
1248.6607	1254.2742	1292.0596
1306.1173	1318.0725	1325.4485
1328.8100	1331.2083	1332.0567
1333.5436	1337.2445	1355.3194
1366.2631	1367.4063	1368.6945
1373.7284	1386.5690	1400.9878
1478.9616	1490.4207	1493.4908
1495.6309	1496.6471	1497.1984
1520.2515	1526.7388	1535.4000
1541.3272	1541.7118	1542.1614
1543.9592	1547.8562	1556.6540
1648.7466	1658.0782	1667.0860
1669.8509	1670.0457	1681.3487
1683.1690	1686.1935	1689.5364
1691.2846	1693.2629	1697.8062
1922.3499	1951.7129	3149.2060
3184.0233	3188.0852	3196.3787
3199.7490	3203.3604	3203.6788
3205.8522	3210.0730	3212.0228
3214.7758	3215.8373	3219.5206
3222.0778	3222.4522	3223.4429
3224.4016	3228.4648	3230.2275
3231.8817	3233.6317	3233.7851
3234.1700	3235.8221	3239.2395
3239.8391	3242.6120	3243.8602
3244.2390	3248.8171	3258.3061
3268.6849	3276.2676	3352.7263

INT23

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.792129	-0.421922	1.725304
2	6	0	-1.904138	-0.528279	0.337521
3	6	0	-1.171439	0.506071	2.416832
4	1	0	-1.404579	-0.829108	-0.584285
5	1	0	-1.959254	-1.382154	1.016200
6	1	0	-1.006200	1.347069	3.077449
7	6	0	-1.300094	0.686414	1.020132
8	6	0	-1.068862	1.829420	0.220251
9	1	0	-1.691462	-0.335022	2.868893
10	6	0	-1.568909	1.797836	-1.187545
11	6	0	-0.931352	1.052086	-2.192039
12	6	0	-2.753012	2.480825	-1.533551

13	6	0	-1.465878	0.971347	-3.476612
14	1	0	-0.007213	0.526522	-1.956430
15	6	0	-3.282047	2.410205	-2.822799
16	1	0	-3.251017	3.066186	-0.762662
17	6	0	-2.641937	1.646290	-3.796742
18	1	0	-0.953218	0.378200	-4.227841
19	1	0	-4.193839	2.949413	-3.063286
20	1	0	-3.054799	1.580914	-4.798587
21	6	0	-0.383305	3.043598	0.648421
22	6	0	0.425237	3.108286	1.809682
23	6	0	-0.406226	4.213340	-0.151863
24	6	0	1.110666	4.265086	2.160547
25	1	0	0.583421	2.220008	2.408519
26	6	0	0.269903	5.369173	0.212665
27	1	0	-0.963458	4.215456	-1.082300
28	6	0	1.029303	5.415912	1.381716
29	1	0	1.729449	4.256119	3.053596
30	1	0	0.207140	6.243026	-0.430572
31	1	0	1.557777	6.320068	1.666420
32	15	0	2.553655	-0.964878	0.311459
33	6	0	3.876359	-2.216869	0.559702
34	6	0	4.239087	-2.511169	1.877507
35	6	0	4.546197	-2.854375	-0.490238
36	6	0	5.265700	-3.413593	2.143841
37	1	0	3.703919	-2.029563	2.693081
38	6	0	5.566746	-3.762866	-0.223749
39	1	0	4.267324	-2.640054	-1.518867
40	6	0	5.929813	-4.040846	1.092804
41	1	0	5.540157	-3.632917	3.171184
42	1	0	6.079370	-4.255409	-1.044587
43	1	0	6.725481	-4.750761	1.297798
44	6	0	3.501322	0.553088	-0.113571
45	6	0	4.889683	0.616092	-0.249880
46	6	0	2.742836	1.718294	-0.283119
47	6	0	5.505652	1.831740	-0.548984
48	1	0	5.493707	-0.277208	-0.115811
49	6	0	3.356628	2.928257	-0.583802
50	1	0	1.662658	1.677362	-0.160301
51	6	0	4.744018	2.985183	-0.715134
52	1	0	6.586521	1.875444	-0.646542
53	1	0	2.747204	3.821728	-0.690735
54	1	0	5.231848	3.929591	-0.937627
55	6	0	1.861487	-1.426107	-1.340070
56	6	0	0.737270	-2.262031	-1.361511
57	6	0	2.342046	-0.912914	-2.549158
58	6	0	0.099614	-2.572244	-2.558875
59	1	0	0.349358	-2.642004	-0.417881
60	6	0	1.706302	-1.225051	-3.750977
61	1	0	3.202746	-0.249316	-2.550141
62	6	0	0.584659	-2.050623	-3.758069
63	1	0	-0.784553	-3.202299	-2.555729
64	1	0	2.085440	-0.814111	-4.682124
65	1	0	0.083528	-2.281412	-4.693652
66	6	0	-5.299398	-0.923394	1.070285
67	6	0	-5.106075	-1.863703	0.048870
68	6	0	-5.964962	-2.952029	-0.104932
69	6	0	-7.016493	-3.072872	0.792588
70	6	0	-7.209226	-2.127398	1.820239
71	6	0	-6.357665	-1.043555	1.971678
72	6	0	-4.286063	0.120459	1.021248
73	6	0	-3.942821	-1.509657	-0.755979
74	1	0	-5.804415	-3.672976	-0.899498
75	1	0	-7.703377	-3.907974	0.706189
76	1	0	-8.040514	-2.254775	2.505843
77	1	0	-6.493999	-0.308939	2.757940
78	8	0	-4.080171	1.090506	1.688749
79	8	0	-3.426991	-2.014496	-1.709160
80	7	0	-3.362050	-0.265693	-0.117008
81	1	0	-3.300020	0.515678	-0.801183

Zero-point correction= 0.649797 (Hartree/Particle)
Thermal correction to Energy= 0.690936
Thermal correction to Enthalpy= 0.691881
Thermal correction to Gibbs Free Energy= 0.570959
Sum of electronic and zero-point Energies= -2292.593566

Sum of electronic and thermal Energies= -2292.552426
Sum of electronic and thermal Enthalpies= -2292.551482
Sum of electronic and thermal Free Energies= -2292.672403
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -2293.29552
Frequencies --

13.2891	14.9849	23.7270
25.9444	30.5763	34.4350
40.6152	44.2192	50.2741
53.7177	56.9523	58.8970
65.7608	74.2445	76.6817
78.7701	82.1999	90.9744
93.3000	97.9955	115.8330
125.0802	138.0090	148.6555
157.3149	165.7189	191.8996
204.9977	216.3943	226.9281
237.3465	252.4103	255.9925
258.2022	259.2417	276.1120
290.1234	295.5512	311.8110
349.7175	360.3914	403.6070
410.0152	412.8683	417.0276
422.4932	427.4957	427.6480
433.5392	436.1151	438.5415
451.0850	460.3576	502.0155
507.9978	515.6601	519.1281
521.8259	525.8428	535.4690
561.4235	582.7426	620.2839
627.0684	628.1183	629.0236
629.5123	632.1491	638.1585
659.9365	671.5922	689.7241
699.9613	708.9704	712.4521
714.5076	715.5688	716.5570
717.5239	721.2569	724.4272
733.9428	756.2251	764.9586
768.0075	773.5453	779.5126
782.7376	787.1868	792.9875
795.6182	821.1690	867.8426
871.8787	876.5058	885.0483
887.1794	887.5583	896.3697
915.4063	919.4958	934.0672
945.4733	950.3911	956.0276
962.2644	969.1795	987.6588
995.2569	998.6249	1002.5991
1003.6318	1005.7259	1007.4434
1012.7968	1014.0451	1014.6724
1014.9849	1015.5723	1017.6964
1020.5482	1024.0357	1027.4602
1030.0282	1030.2166	1048.6211
1056.8752	1068.2839	1070.1308
1070.3412	1074.1769	1080.0541
1090.0397	1114.8162	1120.1705
1122.1075	1123.3621	1128.1476
1135.6195	1137.6957	1138.7829
1143.9330	1168.7902	1187.0065
1188.5771	1189.0404	1189.5650
1190.3114	1205.9762	1210.3781
1218.9003	1222.0710	1222.5370
1222.9676	1226.1541	1243.7628
1277.4652	1289.2283	1298.0523
1311.2000	1327.1509	1330.5133
1332.3305	1332.5834	1336.4460
1355.3183	1357.0298	1362.9326
1365.7370	1367.0701	1374.2543
1375.2539	1395.0635	1399.8466
1472.3814	1491.8170	1493.9087
1494.7231	1495.7069	1510.9834
1516.5715	1520.8457	1532.2527
1538.3249	1542.8240	1543.4084
1543.8024	1546.5815	1562.7514
1647.8675	1658.4891	1664.4122
1668.1420	1669.3587	1669.9440
1674.4547	1684.2583	1686.1461
1686.8623	1689.0110	1691.1525
1870.9450	1904.9300	3142.5632
3174.0053	3191.0303	3200.4117
3203.4861	3203.7090	3205.8588

3208.6400	3210.3223	3211.3486
3212.7041	3214.5326	3215.4048
3216.8493	3217.2707	3218.3198
3221.3582	3222.7891	3224.3717
3224.8282	3225.5521	3230.7772
3231.2314	3235.7799	3236.7163
3237.1724	3238.3717	3238.8743
3242.0833	3244.4327	3246.0835
3253.3327	3260.6766	3278.8284

INT24

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.449276	-0.383211	-1.892540
2	6	0	0.224699	-2.303788	-1.646962
3	6	0	1.333045	-0.837929	-2.974328
4	1	0	-0.120342	-2.891479	-2.500197
5	1	0	-0.055300	-2.740297	-0.688634
6	1	0	2.008104	-0.024358	-3.214731
7	6	0	1.568870	-1.702079	-1.808136
8	6	0	2.569590	-1.675872	-0.861129
9	1	0	0.971228	-1.367412	-3.857149
10	1	0	1.472130	0.419578	-0.239675
11	6	0	2.438763	-2.495128	0.374680
12	6	0	2.757281	-1.939602	1.625686
13	6	0	2.007789	-3.830052	0.347011
14	6	0	2.624031	-2.681700	2.795899
15	1	0	3.110243	-0.911011	1.671437
16	6	0	1.858584	-4.567366	1.518435
17	1	0	1.799435	-4.294325	-0.613323
18	6	0	2.162623	-3.996218	2.751656
19	1	0	2.883558	-2.229068	3.749813
20	1	0	1.519628	-5.598010	1.464538
21	1	0	2.056241	-4.572435	3.665715
22	6	0	3.847033	-0.935517	-1.025279
23	6	0	5.043274	-1.551729	-0.608678
24	6	0	3.958393	0.351173	-1.576939
25	6	0	6.275200	-0.930138	-0.754649
26	1	0	4.991781	-2.544425	-0.170637
27	6	0	5.194983	0.976231	-1.726829
28	1	0	3.069298	0.896561	-1.870247
29	6	0	6.362191	0.341372	-1.320996
30	1	0	7.175422	-1.444026	-0.429607
31	1	0	5.238962	1.973063	-2.156861
32	1	0	7.325224	0.828718	-1.437322
33	15	0	-2.256982	-0.415351	-0.253494
34	6	0	-2.909760	-2.036678	0.278826
35	6	0	-3.071248	-3.022113	-0.700913
36	6	0	-3.261170	-2.319323	1.603099
37	6	0	-3.594975	-4.267022	-0.365005
38	1	0	-2.772887	-2.810084	-1.725382
39	6	0	-3.777811	-3.567809	1.937735
40	1	0	-3.118889	-1.565158	2.372557
41	6	0	-3.947531	-4.540289	0.954408
42	1	0	-3.717320	-5.026532	-1.130596
43	1	0	-4.043612	-3.782995	2.968034
44	1	0	-4.346870	-5.514586	1.218929
45	6	0	-3.744454	0.617041	-0.534684
46	6	0	-4.950567	0.416564	0.143982
47	6	0	-3.637683	1.665220	-1.455578
48	6	0	-6.034556	1.255728	-0.095900
49	1	0	-5.045708	-0.401505	0.852676
50	6	0	-4.722741	2.507533	-1.687144
51	1	0	-2.699314	1.825339	-1.980819
52	6	0	-5.921445	2.301769	-1.009929
53	1	0	-6.970505	1.091099	0.428926
54	1	0	-4.632616	3.317228	-2.404660
55	1	0	-6.770069	2.952532	-1.197582
56	6	0	-1.507158	0.289952	1.261789
57	6	0	-0.506069	-0.442326	1.919436
58	6	0	-1.764481	1.605364	1.654098
59	6	0	0.209667	0.134014	2.961934
60	1	0	-0.264479	-1.457431	1.604798

61	6	0	-1.032649	2.183699	2.691261
62	1	0	-2.526318	2.186985	1.141637
63	6	0	-0.048811	1.450831	3.346813
64	1	0	0.991671	-0.438100	3.450619
65	1	0	-1.226762	3.214521	2.974663
66	1	0	0.530465	1.906665	4.144184
67	6	0	1.586077	3.467690	0.994139
68	6	0	0.598393	3.581273	0.022823
69	6	0	-0.090046	4.763035	-0.181296
70	6	0	0.253667	5.847448	0.632241
71	6	0	1.248735	5.734006	1.606868
72	6	0	1.934033	4.531193	1.804970
73	6	0	2.084293	2.057182	0.988530
74	6	0	0.444106	2.251417	-0.635771
75	1	0	-0.864423	4.837669	-0.937921
76	1	0	-0.259620	6.795348	0.506573
77	1	0	1.491186	6.596072	2.220014
78	1	0	2.704212	4.425116	2.561946
79	8	0	2.931208	1.553291	1.677647
80	8	0	-0.319605	1.973639	-1.551008
81	7	0	1.335975	1.409558	-0.010374

Zero-point correction= 0.649158 (Hartree/Particle)
Thermal correction to Energy= 0.690170
Thermal correction to Enthalpy= 0.691114
Thermal correction to Gibbs Free Energy= 0.571392
Sum of electronic and zero-point Energies= -2292.685390
Sum of electronic and thermal Energies= -2292.644379
Sum of electronic and thermal Enthalpies= -2292.643434
Sum of electronic and thermal Free Energies= -2292.763157
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -2293.363611
Frequencies

13.8287	19.7485	24.6794
27.7332	29.2734	33.1147
39.3329	43.8273	47.9663
56.1734	61.6681	64.9078
72.0857	73.6144	81.1961
86.1799	86.7805	96.6891
02.1986	109.0274	115.7943
28.2131	140.6560	147.2703
61.5541	178.6954	191.6256
04.2799	209.8972	224.0161
234.8366	249.9594	253.3507
255.6901	259.1792	271.4884
280.8692	304.1272	334.8114
373.4773	386.2725	407.4469
409.5359	412.8763	414.6506
417.0893	425.7166	429.0144
434.5768	437.0290	439.3274
458.0880	467.6651	469.9560
504.8837	517.9202	521.8999
531.7665	542.5947	547.1281
563.4442	595.3774	624.9543
626.2016	627.7295	628.0949
631.5380	638.7021	651.3306
673.5757	678.2571	682.2588
696.5135	703.0531	710.7686
714.2562	715.1846	718.9132
720.8508	722.7103	724.6800
725.7755	729.8701	734.8197
767.5137	770.8574	771.2423
776.9516	783.3863	788.8023
793.3380	801.7537	811.3257
828.8520	877.0704	878.0594
883.9399	886.9029	887.3840
918.5986	925.8542	930.3937
945.7376	946.9839	951.0374
955.6926	958.1984	975.7962
993.4444	997.2920	997.7930
1000.2196	1003.6670	1005.9700
1010.4266	1011.4037	1013.0696
1015.4804	1016.1710	1016.6272
1017.5092	1018.9794	1020.3769
1027.7423	1030.8550	1032.2030
1041.4349	1052.4831	1065.5612

1070.0525	1071.3663	1072.0337
1078.1905	1079.8490	1102.9071
1120.1653	1122.0091	1123.1869
1123.4827	1124.4908	1129.9693
1133.9586	1136.9527	1146.9191
1182.6190	1183.6685	1185.1234
1187.1419	1187.7484	1188.6183
1205.9425	1215.7614	1216.4204
1219.3320	1219.7617	1220.4605
1226.0650	1239.5752	1255.3611
1309.9603	1324.5079	1326.8095
1333.0763	1338.2471	1338.5777
1358.4221	1361.4179	1366.1148
1366.3785	1368.9430	1369.4253
1370.6711	1381.5256	1433.3858
1481.8078	1487.7285	1494.7400
1496.4810	1497.6596	1499.2848
1516.0455	1531.7994	1534.0817
1534.2909	1542.8156	1547.3910
1554.3746	1557.1609	1626.8665
1663.9156	1665.1755	1670.0584
1670.7218	1672.9858	1681.4814
1687.0254	1690.4540	1693.0635
1698.8504	1708.7284	1715.7111
1811.1676	1924.7031	3124.8690
3138.7696	3190.6375	3192.1497
3200.6171	3204.0330	3205.9784
3208.9569	3209.0673	3210.4909
3210.8810	3211.8324	3215.5088
3215.7333	3216.2597	3221.0743
3221.6223	3222.2001	3227.1187
3227.4508	3228.4769	3229.3250
3232.1469	3235.1423	3236.1482
3240.5004	3243.0320	3243.6785
3247.6300	3249.3039	3249.5385
3258.4259	3264.1121	3433.2420

TS19

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.271665	-0.542278	-1.789998
2	6	0	0.619622	-2.366864	-1.434403
3	6	0	1.602140	-0.884355	-2.916493
4	1	0	0.329669	-3.011884	-2.263802
5	1	0	0.432342	-2.789615	-0.450932
6	1	0	2.204353	-0.037906	-3.221769
7	6	0	1.778834	-1.504756	-1.650446
8	6	0	2.629799	-1.009455	-0.585076
9	1	0	1.167863	-1.472089	-3.722370
10	1	0	1.887753	0.296596	-0.301730
11	6	0	2.701862	-1.874477	0.644634
12	6	0	2.832702	-1.286003	1.911145
13	6	0	2.713766	-3.276164	0.580307
14	6	0	2.923928	-2.064661	3.062610
15	1	0	2.888987	-0.203045	1.980591
16	6	0	2.798437	-4.057776	1.729606
17	1	0	2.665641	-3.762248	-0.391535
18	6	0	2.895014	-3.454759	2.980779
19	1	0	3.025806	-1.580073	4.030047
20	1	0	2.802428	-5.140758	1.643978
21	1	0	2.961524	-4.061238	3.878951
22	6	0	3.948945	-0.393591	-0.975722
23	6	0	5.159673	-0.993635	-0.593329
24	6	0	4.031795	0.799837	-1.711275
25	6	0	6.386353	-0.446685	-0.951236
26	1	0	5.134407	-1.907021	-0.006899
27	6	0	5.259800	1.345905	-2.076111
28	1	0	3.124953	1.332627	-1.978674
29	6	0	6.446310	0.725622	-1.701317
30	1	0	7.302395	-0.943408	-0.643911
31	1	0	5.284130	2.270234	-2.646338
32	1	0	7.404250	1.152836	-1.981711
33	15	0	-2.123864	-0.634150	-0.268917

34	6	0	-2.629068	-2.253967	0.406177
35	6	0	-2.626920	-3.352893	-0.459161
36	6	0	-3.041142	-2.420427	1.731738
37	6	0	-3.045660	-4.601029	-0.008614
38	1	0	-2.289565	-3.225467	-1.485683
39	6	0	-3.453070	-3.672317	2.181466
40	1	0	-3.033771	-1.572148	2.410748
41	6	0	-3.457699	-4.760899	1.312626
42	1	0	-3.041880	-5.449882	-0.684931
43	1	0	-3.768306	-3.797411	3.212613
44	1	0	-3.777164	-5.735929	1.666979
45	6	0	-3.680808	0.116666	-0.871140
46	6	0	-4.941129	-0.329459	-0.464016
47	6	0	-3.580011	1.205390	-1.746910
48	6	0	-6.089435	0.308455	-0.926856
49	1	0	-5.026703	-1.175725	0.211744
50	6	0	-4.731513	1.843345	-2.199333
51	1	0	-2.599098	1.558098	-2.058477
52	6	0	-5.986206	1.394551	-1.792203
53	1	0	-7.065655	-0.044671	-0.609538
54	1	0	-4.648349	2.687060	-2.877506
55	1	0	-6.883500	1.889037	-2.151522
56	6	0	-1.688007	0.362171	1.204752
57	6	0	-0.527818	0.011845	1.910281
58	6	0	-2.415258	1.489643	1.592284
59	6	0	-0.112912	0.773279	2.996931
60	1	0	0.069099	-0.845413	1.599531
61	6	0	-1.988051	2.259626	2.673719
62	1	0	-3.308393	1.776272	1.045042
63	6	0	-0.841512	1.902696	3.375731
64	1	0	0.795597	0.498318	3.524432
65	1	0	-2.548302	3.145313	2.956999
66	1	0	-0.504604	2.510600	4.209935
67	6	0	1.038752	3.445098	1.037207
68	6	0	0.093966	3.360256	0.029897
69	6	0	-0.902823	4.307008	-0.125260
70	6	0	-0.914256	5.367173	0.784107
71	6	0	0.043626	5.458433	1.799747
72	6	0	1.043065	4.491567	1.942514
73	6	0	1.891160	2.214070	0.936929
74	6	0	0.348985	2.087197	-0.708985
75	1	0	-1.646376	4.215678	-0.910929
76	1	0	-1.678041	6.134583	0.704759
77	1	0	0.005958	6.296676	2.488666
78	1	0	1.786653	4.546285	2.731412
79	8	0	2.820364	1.926500	1.653625
80	8	0	-0.331762	1.726340	-1.680043
81	7	0	1.397173	1.440865	-0.126711

Zero-point correction= 0.644971 (Hartree/Particle)
Thermal correction to Energy= 0.685328
Thermal correction to Enthalpy= 0.686272
Thermal correction to Gibbs Free Energy= 0.569189
Sum of electronic and zero-point Energies= -2292.672875
Sum of electronic and thermal Energies= -2292.632519
Sum of electronic and thermal Enthalpies= -2292.631575
Sum of electronic and thermal Free Energies= -2292.748657
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -2293.34705
Frequencies

-1326.8282	18.4893	21.5866
24.6496	34.6329	36.2964
40.5855	43.6981	49.0171
49.4798	56.2322	61.7819
65.0061	67.2302	76.8584
84.1765	89.8717	96.1240
102.9318	104.0479	116.6617
136.2843	144.5259	145.6875
161.3248	173.6654	200.1779
201.0488	214.7276	221.0498
223.9910	246.6062	253.8018
256.2672	263.7209	267.1728
282.5160	292.0817	301.8734
308.1595	355.5399	391.5738
406.2577	409.3274	412.9931
413.8289	418.6654	422.0034

431.7474	433.7464	447.1716
458.0242	462.4840	466.3921
483.9258	510.7779	516.4684
524.5648	534.1432	548.9691
551.7117	579.6147	608.9226
627.3357	627.6074	628.1972
628.7493	633.8073	640.5460
682.5113	684.9356	702.1464
702.9018	710.7727	713.9350
715.1262	716.3360	723.4057
725.4864	725.9979	727.9757
729.9875	747.0252	755.2011
763.5571	770.3801	773.4589
781.8058	788.6548	792.8564
805.6408	811.5806	853.5220
870.4234	873.8566	878.6125
880.0307	885.9941	886.2703
910.9204	911.6607	924.1999
942.9791	953.5878	954.0256
955.5827	960.3412	980.4612
985.1342	997.1331	998.3557
1000.5350	1001.4845	1010.2394
1010.8553	1012.9555	1015.4976
1015.6750	1016.2770	1017.0164
1017.7665	1020.1382	1023.6041
1028.1528	1029.0629	1030.0752
1035.7367	1052.1366	1070.3829
1070.9616	1072.4891	1077.1593
1081.8049	1098.2703	1106.5655
1124.2302	1124.6850	1127.7929
1129.2748	1131.9930	1142.5991
1143.5441	1145.9297	1147.8155
1182.5889	1185.0215	1186.6781
1190.4396	1191.5263	1191.8166
1208.6133	1221.1167	1221.5624
1224.9464	1227.0294	1228.2716
1229.9351	1243.6181	1277.5891
1310.3120	1319.6682	1321.4712
1333.7843	1337.0390	1340.7301
1352.0918	1367.5814	1368.4159
1370.0050	1373.5681	1374.2750
1376.3178	1383.1892	1432.5782
1445.9372	1494.7239	1496.3968
1498.5771	1500.0881	1507.0232
1508.9789	1531.3746	1534.5084
1539.9068	1543.0416	1545.9724
1546.7739	1556.4297	1558.4507
1563.5645	1668.1700	1669.4998
1670.7130	1672.7382	1675.0851
1684.9392	1687.7464	1688.7531
1695.1378	1702.5641	1710.4364
1714.8528	1754.9720	1900.7864
3155.0323	3180.2527	3194.6281
3197.5188	3198.6811	3204.4143
3208.4629	3208.6861	3209.4191
3210.3878	3215.4957	3216.0456
3217.4610	3220.6204	3221.0695
3221.1905	3221.2557	3227.6078
3228.2743	3231.1956	3232.0532
3232.2391	3232.5542	3235.9803
3236.5510	3236.8886	3239.3002
3240.5003	3246.1101	3246.4173
3247.2666	3254.5171	3305.1079

INT25

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.194254	-0.317792	-1.453948
2	6	0	1.799663	-1.680213	-1.334078
3	6	0	1.961583	0.294773	-2.655607
4	1	0	1.628682	-2.304593	-2.211196
5	1	0	1.930437	-2.207787	-0.394675
6	1	0	2.157608	1.358457	-2.750484

7	6	0	2.390235	-0.394783	-1.517968
8	6	0	3.124979	0.379104	-0.428070
9	1	0	1.687438	-0.240728	-3.562177
10	1	0	2.658535	1.372665	-0.405687
11	6	0	2.968833	-0.211111	0.964001
12	6	0	2.187130	0.455527	1.908919
13	6	0	3.603669	-1.403659	1.323989
14	6	0	2.013698	-0.085954	3.183518
15	1	0	1.732534	1.410202	1.647180
16	6	0	3.422808	-1.946564	2.591955
17	1	0	4.252564	-1.903494	0.607557
18	6	0	2.619013	-1.291485	3.523903
19	1	0	1.406418	0.444946	3.911771
20	1	0	3.916703	-2.876802	2.856300
21	1	0	2.480903	-1.713011	4.514980
22	6	0	4.594796	0.555757	-0.787749
23	6	0	5.290574	-0.351876	-1.587062
24	6	0	5.281803	1.650427	-0.255687
25	6	0	6.647784	-0.170466	-1.849247
26	1	0	4.770279	-1.204500	-2.016997
27	6	0	6.634237	1.834649	-0.518002
28	1	0	4.742997	2.357678	0.370677
29	6	0	7.322691	0.922685	-1.316649
30	1	0	7.175301	-0.884847	-2.474192
31	1	0	7.151676	2.692918	-0.100240
32	1	0	8.378495	1.066865	-1.523789
33	15	0	-1.499631	-1.342951	-0.119969
34	6	0	-1.014130	-2.727157	0.967530
35	6	0	-0.357090	-3.815638	0.379377
36	6	0	-1.240353	-2.725034	2.344856
37	6	0	0.059360	-4.889455	1.157118
38	1	0	-0.176306	-3.818352	-0.693957
39	6	0	-0.807912	-3.797015	3.124103
40	1	0	-1.746695	-1.885541	2.811234
41	6	0	-0.161523	-4.878160	2.534229
42	1	0	0.562703	-5.730894	0.691430
43	1	0	-0.981496	-3.784819	4.195586
44	1	0	0.171801	-5.711768	3.144434
45	6	0	-2.872887	-1.993415	-1.134406
46	6	0	-3.562874	-3.166569	-0.819573
47	6	0	-3.248216	-1.241985	-2.256141
48	6	0	-4.617321	-3.590031	-1.625981
49	1	0	-3.276495	-3.749225	0.051524
50	6	0	-4.307276	-1.667724	-3.051765
51	1	0	-2.720898	-0.317578	-2.484393
52	6	0	-4.989019	-2.842926	-2.740801
53	1	0	-5.149493	-4.503797	-1.380576
54	1	0	-4.596883	-1.082691	-3.919018
55	1	0	-5.810942	-3.175868	-3.367120
56	6	0	-2.276679	-0.097763	0.965150
57	6	0	-1.430047	0.656536	1.787197
58	6	0	-3.645632	0.178305	0.943446
59	6	0	-1.948340	1.674628	2.579995
60	1	0	-0.360649	0.461477	1.780836
61	6	0	-4.158715	1.205726	1.733623
62	1	0	-4.308893	-0.395621	0.303106
63	6	0	-3.313671	1.955660	2.546337
64	1	0	-1.276684	2.275270	3.186921
65	1	0	-5.220980	1.427480	1.702084
66	1	0	-3.713882	2.772123	3.139621
67	6	0	-1.252103	4.008140	0.426132
68	6	0	-1.914088	3.287072	-0.557086
69	6	0	-3.225044	3.556770	-0.901349
70	6	0	-3.859909	4.604469	-0.222594
71	6	0	-3.191518	5.335911	0.761549
72	6	0	-1.866645	5.041236	1.106693
73	6	0	0.100496	3.346187	0.586721
74	6	0	-0.948069	2.220475	-0.984680
75	1	0	-3.740895	2.971909	-1.656783
76	1	0	-4.889745	4.852988	-0.461489
77	1	0	-3.713012	6.142016	1.269217
78	1	0	-1.341102	5.589388	1.882807
79	8	0	0.924888	3.645628	1.431432
80	8	0	-1.245091	1.322978	-1.817704
81	7	0	0.207805	2.305582	-0.324037

Zero-point correction= 0.650377 (Hartree/Particle)
Thermal correction to Energy= 0.691382
Thermal correction to Enthalpy= 0.692326
Thermal correction to Gibbs Free Energy= 0.571972
Sum of electronic and zero-point Energies= -2292.711458
Sum of electronic and thermal Energies= -2292.670453
Sum of electronic and thermal Enthalpies= -2292.669508
Sum of electronic and thermal Free Energies= -2292.789863
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -2293.393609
Frequencies --

10.2317	15.2154	25.2019
29.5292	35.6364	36.5486
39.2721	44.5016	48.4170
51.4347	59.3569	62.2077
67.7344	71.5441	75.1922
80.2273	88.0634	92.3453
100.5130	106.2541	110.8449
128.0436	142.9240	149.1736
162.0234	170.6699	202.4538
215.0553	215.5447	221.4667
224.0636	238.5597	250.5165
257.0590	273.1342	278.5537
283.5702	291.1386	303.5664
325.6573	363.7273	402.3655
406.8934	409.0835	411.9818
414.9785	415.3447	422.4108
424.1178	426.7209	456.4653
458.3655	471.2169	483.5808
492.8515	507.4133	513.4813
533.6168	537.2598	552.2643
578.1415	594.8316	626.1759
628.2313	629.4825	629.8197
630.0241	649.0615	671.3045
683.6367	700.7879	702.6903
706.1208	712.5159	714.0391
715.1836	719.1343	723.9387
726.0264	731.2230	739.3814
766.8024	767.9405	768.2579
770.8286	772.6572	773.9936
787.9995	794.3724	813.6178
815.3765	846.1068	864.0880
871.0800	877.1741	884.1307
885.1284	888.8831	895.5215
914.3489	929.6270	944.4211
950.5063	952.7118	957.7894
961.7136	972.9068	975.9329
991.4509	997.6201	1001.4345
1003.4477	1008.8015	1010.3068
1012.0952	1014.3567	1015.4767
1015.9391	1016.8222	1018.9870
1019.6745	1021.1236	1023.2831
1026.3704	1032.4158	1036.9106
1048.9519	1070.5153	1071.8909
1074.0875	1074.2323	1076.4800
1077.5123	1100.8284	1121.9661
1125.8200	1127.6683	1128.2343
1134.0418	1141.2284	1143.7685
1145.7669	1165.8218	1180.2937
1185.2516	1186.8514	1188.1753
1193.4540	1198.7296	1200.5645
1214.8903	1217.2928	1224.2537
1227.1762	1231.2776	1236.1349
1241.1064	1259.9570	1301.9213
1308.0410	1315.8089	1335.5075
1341.7514	1343.2884	1358.4534
1367.9666	1369.6004	1370.9829
1375.1350	1381.9088	1382.7838
1384.8486	1387.3990	1437.2092
1449.9945	1493.5991	1497.8969
1504.6593	1512.1937	1516.5889
1523.1429	1530.2208	1535.7259
1546.0326	1547.0753	1553.0916
1558.1696	1560.0823	1568.2733
1660.7385	1670.7224	1674.4205

1676.0323	1685.2782	1686.5971
1686.8520	1690.6053	1692.0256
1698.1621	1706.2229	1706.9384
1714.9597	1849.7048	3102.1068
3152.7538	3175.0318	3192.2306
3193.8429	3196.5658	3200.3717
3202.6306	3206.9901	3212.1373
3212.9178	3213.5673	3215.0171
3215.4466	3216.2332	3218.6884
3221.5144	3224.2904	3227.3435
3228.3949	3229.5051	3231.0296
3232.7046	3236.8195	3239.5801
3239.7096	3240.0505	3240.8467
3241.9570	3243.7283	3248.6893
3249.8835	3264.0176	3273.1020

INT26

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.970962	-3.808132	-0.530474
2	1	0	3.782196	-4.207726	-1.134279
3	1	0	2.060964	-4.401346	-0.545330
4	6	0	3.331300	-3.125109	0.787258
5	1	0	2.655083	-3.274495	1.625357
6	6	0	2.870382	-2.347413	-0.376480
7	6	0	3.022395	-1.169896	-1.053164
8	46	0	0.885053	-1.344736	-0.308125
9	1	0	4.383001	-3.063955	1.059704
10	15	0	-1.109844	-0.093529	-0.030314
11	6	0	-0.827352	1.714648	-0.210183
12	6	0	0.416603	2.221294	0.184906
13	6	0	-1.795632	2.591605	-0.711357
14	6	0	0.677438	3.586261	0.100436
15	1	0	1.187191	1.544082	0.550862
16	6	0	-1.527862	3.955232	-0.802407
17	1	0	-2.758205	2.208527	-1.039233
18	6	0	-0.293420	4.454245	-0.393473
19	1	0	1.647748	3.962135	0.409703
20	1	0	-2.283564	4.627744	-1.196950
21	1	0	-0.086247	5.517606	-0.467952
22	6	0	-1.898032	-0.231857	1.624657
23	6	0	-2.496104	0.841469	2.291607
24	6	0	-1.901160	-1.495039	2.226117
25	6	0	-3.096124	0.648292	3.534541
26	1	0	-2.488380	1.831112	1.842331
27	6	0	-2.507674	-1.688615	3.463211
28	1	0	-1.415802	-2.326791	1.719201
29	6	0	-3.105549	-0.614901	4.119775
30	1	0	-3.555235	1.488385	4.046818
31	1	0	-2.504521	-2.673952	3.919135
32	1	0	-3.571090	-0.761177	5.089624
33	6	0	-2.517688	-0.408688	-1.169559
34	6	0	-2.205867	-0.806362	-2.474025
35	6	0	-3.859220	-0.261218	-0.803683
36	6	0	-3.216227	-1.031402	-3.404226
37	1	0	-1.162679	-0.947747	-2.749191
38	6	0	-4.869956	-0.494926	-1.733505
39	1	0	-4.115373	0.031151	0.211336
40	6	0	-4.550103	-0.876137	-3.034304
41	1	0	-2.962410	-1.337495	-4.414442
42	1	0	-5.909087	-0.381537	-1.439615
43	1	0	-5.339571	-1.058973	-3.756859
44	6	0	3.474782	0.108814	-0.468301
45	6	0	3.636490	1.221134	-1.302987
46	6	0	3.729556	0.262201	0.903740
47	6	0	4.032349	2.451639	-0.788438
48	1	0	3.433910	1.118072	-2.366019
49	6	0	4.123539	1.491000	1.417035
50	1	0	3.591244	-0.585734	1.567484
51	6	0	4.278093	2.593500	0.574749
52	1	0	4.143386	3.302035	-1.454756
53	1	0	4.309865	1.592297	2.482097
54	1	0	4.588416	3.552207	0.979322

55	1	0	2.928838	-1.183465	-2.138653

Zero-point correction= 0.447664 (Hartree/Particle)
Thermal correction to Energy= 0.475891
Thermal correction to Enthalpy= 0.476835
Thermal correction to Gibbs Free Energy= 0.382562
Sum of electronic and zero-point Energies= -1549.035763
Sum of electronic and thermal Energies= -1549.007536
Sum of electronic and thermal Enthalpies= -1549.006592
Sum of electronic and thermal Free Energies= -1549.100866
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1549.470314
Frequencies

7.6905	16.4603	25.4161
30.8657	35.3265	38.3717
48.7866	51.0626	57.3590
61.5853	63.4224	76.9401
92.6863	104.2292	128.2654
153.3286	164.5589	177.6550
188.8983	217.5196	218.5502
235.1196	257.3364	265.7674
266.6678	305.0365	380.5588
400.4521	407.0755	408.7279
413.2135	414.9916	439.8922
441.1455	442.0762	514.5702
516.2546	521.0298	533.4805
617.0423	627.8049	628.8726
629.4615	630.2629	701.2811
708.3670	714.4011	714.5557
717.9907	718.8305	719.7148
768.2400	769.9133	773.0104
775.7958	778.0923	795.3830
844.7516	859.0254	862.9352
877.6128	879.1819	888.6243
933.2010	954.6212	956.2508
959.5352	961.3468	985.7503
999.5838	1000.6305	1007.2196
1008.4448	1013.7693	1015.0161
1015.4063	1016.8565	1017.3738
1024.0442	1026.4913	1027.5736
1049.3859	1070.1438	1070.4766
1070.8806	1071.0976	1083.6342
1086.5613	1114.3638	1121.9297
1123.4123	1124.6179	1131.6125
1136.1261	1138.3062	1142.9867
1178.5293	1186.1939	1188.9275
1189.9947	1192.9056	1210.6017
1219.0742	1221.0302	1222.0753
1249.8156	1330.4234	1330.9050
1333.2412	1334.6993	1365.1614
1365.7193	1367.5908	1367.8070
1387.8590	1475.6300	1494.1823
1495.2650	1495.9809	1498.4330
1517.4071	1540.9751	1543.2001
1544.1653	1556.7933	1669.6497
1673.0109	1673.2090	1674.0163
1685.8649	1686.4936	1687.7866
1698.8757	1752.1207	3143.3628
3153.3145	3177.3782	3194.0696
3200.0116	3200.5159	3202.3249
3207.7623	3208.1976	3209.2320
3210.2828	3216.3465	3217.1762
3222.2102	3222.3640	3223.3450
3225.0188	3226.8677	3228.1480
3231.6380	3233.1728	3237.5758
3238.0229	3240.5903	3245.2227

INT27

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.864134	0.018003	0.013566
2	46	0	-0.359374	-0.384089	0.118535
3	6	0	-2.616731	-1.662493	0.113994
4	6	0	-2.938561	-0.130033	0.206107

5	1	0	-2.270257	-2.160878	1.017698
6	1	0	-2.188990	-2.043266	-0.813085
7	1	0	-2.724577	0.496981	-0.660028
8	6	0	-3.980541	-1.145615	0.084367
9	6	0	-5.271219	-1.435101	-0.009440
10	1	0	-2.802267	0.359659	1.169427
11	1	0	-5.554497	-2.482781	-0.102264
12	6	0	2.864996	-1.285306	-0.819804
13	6	0	2.499619	-2.617849	-0.598138
14	6	0	3.971925	-1.011299	-1.628815
15	6	0	3.236467	-3.656871	-1.157075
16	1	0	1.624427	-2.832217	0.011785
17	6	0	4.702562	-2.052482	-2.198095
18	1	0	4.263985	0.017895	-1.818370
19	6	0	4.339442	-3.375277	-1.960862
20	1	0	2.944213	-4.686431	-0.973866
21	1	0	5.557401	-1.826813	-2.828529
22	1	0	4.909261	-4.184781	-2.406881
23	6	0	2.379938	1.533501	-0.896518
24	6	0	3.484026	2.312885	-0.537750
25	6	0	1.628911	1.894370	-2.020670
26	6	0	3.833076	3.428658	-1.296304
27	1	0	4.071675	2.049898	0.337530
28	6	0	1.984880	3.001738	-2.784111
29	1	0	0.756243	1.301155	-2.285496
30	6	0	3.087812	3.772202	-2.421286
31	1	0	4.689572	4.029898	-1.006674
32	1	0	1.395944	3.269687	-3.655887
33	1	0	3.361485	4.642353	-3.010034
34	6	0	2.750940	0.208333	1.616098
35	6	0	2.085247	0.878666	2.648719
36	6	0	4.047058	-0.265782	1.839489
37	6	0	2.709656	1.087844	3.874490
38	1	0	1.067550	1.226476	2.484114
39	6	0	4.667241	-0.066047	3.071377
40	1	0	4.573911	-0.796907	1.051684
41	6	0	4.001965	0.613115	4.088529
42	1	0	2.183354	1.611020	4.666974
43	1	0	5.671666	-0.444633	3.235314
44	1	0	4.485670	0.765849	5.048471
45	6	0	-6.380116	-0.468195	-0.005474
46	6	0	-7.689945	-0.937770	-0.156774
47	6	0	-6.178205	0.911189	0.143100
48	6	0	-8.769405	-0.060557	-0.162629
49	1	0	-7.859028	-2.005491	-0.272367
50	6	0	-7.255624	1.787509	0.138342
51	1	0	-5.169857	1.294153	0.263732
52	6	0	-8.555961	1.306695	-0.014868
53	1	0	-9.777114	-0.446350	-0.282270
54	1	0	-7.081671	2.852919	0.255309
55	1	0	-9.395647	1.994479	-0.018376

Zero-point correction= 0.448177 (Hartree/Particle)
Thermal correction to Energy= 0.475772
Thermal correction to Enthalpy= 0.476716
Thermal correction to Gibbs Free Energy= 0.382954
Sum of electronic and zero-point Energies= -1549.016618
Sum of electronic and thermal Energies= -1548.989023
Sum of electronic and thermal Enthalpies= -1548.988079
Sum of electronic and thermal Free Energies= -1549.081841
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1549.455166
Frequencies

-10.1787	11.1064	16.2124
21.2352	30.4870	32.6338
33.3021	44.1341	49.7311
52.3343	59.6828	65.4393
76.5762	86.9992	99.3450
125.1320	155.2988	176.9166
202.7504	218.8968	223.2423
249.4281	258.9242	267.8430
275.0788	315.9748	362.4063
398.6804	407.5676	408.6937
413.3667	417.0284	439.8468
442.8779	445.6109	514.7099
516.1529	525.0779	527.9038

625.5995	629.1518	629.5700
630.3545	633.9398	702.9184
712.3003	712.9588	714.2859
717.0181	718.6564	719.9160
756.1175	767.3663	768.7462
775.4293	777.9704	782.2478
847.9946	849.9958	874.0189
879.2509	885.4143	889.3640
945.5833	950.9426	956.8400
960.2824	983.1429	995.4548
1000.8706	1005.8217	1008.3655
1014.2860	1015.0787	1016.7600
1018.4694	1020.2465	1021.5564
1022.2646	1028.7754	1030.1196
1051.6162	1061.5615	1070.2942
1071.0848	1071.1865	1074.2080
1087.3649	1113.5910	1122.2638
1123.7367	1130.1800	1131.7468
1136.0521	1139.3777	1145.9138
1161.8555	1186.8912	1190.1010
1193.5079	1199.2947	1217.5216
1220.6694	1221.6844	1231.7862
1256.8264	1330.4006	1333.8535
1338.6036	1339.2484	1364.4349
1366.5308	1370.2663	1375.3208
1396.7865	1461.1854	1487.0608
1494.7965	1497.5672	1503.4531
1515.9011	1542.1015	1544.4244
1552.2203	1564.5456	1669.4819
1672.2052	1674.1305	1678.2691
1687.7424	1688.6001	1690.7476
1706.1727	1884.3980	3133.0818
3137.2489	3177.1230	3198.4926
3203.0639	3204.9659	3212.4438
3213.2983	3215.9973	3216.4357
3216.6466	3220.5579	3222.9224
3223.6459	3228.2297	3228.3133
3232.3038	3234.4713	3237.5755
3237.7585	3239.9633	3240.5237
3244.7444	3248.1983	3254.3057

TS20

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.597466	-0.275580	0.148761
2	6	0	-2.246580	-1.685289	0.244901
3	6	0	-2.698016	0.200722	0.198701
4	1	0	-1.963602	-2.138890	1.196825
5	1	0	-1.952288	-2.252318	-0.640665
6	1	0	-2.698306	0.802535	-0.714567
7	6	0	-3.541803	-0.999707	0.199321
8	6	0	-4.824757	-1.349742	0.128972
9	1	0	-2.672991	0.780680	1.125242
10	6	0	-5.985290	-0.451371	0.051058
11	6	0	-7.262490	-1.007247	-0.101827
12	6	0	-5.877264	0.945786	0.125355
13	6	0	-8.393666	-0.202717	-0.183242
14	1	0	-7.363096	-2.088305	-0.158648
15	6	0	-7.007348	1.750172	0.044853
16	1	0	-4.901694	1.402674	0.252267
17	6	0	-8.270886	1.181901	-0.110504
18	1	0	-9.372044	-0.658171	-0.303038
19	1	0	-6.901891	2.829293	0.106236
20	1	0	-9.151328	1.813957	-0.171007
21	15	0	1.807825	0.023680	0.022011
22	6	0	2.716413	0.173975	1.610866
23	6	0	2.067005	0.834205	2.659979
24	6	0	4.009011	-0.319586	1.811190
25	6	0	2.706867	1.016839	3.882097
26	1	0	1.050984	1.195159	2.513978
27	6	0	4.644310	-0.144909	3.038670
28	1	0	4.519017	-0.846305	1.009360
29	6	0	3.996483	0.525770	4.073194

30	1	0	2.194280	1.531629	4.688721
31	1	0	5.645817	-0.537154	3.186730
32	1	0	4.492125	0.658668	5.029916
33	6	0	2.343842	1.519102	-0.901893
34	6	0	3.459465	2.285271	-0.551890
35	6	0	1.587371	1.883357	-2.021753
36	6	0	3.816462	3.393558	-1.317576
37	1	0	4.047540	2.018663	0.322022
38	6	0	1.951185	2.984414	-2.790342
39	1	0	0.706095	1.300514	-2.281423
40	6	0	3.066289	3.742145	-2.437731
41	1	0	4.681805	3.985815	-1.036261
42	1	0	1.358715	3.257234	-3.658028
43	1	0	3.345583	4.607331	-3.030995
44	6	0	2.705600	-1.326481	-0.841725
45	6	0	2.215686	-2.628024	-0.690376
46	6	0	3.849274	-1.113407	-1.617427
47	6	0	2.869238	-3.702108	-1.287100
48	1	0	1.310562	-2.791834	-0.108741
49	6	0	4.497633	-2.188603	-2.220678
50	1	0	4.231667	-0.105310	-1.754331
51	6	0	4.011356	-3.483024	-2.053749
52	1	0	2.479962	-4.707765	-1.162456
53	1	0	5.382944	-2.012688	-2.824261
54	1	0	4.516985	-4.318505	-2.528017
55	1	0	-5.053105	-2.415467	0.119927

Zero-point correction= 0.446162 (Hartree/Particle)
Thermal correction to Energy= 0.473872
Thermal correction to Enthalpy= 0.474816
Thermal correction to Gibbs Free Energy= 0.380616
Sum of electronic and zero-point Energies= -1548.998055
Sum of electronic and thermal Energies= -1548.970345
Sum of electronic and thermal Enthalpies= -1548.969401
Sum of electronic and thermal Free Energies= -1549.063601
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1549.435355
Frequencies

-214.4048	11.1339	16.1801
20.8684	25.5352	30.6684
33.1040	41.8310	45.4265
52.4881	59.3748	64.1954
70.2605	81.1605	104.7210
117.6934	132.9686	194.6105
219.2654	220.0995	247.8893
258.6046	267.7912	275.7077
283.2288	352.9877	404.7096
407.6819	409.0113	412.8002
417.8613	426.9633	440.4218
441.8860	443.4779	513.5941
516.3673	518.4932	527.7858
535.1382	590.9314	629.6833
630.4884	631.1548	633.3749
637.2730	704.6183	709.1276
715.4595	715.6824	718.4709
720.7136	722.6170	739.9939
773.6157	777.6013	778.3637
790.7283	838.4364	876.1836
882.0039	886.3246	890.2104
897.4335	945.8247	948.4973
951.4640	957.9253	958.7101
961.1572	963.1725	993.8980
1003.2034	1007.2744	1009.7481
1015.3466	1015.6121	1016.6541
1017.5063	1018.1366	1021.2535
1029.4386	1031.2197	1032.3602
1070.6737	1072.0784	1074.1433
1075.6317	1122.4412	1122.8444
1125.8362	1129.8862	1132.9144
1141.0765	1143.5434	1147.7173
1173.4593	1189.3390	1189.9759
1193.8544	1200.1429	1215.9314
1219.8857	1225.1835	1232.9554
1265.6569	1332.0210	1335.8684
1340.2361	1342.5394	1365.2452
1368.0153	1369.5512	1377.0327

1393.1930	1415.1490	1447.3488
1494.0941	1498.6035	1504.4038
1513.6791	1543.5123	1547.1906
1552.8144	1563.3423	1671.3703
1672.0030	1674.3623	1675.4060
1688.0035	1689.9670	1691.0366
1704.0057	1834.9525	3085.4677
3104.6121	3177.1934	3179.2010
3194.5670	3197.7313	3198.4708
3209.3037	3210.5047	3214.6044
3217.3444	3220.2258	3223.8771
3228.6237	3230.3522	3230.7959
3233.5936	3238.8213	3242.6713
3243.8329	3244.6507	3246.8298
3251.2912	3256.1616	3258.9260

INT28

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.587711	-0.711528	-1.036200
2	6	0	1.436274	-1.490236	0.670957
3	6	0	2.563400	-1.312556	-1.280816
4	1	0	1.150833	-2.545281	0.635765
5	1	0	1.070479	-0.982771	1.566782
6	1	0	3.130114	-0.638533	-1.927182
7	6	0	2.798810	-1.185454	0.182918
8	6	0	3.788224	-0.591465	0.877911
9	1	0	2.537555	-2.339761	-1.656605
10	6	0	5.075414	-0.123504	0.351350
11	6	0	5.772344	0.890237	1.026763
12	6	0	5.677322	-0.675871	-0.791713
13	6	0	7.000421	1.354888	0.568815
14	1	0	5.333470	1.319610	1.924262
15	6	0	6.904547	-0.212128	-1.250484
16	1	0	5.184332	-1.493760	-1.307568
17	6	0	7.572158	0.810371	-0.578190
18	1	0	7.512992	2.145192	1.109794
19	1	0	7.348884	-0.659567	-2.135042
20	1	0	8.530187	1.171130	-0.939270
21	15	0	-1.628442	0.029841	-0.188838
22	6	0	-2.145015	-1.034964	1.210484
23	6	0	-1.981760	-2.417059	1.057942
24	6	0	-2.686710	-0.536023	2.397924
25	6	0	-2.371904	-3.288008	2.069809
26	1	0	-1.539332	-2.806188	0.143193
27	6	0	-3.068040	-1.410194	3.413809
28	1	0	-2.806286	0.535262	2.533239
29	6	0	-2.914516	-2.784180	3.250413
30	1	0	-2.242804	-4.358144	1.941188
31	1	0	-3.482888	-1.014893	4.335828
32	1	0	-3.210864	-3.462028	4.044904
33	6	0	-3.121392	0.089140	-1.252271
34	6	0	-4.377040	-0.365925	-0.840450
35	6	0	-2.976516	0.630623	-2.535062
36	6	0	-5.470954	-0.273001	-1.698460
37	1	0	-4.500962	-0.794983	0.149889
38	6	0	-4.071482	0.730966	-3.386430
39	1	0	-1.999798	0.977433	-2.866844
40	6	0	-5.321177	0.276848	-2.968681
41	1	0	-6.441995	-0.631743	-1.371522
42	1	0	-3.948161	1.155928	-4.377584
43	1	0	-6.175291	0.346502	-3.635050
44	6	0	-1.569682	1.711104	0.539684
45	6	0	-0.338749	2.172036	1.020984
46	6	0	-2.699778	2.528091	0.646814
47	6	0	-0.245754	3.426517	1.617773
48	1	0	0.548345	1.549263	0.918649
49	6	0	-2.601636	3.784453	1.238649
50	1	0	-3.655809	2.181412	0.263186
51	6	0	-1.375985	4.232783	1.726739
52	1	0	0.712298	3.777252	1.988020
53	1	0	-3.482277	4.414847	1.314383
54	1	0	-1.299946	5.213989	2.185122

55	1	0	3.613887	-0.402431	1.937154

Zero-point correction= 0.447613 (Hartree/Particle)
Thermal correction to Energy= 0.475283
Thermal correction to Enthalpy= 0.476227
Thermal correction to Gibbs Free Energy= 0.382642
Sum of electronic and zero-point Energies= -1549.006612
Sum of electronic and thermal Energies= -1548.978942
Sum of electronic and thermal Enthalpies= -1548.977998
Sum of electronic and thermal Free Energies= -1549.071583
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1549.455573
Frequencies

8.2212	9.7857	23.1436
34.0211	37.5548	39.7478
48.2260	48.7693	49.1666
59.8516	62.8719	71.3761
96.2511	129.4217	134.9910
144.9195	190.8627	214.4790
218.6682	246.9780	255.4521
264.1377	270.1447	284.4629
329.8639	407.6051	408.7185
412.2634	418.4285	432.2340
436.1645	444.1464	446.2225
462.8345	477.6092	512.4201
515.5655	526.2684	539.1512
607.2243	628.2817	628.6395
629.5583	634.0696	650.3141
698.2282	702.7635	713.9690
716.2687	718.3797	720.7534
721.4065	723.1590	742.6587
771.9029	776.1261	778.0993
779.0887	839.9932	855.6809
876.1736	883.1186	886.6130
889.7779	924.9950	942.2450
953.2784	957.6696	961.5467
981.2143	991.5166	1002.6458
1006.2499	1007.8679	1009.2997
1014.3851	1014.6063	1015.1128
1015.8380	1017.9974	1028.0052
1031.3278	1033.6395	1034.7324
1069.7369	1070.9752	1071.5720
1079.2649	1097.7088	1123.5699
1124.0966	1125.5357	1129.4271
1138.7237	1141.6228	1146.8021
1189.0076	1191.6001	1192.1642
1196.4450	1207.2823	1222.7725
1224.9995	1226.0455	1226.5940
1275.1753	1332.0392	1335.2679
1336.7203	1347.2623	1367.3819
1368.5553	1368.6455	1378.0279
1395.8803	1451.1044	1472.3117
1494.8496	1495.8756	1496.6957
1514.1977	1543.0425	1544.6184
1547.2076	1566.7426	1669.6070
1670.0650	1670.8124	1672.7127
1686.2656	1689.2339	1690.5253
1703.1275	1741.6634	3092.8887
3104.2597	3165.7412	3173.9243
3180.3897	3196.5945	3197.3811
3197.6699	3202.6415	3204.7596
3214.3036	3217.8335	3218.9535
3226.4805	3226.5851	3229.8396
3231.5795	3234.9007	3237.4509
3242.1364	3243.3700	3243.6649
3247.5236	3248.5413	3249.1819

TS21

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.057410	-0.003249	-1.848313
2	6	0	1.850136	-1.327028	-0.605626
3	6	0	2.072869	0.238510	-2.403945
4	1	0	1.211633	-1.503090	0.259523

5	1	0	1.768510	-2.064106	-1.400472
6	1	0	2.338263	1.181777	-2.864867
7	6	0	2.167268	0.063019	-0.991110
8	6	0	2.488689	0.911928	0.077104
9	1	0	2.274932	-0.638145	-3.017183
10	1	0	3.852364	-0.934798	0.206696
11	6	0	3.905927	-4.207251	0.057476
12	6	0	2.936676	-3.943279	1.214064
13	6	0	3.190531	-2.469594	1.552787
14	7	0	3.425291	-1.875151	0.224361
15	1	0	3.568779	-4.947202	-0.671002
16	1	0	4.893616	-4.521302	0.415360
17	1	0	1.898705	-4.063391	0.886538
18	1	0	3.098012	-4.594235	2.074722
19	6	0	2.637655	2.350451	0.081069
20	6	0	2.258714	3.192331	-0.987051
21	6	0	3.111839	2.990990	1.249162
22	6	0	2.379620	4.576484	-0.896183
23	1	0	1.808827	2.764581	-1.875258
24	6	0	3.229567	4.368765	1.336283
25	1	0	3.393834	2.373639	2.099697
26	6	0	2.870890	5.181301	0.257202
27	1	0	2.070944	5.188867	-1.739242
28	1	0	3.604956	4.816293	2.252875
29	1	0	2.967706	6.260448	0.320181
30	15	0	-1.840850	-0.101724	-0.308253
31	6	0	-1.957813	1.520921	0.546063
32	6	0	-0.794122	2.301101	0.557520
33	6	0	-3.104435	1.991623	1.191136
34	6	0	-0.765551	3.524318	1.221101
35	1	0	0.098968	1.945325	0.049533
36	6	0	-3.079775	3.223105	1.841727
37	1	0	-4.019373	1.406325	1.178510
38	6	0	-1.913083	3.986168	1.862625
39	1	0	0.152262	4.107532	1.217576
40	1	0	-3.976595	3.588216	2.333485
41	1	0	-1.902920	4.944464	2.373495
42	6	0	-1.280036	-1.221406	1.049397
43	6	0	-0.674270	-0.744418	2.214797
44	6	0	-1.338298	-2.606370	0.835983
45	6	0	-0.144331	-1.634897	3.151391
46	1	0	-0.613745	0.325000	2.395278
47	6	0	-0.813792	-3.492483	1.771081
48	1	0	-1.800259	-2.989036	-0.071814
49	6	0	-0.210162	-3.008406	2.933555
50	1	0	0.312642	-1.247895	4.057877
51	1	0	-0.879710	-4.562821	1.596584
52	1	0	0.196097	-3.699929	3.666173
53	6	0	-3.586649	-0.627930	-0.519713
54	6	0	-4.158170	-0.487267	-1.787764
55	6	0	-4.362755	-1.143909	0.525086
56	6	0	-5.487446	-0.840903	-2.006378
57	1	0	-3.549891	-0.106366	-2.605115
58	6	0	-5.688765	-1.503133	0.304908
59	1	0	-3.924145	-1.267724	1.512206
60	6	0	-6.252872	-1.349757	-0.960877
61	1	0	-5.921847	-0.726472	-2.994606
62	1	0	-6.283103	-1.903155	1.120868
63	1	0	-7.287326	-1.631682	-1.132090
64	6	0	4.071641	-2.852936	-0.611649
65	8	0	4.593793	-2.575900	-1.652992
66	1	0	4.084815	-2.343297	2.173188
67	1	0	2.342363	-1.983074	2.040156
68	1	0	2.388736	0.473525	1.073407

Zero-point correction= 0.561663 (Hartree/Particle)
Thermal correction to Energy= 0.595350
Thermal correction to Enthalpy= 0.596295
Thermal correction to Gibbs Free Energy= 0.491425
Sum of electronic and zero-point Energies= -1835.355265
Sum of electronic and thermal Energies= -1835.321577
Sum of electronic and thermal Enthalpies= -1835.320633
Sum of electronic and thermal Free Energies= -1835.425503
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1835.907531
Frequencies

-491.5859	11.4326	25.0227
27.3462	29.4516	35.5547
40.5046	45.2417	47.4485
52.4141	57.8799	65.4323
71.6289	72.7824	78.8765
84.8697	94.7237	110.3169
120.6847	128.3575	151.5176
169.1402	189.2256	197.7372
203.8695	224.5789	229.2806
252.2168	264.8717	278.1503
286.6883	295.7302	332.6206
352.0867	374.7651	404.6408
409.5506	413.4529	421.5008
424.3497	431.5897	460.2392
480.9193	503.5300	508.4402
513.3602	522.7308	532.1924
546.6116	603.7217	619.3643
628.1733	628.2829	629.7482
630.4858	649.2059	666.3977
680.0636	695.4965	696.7623
710.5163	713.4882	716.4480
717.8743	720.0081	723.2591
769.9238	770.7325	777.4541
778.2711	804.7733	835.8692
845.1776	862.6544	864.2039
878.2866	879.9384	884.4447
905.8204	911.0895	940.0420
946.5716	947.7296	952.0231
958.1774	965.4254	983.8510
998.9430	999.8704	1001.3381
1005.2253	1008.2829	1013.0535
1013.8067	1015.4597	1016.3665
1021.3025	1027.4071	1028.1706
1035.4854	1067.6702	1069.4726
1069.8386	1075.9055	1079.9263
1093.9768	1110.3130	1120.1674
1122.2176	1124.9508	1126.0260
1132.9662	1138.6911	1140.2575
1141.2245	1173.0372	1184.6097
1188.0402	1188.8283	1189.4162
1217.0272	1218.6128	1221.0603
1223.1815	1224.7519	1227.4224
1233.8387	1243.8383	1276.6559
1288.3688	1323.4292	1328.3490
1338.2160	1338.3657	1354.7135
1356.3888	1366.2122	1367.6125
1368.6009	1370.5124	1371.4560
1433.7055	1442.1299	1485.3441
1486.1000	1491.0099	1492.6744
1493.9999	1497.0835	1521.1163
1531.2158	1541.1485	1541.7398
1542.8640	1543.4739	1558.7631
1576.9831	1652.5696	1666.6692
1667.4952	1671.3118	1681.1884
1686.5277	1688.8909	1693.3725
1931.1566	3096.6792	3102.4468
3110.3438	3126.3102	3159.6255
3170.1480	3174.3768	3176.7879
3178.9593	3194.5621	3197.9971
3200.5668	3202.9376	3208.5857
3209.6035	3209.9259	3215.2000
3215.2418	3216.7261	3223.3322
3226.3533	3227.3495	3232.4517
3233.5370	3234.2707	3237.0658
3239.1490	3243.3460	3245.8166
3271.5408	3276.2907	3317.2400

INT29

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.600085	-0.555454	-2.053000
2	6	0	1.932120	-1.259857	-0.592540
3	6	0	1.412669	-1.319359	-2.987195

4	1	0	1.878512	-0.612205	0.283828
5	1	0	1.150336	-2.018797	-0.526476
6	1	0	1.562532	-0.983104	-4.009337
7	6	0	1.940164	-0.550248	-1.929262
8	6	0	2.624740	0.668973	-2.031599
9	1	0	1.263396	-2.391380	-2.856389
10	1	0	3.243938	-2.765343	-1.180719
11	6	0	3.922910	-1.847887	1.892645
12	6	0	4.532855	-0.719017	1.046061
13	6	0	4.511777	-1.263828	-0.386097
14	7	0	3.249010	-2.070802	-0.426318
15	1	0	3.200825	-1.500314	2.638467
16	1	0	4.667378	-2.461185	2.410319
17	1	0	3.934975	0.194805	1.109047
18	1	0	5.551669	-0.473370	1.347830
19	6	0	2.899955	1.587310	-0.945903
20	6	0	2.023022	1.762020	0.151195
21	6	0	4.085467	2.359591	-0.924283
22	6	0	2.347591	2.578140	1.228982
23	1	0	1.052423	1.274138	0.122662
24	6	0	4.400428	3.186303	0.145806
25	1	0	4.771445	2.281947	-1.765730
26	6	0	3.547186	3.288856	1.247532
27	1	0	1.637848	2.685170	2.046882
28	1	0	5.327153	3.754052	0.126616
29	1	0	3.799832	3.931128	2.084894
30	15	0	-1.956602	0.012952	-0.323939
31	6	0	-3.658633	-0.626380	-0.025448
32	6	0	-4.500046	-0.732392	-1.137450
33	6	0	-4.148125	-0.995755	1.232511
34	6	0	-5.812009	-1.175009	-0.993989
35	1	0	-4.112112	-0.474792	-2.120518
36	6	0	-5.457536	-1.448516	1.374743
37	1	0	-3.500760	-0.936780	2.104068
38	6	0	-6.292244	-1.534583	0.262889
39	1	0	-6.455562	-1.248898	-1.865329
40	1	0	-5.825621	-1.735828	2.355206
41	1	0	-7.312235	-1.889442	0.375204
42	6	0	-2.116897	1.796199	0.112023
43	6	0	-3.008079	2.279349	1.077044
44	6	0	-1.242216	2.688827	-0.515526
45	6	0	-3.013446	3.629018	1.415350
46	1	0	-3.703111	1.599371	1.562408
47	6	0	-1.235435	4.037398	-0.163096
48	1	0	-0.560370	2.314358	-1.276960
49	6	0	-2.121722	4.507881	0.801429
50	1	0	-3.712507	3.996670	2.160620
51	1	0	-0.538316	4.715726	-0.645073
52	1	0	-2.123132	5.559542	1.072311
53	6	0	-1.059090	-0.636646	1.161784
54	6	0	-0.909532	-2.028297	1.278654
55	6	0	-0.408427	0.183414	2.087535
56	6	0	-0.130697	-2.582642	2.286691
57	1	0	-1.399863	-2.677357	0.555362
58	6	0	0.390783	-0.370520	3.091091
59	1	0	-0.516121	1.263277	2.024227
60	6	0	0.530306	-1.751370	3.195757
61	1	0	-0.026005	-3.660960	2.360625
62	1	0	0.892768	0.285271	3.797542
63	1	0	1.134481	-2.184597	3.988795
64	6	0	3.190463	-2.744539	0.923646
65	8	0	2.641089	-3.788035	1.059386
66	1	0	5.335306	-1.961386	-0.567729
67	1	0	4.458263	-0.500517	-1.164340
68	1	0	2.933976	0.978671	-3.027941

Zero-point correction= 0.563768 (Hartree/Particle)
Thermal correction to Energy= 0.597409
Thermal correction to Enthalpy= 0.598353
Thermal correction to Gibbs Free Energy= 0.494497
Sum of electronic and zero-point Energies= -1835.364535
Sum of electronic and thermal Energies= -1835.330895
Sum of electronic and thermal Enthalpies= -1835.329951
Sum of electronic and thermal Free Energies= -1835.433807
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1835.918289

Frequencies

12.8435	21.6472	27.8839
29.7712	41.5729	42.9320
47.6199	50.8523	55.0391
58.9090	65.3177	76.7914
81.4963	91.7338	95.1133
97.5453	109.6351	113.7281
143.0836	168.2423	180.3031
195.0076	211.3625	218.7204
225.8490	230.3534	251.9407
256.0104	260.3576	280.4735
307.0726	334.8278	358.6089
400.9090	408.2373	410.5580
414.8272	429.3659	433.7376
434.3925	452.2379	474.3260
481.8263	502.1578	513.7108
519.3961	528.6649	540.6741
590.3939	613.3635	624.2175
628.2593	628.6830	630.7060
633.9975	634.2950	648.3003
677.3025	695.9070	708.9889
715.3278	716.2656	718.2617
719.8282	727.2651	729.2310
766.0219	768.1672	770.2932
772.8879	776.6384	825.3861
829.2941	844.4952	868.2891
876.3784	878.1976	886.3480
911.2567	918.7161	922.0346
936.8326	945.8235	951.3299
960.0394	962.0465	983.8049
996.0433	998.8676	999.6418
1008.1823	1009.5897	1011.2361
1012.1926	1015.0091	1015.3742
1016.0184	1021.5870	1027.5895
1038.2939	1066.0621	1067.8532
1069.5260	1070.9206	1073.5322
1103.8167	1118.1021	1120.6965
1121.8675	1123.8364	1127.1721
1130.5792	1135.1802	1139.4899
1183.6921	1185.1384	1188.6145
1189.8892	1197.8854	1214.3448
1219.4534	1220.5641	1220.7864
1223.7868	1232.3187	1257.0036
1290.7299	1293.3902	1319.5791
1326.6360	1333.2808	1335.3772
1336.0661	1343.0565	1351.9713
1364.6247	1365.2258	1366.3876
1369.8346	1372.8780	1382.8406
1404.2174	1429.8110	1468.6765
1488.1521	1491.5106	1494.5858
1495.6141	1496.4957	1509.6947
1515.4702	1537.2072	1538.3943
1542.0425	1542.7632	1549.4744
1584.3365	1645.2121	1659.9827
1671.0290	1671.5901	1681.6553
1683.3397	1688.9231	1690.0622
1985.5558	3109.2502	3111.3666
3138.7970	3140.7772	3160.0650
3160.4732	3180.0040	3184.3405
3188.3272	3191.8284	3195.3023
3198.6367	3199.1057	3199.1125
3201.0373	3204.6896	3208.5475
3212.3472	3213.6931	3215.1150
3215.4455	3222.3918	3223.3395
3224.3150	3227.0051	3231.8339
3232.4440	3232.9709	3233.4344
3234.8333	3244.3997	3458.5168

INT30

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.109494	-0.472450	-1.920928
2	6	0	-1.071948	1.180658	-2.319650

3	6	0	-1.548370	-0.889220	-3.165606
4	1	0	-0.764357	1.572508	-3.291076
5	1	0	-1.059467	1.935828	-1.535152
6	1	0	-1.968137	-1.893447	-3.086664
7	6	0	-2.159022	0.181720	-2.367531
8	6	0	-3.232156	-0.007913	-1.533482
9	1	0	-1.232777	-0.619952	-4.174099
10	1	0	-1.815358	-1.595280	-0.575564
11	6	0	-0.165350	-4.218677	0.562459
12	6	0	-1.612502	-4.533795	0.957691
13	6	0	-2.331589	-3.177440	0.824829
14	7	0	-1.518902	-2.482987	-0.163996
15	1	0	0.358175	-5.028694	0.052624
16	1	0	0.437889	-3.907418	1.423427
17	1	0	-2.042149	-5.246341	0.247922
18	1	0	-1.707312	-4.953415	1.960491
19	6	0	-3.717423	0.837712	-0.450290
20	6	0	-4.523059	0.259817	0.552691
21	6	0	-3.449714	2.216451	-0.327997
22	6	0	-5.004604	0.998237	1.626095
23	1	0	-4.770844	-0.797125	0.474878
24	6	0	-3.914796	2.950504	0.757813
25	1	0	-2.900399	2.724907	-1.112338
26	6	0	-4.688673	2.350924	1.750030
27	1	0	-5.625495	0.513579	2.375205
28	1	0	-3.683649	4.010438	0.818725
29	1	0	-5.053673	2.930208	2.592106
30	15	0	1.507936	0.424525	-0.129651
31	6	0	1.595407	2.239562	0.076194
32	6	0	1.656552	3.026505	-1.077981
33	6	0	1.610830	2.857996	1.331277
34	6	0	1.751529	4.412377	-0.979295
35	1	0	1.614190	2.546484	-2.053390
36	6	0	1.702416	4.243128	1.427803
37	1	0	1.545114	2.252494	2.231821
38	6	0	1.775144	5.020379	0.272996
39	1	0	1.795409	5.016530	-1.879975
40	1	0	1.712981	4.716844	2.404626
41	1	0	1.841919	6.101252	0.350718
42	6	0	3.219128	-0.159865	0.165542
43	6	0	4.198556	0.622445	0.784316
44	6	0	3.536343	-1.458169	-0.255420
45	6	0	5.478393	0.111333	0.984108
46	1	0	3.967283	1.635158	1.101279
47	6	0	4.814677	-1.967163	-0.042052
48	1	0	2.775683	-2.067263	-0.739106
49	6	0	5.787209	-1.183235	0.574225
50	1	0	6.235565	0.727610	1.459199
51	1	0	5.053338	-2.974849	-0.368135
52	1	0	6.786180	-1.579132	0.729728
53	6	0	0.584609	-0.114116	1.363731
54	6	0	-0.715361	0.385847	1.527768
55	6	0	1.073213	-1.059876	2.266370
56	6	0	-1.503979	-0.031315	2.593862
57	1	0	-1.119826	1.109540	0.821911
58	6	0	0.273724	-1.490457	3.327493
59	1	0	2.077579	-1.457779	2.148214
60	6	0	-1.006729	-0.972328	3.498457
61	1	0	-2.504422	0.377011	2.704103
62	1	0	0.663847	-2.221312	4.030204
63	1	0	-1.619004	-1.300258	4.333523
64	1	0	-3.360432	-3.279485	0.469158
65	1	0	-2.340889	-2.618535	1.767158
66	6	0	-0.296711	-3.006757	-0.343414
67	8	0	0.594070	-2.585651	-1.093554
68	1	0	-3.767442	-0.950777	-1.655845

Zero-point correction= 0.563062 (Hartree/Particle)
Thermal correction to Energy= 0.596676
Thermal correction to Enthalpy= 0.597621
Thermal correction to Gibbs Free Energy= 0.494497
Sum of electronic and zero-point Energies= -1835.437410
Sum of electronic and thermal Energies= -1835.403796
Sum of electronic and thermal Enthalpies= -1835.402852
Sum of electronic and thermal Free Energies= -1835.505976

M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1835.973223
Frequencies

12.5471	22.9183	29.4105
33.0979	39.6426	42.6700
51.6371	54.5916	61.0340
65.8737	70.0871	72.2403
90.4189	98.0589	106.0509
114.3477	120.2894	136.6035
146.1598	148.7707	167.8542
186.2334	197.7407	205.8907
214.1709	225.9483	240.7531
255.8113	257.3045	284.1645
285.2119	319.5767	338.7774
407.4883	408.5468	412.4375
420.0141	421.5192	427.9828
439.7420	450.8141	462.9683
501.1228	506.6441	516.0188
522.1158	533.4835	541.3452
553.2714	623.1236	626.6867
628.3124	629.4632	629.9541
643.6013	662.3337	700.3255
702.3991	713.2338	714.0394
715.1549	717.7956	722.3226
725.3005	736.5913	742.2261
763.8494	769.3348	772.5286
776.7942	777.8462	816.1853
837.1543	839.1694	866.6615
877.7558	886.7540	889.6528
918.2519	919.5111	927.0754
935.9424	949.7677	952.3517
955.2543	959.4377	965.9224
977.7779	982.7358	999.9299
1001.4786	1007.1247	1010.0691
1010.2965	1014.3674	1015.4095
1016.4361	1024.6233	1027.0972
1031.5085	1031.8270	1032.9085
1069.2512	1070.4031	1070.8096
1071.0282	1095.0049	1109.9056
1121.1070	1122.1831	1124.8493
1130.3244	1131.0851	1137.3820
1144.6261	1147.3691	1180.1044
1187.8653	1190.8932	1196.5499
1205.7132	1213.4163	1216.1087
1222.0599	1225.9830	1233.8201
1237.5856	1266.9632	1278.6068
1313.3792	1333.3800	1333.5064
1342.0976	1342.9641	1348.0208
1364.8115	1366.2062	1367.4517
1371.4762	1375.5206	1400.3563
1415.3237	1478.9405	1492.9365
1493.2481	1494.8400	1498.2072
1500.2775	1507.3920	1510.8956
1532.6104	1543.5545	1544.6180
1547.7693	1552.7711	1556.3077
1639.5871	1662.2826	1667.8979
1671.3934	1672.9267	1684.4089
1686.9734	1688.1521	1697.9703
1779.1371	3096.8857	3105.2428
3121.4686	3123.2475	3130.2036
3144.5469	3145.0583	3176.8139
3182.5261	3189.1738	3200.9907
3204.0086	3205.7346	3207.5043
3208.3496	3209.7369	3212.6830
3215.0835	3215.4011	3222.7788
3223.3163	3223.9132	3224.6688
3226.7826	3229.2428	3230.8862
3238.4532	3238.8226	3244.7228
3245.5301	3254.3703	3481.9384

TS22

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.193735	0.572957	-1.352245

2	6	0	-0.758933	2.493314	-0.774691
3	6	0	-2.107363	1.285375	-2.250921
4	1	0	-0.440342	3.159531	-1.575832
5	1	0	-0.452244	2.808043	0.221884
6	1	0	-2.860233	0.557229	-2.525677
7	6	0	-2.028288	1.809298	-0.938813
8	6	0	-2.773867	1.305948	0.201782
9	1	0	-1.677739	1.856133	-3.071243
10	1	0	-2.271698	-0.048796	0.192405
11	6	0	-1.305832	-3.509311	-0.278262
12	6	0	-1.996772	-3.470443	1.085939
13	6	0	-2.778224	-2.144461	1.030191
14	7	0	-2.026550	-1.308937	0.099034
15	1	0	-1.910415	-4.011697	-1.043047
16	1	0	-0.315121	-3.969694	-0.277263
17	1	0	-2.638518	-4.332159	1.283341
18	1	0	-1.240802	-3.414130	1.875983
19	6	0	-4.234404	1.039591	0.108229
20	6	0	-5.128236	1.710105	0.959072
21	6	0	-4.777422	0.075293	-0.758396
22	6	0	-6.494271	1.456048	0.929635
23	1	0	-4.733899	2.453193	1.648036
24	6	0	-6.147758	-0.171917	-0.798673
25	1	0	-4.115718	-0.523267	-1.376836
26	6	0	-7.016549	0.517582	0.040966
27	1	0	-7.155970	2.000186	1.597938
28	1	0	-6.535048	-0.920173	-1.484691
29	1	0	-8.083864	0.321867	0.010721
30	15	0	1.782692	0.245349	-0.073991
31	6	0	2.596420	1.712143	0.654326
32	6	0	2.631263	2.884419	-0.108300
33	6	0	3.196181	1.694774	1.917107
34	6	0	3.268401	4.021325	0.379201
35	1	0	2.148296	2.901704	-1.082987
36	6	0	3.827330	2.836047	2.405553
37	1	0	3.165853	0.789791	2.518294
38	6	0	3.865203	3.998006	1.637572
39	1	0	3.290033	4.926957	-0.218675
40	1	0	4.288042	2.817794	3.388426
41	1	0	4.354411	4.887270	2.022866
42	6	0	3.137079	-0.660462	-0.906002
43	6	0	4.485551	-0.346913	-0.715195
44	6	0	2.779894	-1.720559	-1.750500
45	6	0	5.470950	-1.089228	-1.362406
46	1	0	4.768626	0.477198	-0.066867
47	6	0	3.771760	-2.461247	-2.386611
48	1	0	1.728226	-1.961812	-1.896144
49	6	0	5.115828	-2.145948	-2.196256
50	1	0	6.517030	-0.839591	-1.213875
51	1	0	3.492042	-3.283530	-3.037795
52	1	0	5.886500	-2.721487	-2.699923
53	6	0	1.373284	-0.791256	1.380907
54	6	0	0.245692	-0.441415	2.135322
55	6	0	2.139725	-1.895291	1.761289
56	6	0	-0.088530	-1.168329	3.273312
57	1	0	-0.376409	0.396449	1.824900
58	6	0	1.789708	-2.634505	2.890558
59	1	0	3.009669	-2.178780	1.175916
60	6	0	0.682757	-2.267746	3.651088
61	1	0	-0.958305	-0.884096	3.857747
62	1	0	2.387492	-3.494011	3.177389
63	1	0	0.415279	-2.841158	4.533414
64	1	0	-3.804781	-2.285072	0.664241
65	1	0	-2.846537	-1.651369	2.006732
66	6	0	-1.204531	-2.032539	-0.640996
67	8	0	-0.421576	-1.630953	-1.547203
68	1	0	-2.520261	1.855222	1.111966

Zero-point correction= 0.558719 (Hartree/Particle)
Thermal correction to Energy= 0.591633
Thermal correction to Enthalpy= 0.592577
Thermal correction to Gibbs Free Energy= 0.492010
Sum of electronic and zero-point Energies= -1835.419288
Sum of electronic and thermal Energies= -1835.386374
Sum of electronic and thermal Enthalpies= -1835.385429

Sum of electronic and thermal Free Energies= -1835.485996
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1835.950937
Frequencies

-1326.6490	21.5445	25.5549
32.7094	37.1525	43.8683
48.3323	50.6693	56.2728
63.4630	69.6730	71.3765
82.1754	87.2662	94.2687
111.2007	122.6545	141.1421
152.6893	155.3224	169.4208
188.8210	203.3021	209.6454
220.6787	224.7932	257.0102
257.8830	266.4290	268.3687
282.4703	285.8822	315.8261
341.3404	409.6126	411.8852
415.6768	420.0890	429.4274
438.5961	442.3103	448.4551
457.0753	514.6597	518.9008
521.9418	532.5423	534.1031
555.9420	577.5237	599.3134
628.1149	629.4967	632.4637
636.3389	657.1867	692.3846
705.7299	713.6745	718.0321
718.6242	719.9031	725.2666
727.3495	729.0426	752.5141
765.9894	772.8992	774.2162
777.9924	797.1697	831.2182
862.4698	880.8765	883.3736
884.8122	888.8883	891.4947
910.2352	916.2354	940.3253
947.6734	955.4761	956.4322
961.4231	964.8171	967.8018
992.5327	1003.7034	1005.9178
1009.7782	1012.5962	1013.8688
1014.4537	1015.9901	1016.3261
1018.3058	1021.3849	1030.2875
1030.4528	1034.5846	1042.2303
1054.4034	1070.1602	1073.1409
1073.9846	1081.7750	1101.6614
1123.9442	1126.9042	1129.7878
1134.7541	1143.7937	1143.9917
1146.4764	1149.6515	1186.4015
1189.8408	1192.6790	1193.8031
1199.3752	1222.9271	1223.8079
1233.6980	1234.6683	1238.0412
1243.8831	1262.0875	1279.0997
1313.8240	1334.5546	1338.1261
1339.7393	1342.6753	1349.8293
1364.7723	1369.7756	1370.0049
1378.8260	1380.2545	1406.7039
1419.3231	1460.9799	1491.5053
1495.0001	1496.2042	1496.6516
1503.5996	1507.9292	1519.5784
1524.9884	1543.5120	1545.9304
1550.0596	1552.5597	1552.7825
1564.8950	1586.8695	1668.7656
1669.8513	1672.6285	1673.5995
1688.5091	1689.4564	1690.5676
1702.2509	1724.6665	3065.4479
3088.3171	3107.1449	3116.5377
3125.6610	3141.7020	3150.9279
3165.3423	3178.5515	3198.1524
3199.3021	3204.9229	3207.7862
3208.6325	3211.7561	3212.5041
3219.2558	3221.7058	3222.6230
3226.2938	3227.6702	3228.4930
3230.5823	3232.5636	3237.5665
3239.2127	3244.0704	3244.3008
3247.1447	3254.9459	3285.9496

INT31

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

1	46	0	0.192612	0.753258	-1.533149
2	6	0	1.955762	-0.073423	-2.441903
3	6	0	1.132436	2.106991	-2.980860
4	1	0	1.530649	-0.510470	-3.344248
5	1	0	2.599771	-0.717050	-1.852303
6	1	0	1.051360	3.165262	-2.754509
7	6	0	2.131275	1.332096	-2.371268
8	6	0	3.102165	1.967719	-1.386700
9	1	0	0.631630	1.755469	-3.880225
10	1	0	2.648687	2.895008	-1.020281
11	6	0	-2.465160	3.481965	0.503263
12	6	0	-1.728038	4.640945	1.176241
13	6	0	-0.272667	4.116629	1.239221
14	7	0	-0.137398	3.106326	0.196598
15	1	0	-3.244747	3.780884	-0.201756
16	1	0	-2.915757	2.788264	1.225470
17	1	0	-1.771640	5.531050	0.540100
18	1	0	-2.128005	4.911261	2.157573
19	6	0	3.447018	1.063071	-0.228702
20	6	0	2.620354	1.050630	0.898353
21	6	0	4.513445	0.165905	-0.298783
22	6	0	2.841306	0.133388	1.922716
23	1	0	1.796417	1.763659	0.933833
24	6	0	4.735519	-0.752323	0.725978
25	1	0	5.164624	0.175687	-1.170455
26	6	0	3.893920	-0.776065	1.834957
27	1	0	2.186948	0.120210	2.790559
28	1	0	5.563609	-1.451455	0.655519
29	1	0	4.051807	-1.503827	2.625009
30	15	0	-0.665669	-0.915658	-0.040220
31	6	0	0.469777	-2.157615	0.678529
32	6	0	1.394391	-2.767145	-0.177049
33	6	0	0.472367	-2.490245	2.035682
34	6	0	2.308727	-3.692199	0.314452
35	1	0	1.392935	-2.513900	-1.234292
36	6	0	1.395558	-3.411522	2.527922
37	1	0	-0.240437	-2.026209	2.711005
38	6	0	2.314624	-4.010567	1.671508
39	1	0	3.023184	-4.155270	-0.359055
40	1	0	1.393534	-3.660564	3.584816
41	1	0	3.034670	-4.724488	2.059717
42	6	0	-1.964960	-1.881029	-0.888761
43	6	0	-2.072954	-3.269829	-0.800908
44	6	0	-2.884408	-1.152561	-1.656919
45	6	0	-3.092084	-3.931249	-1.484708
46	1	0	-1.363308	-3.835285	-0.203254
47	6	0	-3.903689	-1.820408	-2.328005
48	1	0	-2.799447	-0.067094	-1.705222
49	6	0	-4.005465	-3.209044	-2.247058
50	1	0	-3.171642	-5.012045	-1.418222
51	1	0	-4.617313	-1.255255	-2.919527
52	1	0	-4.798246	-3.727219	-2.777871
53	6	0	-1.528242	-0.204393	1.410277
54	6	0	-0.850614	0.748507	2.179846
55	6	0	-2.819317	-0.590221	1.778855
56	6	0	-1.452871	1.298993	3.307042
57	1	0	0.138133	1.075935	1.877833
58	6	0	-3.423989	-0.028605	2.902361
59	1	0	-3.358328	-1.325145	1.188577
60	6	0	-2.743047	0.913426	3.667856
61	1	0	-0.917899	2.038096	3.895718
62	1	0	-4.430038	-0.329884	3.177240
63	1	0	-3.216676	1.350182	4.541738
64	1	0	0.462327	4.918676	1.105302
65	1	0	-0.065277	3.666535	2.225126
66	6	0	-1.325205	2.752571	-0.197466
67	8	0	-1.591097	1.832262	-1.059052
68	1	0	4.008290	2.235267	-1.945345

Zero-point correction= 0.563551 (Hartree/Particle)
Thermal correction to Energy= 0.596953
Thermal correction to Enthalpy= 0.597897
Thermal correction to Gibbs Free Energy= 0.496774
Sum of electronic and zero-point Energies= -1835.454570
Sum of electronic and thermal Energies= -1835.421168

Sum of electronic and thermal Enthalpies= -1835.420224
Sum of electronic and thermal Free Energies= -1835.521347
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1835.987602
Frequencies

20.2143	32.0143	40.9102
44.3254	48.3209	50.8218
54.3274	56.7305	62.9033
67.3111	74.4190	77.6826
81.4748	91.6581	102.9086
112.2085	116.3977	121.1754
138.1911	154.9357	173.0690
191.5386	205.9292	220.2041
225.9219	251.6598	259.6926
271.7833	274.5249	276.9378
287.2446	308.1549	339.3718
365.5045	378.4171	408.0601
409.9693	415.8609	421.2242
428.6724	453.4175	457.8588
465.1739	509.4580	515.6277
516.3385	534.0203	557.8965
560.2645	575.5127	626.5631
627.1708	629.8691	630.4912
635.1993	652.9339	702.0338
707.7994	715.5134	720.1300
720.6341	723.4050	724.9437
725.8205	762.4314	764.2237
774.1964	775.4958	777.3141
817.4107	835.4223	849.9014
860.1363	880.0661	881.6648
884.6355	890.3584	904.3943
918.3409	925.6808	936.4102
945.1508	949.5001	958.5682
960.3805	967.2411	976.8004
985.6501	997.1477	999.7330
1010.0408	1013.0244	1014.2163
1015.5380	1017.1598	1017.8063
1020.1764	1025.7041	1029.6746
1032.0541	1039.9149	1070.4480
1071.2894	1072.5637	1075.8818
1082.8302	1092.0741	1116.3118
1126.4214	1127.0516	1127.2551
1129.4598	1140.2161	1144.3116
1146.0927	1182.5156	1193.9561
1194.7116	1194.8483	1196.7803
1221.3020	1225.2550	1225.9791
1227.7557	1229.3255	1230.5949
1255.1970	1256.2692	1303.1627
1331.3989	1332.5921	1337.3109
1340.6095	1346.4620	1356.6338
1367.0906	1371.2166	1371.6466
1377.3129	1382.6884	1386.6264
1434.4136	1477.2620	1494.8209
1497.6405	1497.8186	1498.0684
1499.5136	1521.0806	1522.5532
1541.3944	1546.3774	1546.8380
1547.5207	1548.8468	1561.1438
1567.3327	1671.0020	1672.7662
1674.6581	1680.6094	1685.1163
1687.3623	1687.7021	1690.4437
1707.4017	3016.8442	3078.3810
3085.4526	3089.4693	3100.2489
3138.2992	3138.6117	3150.9499
3164.5205	3173.3419	3182.8187
3201.4713	3206.0323	3208.1438
3215.1525	3215.2907	3218.3156
3219.7636	3220.0326	3222.0621
3224.8101	3226.2825	3231.1279
3234.0073	3235.6253	3238.5980
3239.1611	3248.3880	3250.9605
3257.1529	3272.2037	3281.1897

INT32

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

1	6	0	1.351569	4.938075	0.034548
2	1	0	1.319347	5.845752	-0.563320
3	1	0	2.337951	4.491930	0.127267
4	6	0	0.434239	4.853783	1.257060
5	1	0	0.829828	4.348675	2.134127
6	6	0	0.163483	4.068827	0.041512
7	6	0	-0.818274	3.500495	-0.700801
8	46	0	0.673105	1.860010	0.047560
9	1	0	-0.204356	5.706880	1.474259
10	15	0	1.383439	-0.380743	0.032507
11	6	0	0.324102	-1.423737	-1.047576
12	6	0	-1.044923	-1.468530	-0.752165
13	6	0	0.799613	-2.107982	-2.167878
14	6	0	-1.925030	-2.177411	-1.560184
15	1	0	-1.427573	-0.942893	0.119685
16	6	0	-0.084445	-2.816991	-2.981447
17	1	0	1.857302	-2.085877	-2.413597
18	6	0	-1.442584	-2.851208	-2.682670
19	1	0	-2.983399	-2.192364	-1.315463
20	1	0	0.294493	-3.342109	-3.853336
21	1	0	-2.126229	-3.400625	-3.322884
22	6	0	1.370512	-1.315238	1.614525
23	6	0	1.067891	-2.678407	1.701797
24	6	0	1.693608	-0.613725	2.780613
25	6	0	1.102288	-3.327794	2.933400
26	1	0	0.797349	-3.230213	0.805069
27	6	0	1.735573	-1.265041	4.009742
28	1	0	1.902000	0.452333	2.717222
29	6	0	1.439306	-2.623913	4.087383
30	1	0	0.863297	-4.385456	2.991419
31	1	0	1.989231	-0.709892	4.907515
32	1	0	1.463451	-3.132343	5.046475
33	6	0	3.069200	-0.703415	-0.625133
34	6	0	3.606667	0.236849	-1.510264
35	6	0	3.806021	-1.851950	-0.318697
36	6	0	4.853491	0.025096	-2.093659
37	1	0	3.037413	1.136880	-1.734381
38	6	0	5.056717	-2.057618	-0.894425
39	1	0	3.403923	-2.584611	0.375580
40	6	0	5.579944	-1.122003	-1.785041
41	1	0	5.259813	0.759243	-2.782520
42	1	0	5.624250	-2.949396	-0.646634
43	1	0	6.555609	-1.284527	-2.232917
44	1	0	-0.662794	3.375569	-1.773059
45	6	0	-2.211199	3.240328	-0.183129
46	6	0	-2.654081	1.778860	-0.284167
47	1	0	-2.913186	3.867213	-0.753705
48	1	0	-2.270215	3.567776	0.862291
49	6	0	-4.127735	1.583574	0.088784
50	1	0	-2.473209	1.391857	-1.296071
51	1	0	-2.019661	1.184045	0.384748
52	1	0	-4.299424	2.009143	1.086618
53	1	0	-4.761141	2.148613	-0.606045
54	6	0	-4.539789	0.130993	0.085403
55	6	0	-5.354202	-0.392908	-0.919911
56	6	0	-4.094541	-0.729704	1.095109
57	6	0	-5.729066	-1.735755	-0.912365
58	1	0	-5.707071	0.262285	-1.712590
59	6	0	-4.458990	-2.072543	1.104720
60	1	0	-3.459897	-0.336727	1.887376
61	6	0	-5.284358	-2.579621	0.101738
62	1	0	-6.372029	-2.120540	-1.698413
63	1	0	-4.103428	-2.722997	1.898062
64	1	0	-5.576095	-3.625268	0.110942

Zero-point correction= 0.535112 (Hartree/Particle)
Thermal correction to Energy= 0.567102
Thermal correction to Enthalpy= 0.568047
Thermal correction to Gibbs Free Energy= 0.466570
Sum of electronic and zero-point Energies= -1666.822513
Sum of electronic and thermal Energies= -1666.790523
Sum of electronic and thermal Enthalpies= -1666.789579
Sum of electronic and thermal Free Energies= -1666.891056
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1667.299688

Frequencies

14.4441	21.3792	27.3464
33.0420	36.9364	42.8508
47.5357	52.4413	57.2684
58.9583	64.5876	66.5758
74.4526	81.6567	86.3167
100.7221	111.2407	116.5109
157.3061	162.5062	181.9711
196.4237	211.1079	216.3812
225.7414	242.7747	255.7162
264.5112	266.1106	280.3533
320.7644	357.5476	409.6402
411.5767	414.1250	415.2580
435.4717	437.4865	450.6511
451.1281	499.6918	506.7516
518.6142	527.6442	529.3840
601.5225	629.7439	630.0014
631.7881	633.7541	702.9883
714.2693	716.1502	718.1156
719.3055	720.0857	722.0011
742.6872	766.5725	767.8939
772.1162	774.4772	779.9307
784.0438	826.0211	839.4451
866.2547	874.5639	881.8809
885.8862	890.2829	939.7859
947.3370	955.1867	963.3145
963.4014	990.3686	998.5697
1002.4026	1007.2024	1009.3398
1010.2159	1013.6699	1015.5172
1015.7036	1016.3967	1020.2327
1020.7139	1026.6818	1031.6923
1050.4745	1069.7895	1070.8526
1071.3163	1072.9249	1074.1426
1079.8392	1088.3803	1098.3435
1102.4283	1121.8520	1122.5433
1128.4907	1130.3570	1138.7979
1140.9323	1142.6102	1145.4780
1177.8576	1187.5516	1188.0755
1188.5096	1192.5117	1197.6638
1214.8651	1217.7823	1220.9415
1230.2144	1246.6161	1267.7114
1296.4927	1330.3945	1336.6338
1338.2361	1338.9070	1347.8022
1363.6584	1366.2709	1366.4219
1368.6353	1373.1108	1391.9083
1415.7846	1478.0212	1492.9628
1497.0359	1500.7147	1500.9346
1506.8880	1509.4582	1513.8762
1526.3105	1540.6391	1543.4368
1549.8353	1561.5366	1669.4778
1671.9429	1673.5084	1685.0299
1687.6335	1688.6374	1690.7080
1703.2145	1785.6258	3044.3379
3063.6060	3075.6032	3099.7197
3108.2899	3128.9653	3149.2547
3160.9279	3173.5666	3187.3620
3195.6811	3197.9602	3203.5107
3205.8818	3208.8311	3213.1681
3215.1629	3218.9942	3219.3956
3222.2609	3224.7526	3229.1328
3230.3260	3234.4216	3237.5286
3238.7185	3242.0088	3242.1969
3245.3594	3247.7778	3250.2724

INT33

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.844231	0.036432	0.336638
2	46	0	-0.647925	-0.347706	-0.030022
3	6	0	1.486408	-1.069026	-1.333623
4	6	0	1.926880	-0.559374	0.086794
5	1	0	1.129320	-0.331537	-2.050669
6	1	0	0.996328	-2.039144	-1.394655

7	1	0	1.725330	-1.201561	0.943048
8	6	0	2.883668	-1.019176	-0.919834
9	6	0	4.153497	-1.225792	-1.220619
10	1	0	1.862313	0.509187	0.289286
11	1	0	4.403814	-1.624851	-2.203931
12	6	0	5.293316	-0.972261	-0.276194
13	6	0	6.078231	-2.249866	0.040412
14	1	0	4.905531	-0.534000	0.651291
15	1	0	5.980738	-0.235807	-0.716100
16	6	0	7.266704	-1.990104	0.973675
17	1	0	5.407823	-2.987116	0.499249
18	1	0	6.444451	-2.702086	-0.890834
19	1	0	7.937270	-1.257466	0.507080
20	1	0	6.900165	-1.536917	1.903297
21	6	0	8.027254	-3.254848	1.286076
22	6	0	9.081229	-3.675133	0.471589
23	6	0	7.657631	-4.060075	2.365969
24	6	0	9.752875	-4.866676	0.730239
25	1	0	9.380060	-3.057222	-0.372318
26	6	0	8.325462	-5.252437	2.629673
27	1	0	6.838888	-3.743946	3.008626
28	6	0	9.376534	-5.659358	1.811661
29	1	0	10.573723	-5.174505	0.089523
30	1	0	8.027898	-5.862389	3.477248
31	1	0	9.901067	-6.587164	2.017448
32	6	0	-3.854220	0.201148	-1.195797
33	6	0	-3.286195	0.911839	-2.259477
34	6	0	-5.144525	-0.317550	-1.338844
35	6	0	-3.999126	1.118271	-3.435333
36	1	0	-2.273135	1.295372	-2.156845
37	6	0	-5.853139	-0.122034	-2.523212
38	1	0	-5.598634	-0.878293	-0.526465
39	6	0	-5.285400	0.598638	-3.570022
40	1	0	-3.547184	1.674577	-4.250931
41	1	0	-6.851980	-0.535292	-2.626418
42	1	0	-5.839601	0.749693	-4.491388
43	6	0	-3.764278	-1.256151	1.271347
44	6	0	-4.840653	-0.974959	2.118661
45	6	0	-3.365718	-2.585915	1.097964
46	6	0	-5.509397	-2.007347	2.773199
47	1	0	-5.156035	0.053512	2.271835
48	6	0	-4.041026	-3.617448	1.743395
49	1	0	-2.512561	-2.802527	0.458351
50	6	0	-5.113580	-3.328886	2.584420
51	1	0	-6.340842	-1.776737	3.432484
52	1	0	-3.722718	-4.645389	1.598794
53	1	0	-5.634904	-4.131717	3.096776
54	6	0	-3.308445	1.566584	1.251461
55	6	0	-2.501539	1.951110	2.328084
56	6	0	-4.430597	2.338454	0.934595
57	6	0	-2.820600	3.073913	3.085706
58	1	0	-1.615400	1.364967	2.561908
59	6	0	-4.742822	3.469237	1.686479
60	1	0	-5.061959	2.058400	0.096057
61	6	0	-3.941931	3.836435	2.764347
62	1	0	-2.188878	3.359838	3.921120
63	1	0	-5.613882	4.063578	1.427690
64	1	0	-4.186841	4.718070	3.348680

Zero-point correction= 0.534606 (Hartree/Particle)
Thermal correction to Energy= 0.566199
Thermal correction to Enthalpy= 0.567143
Thermal correction to Gibbs Free Energy= 0.463715
Sum of electronic and zero-point Energies= -1666.802376
Sum of electronic and thermal Energies= -1666.770783
Sum of electronic and thermal Enthalpies= -1666.769839
Sum of electronic and thermal Free Energies= -1666.873267
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1667.297308
Frequencies

-3.2851	12.9178	16.1926
20.7159	21.8097	25.9522
29.9380	40.4884	46.1591
52.1302	54.8700	58.7789
62.9571	71.8145	79.4312
85.9364	94.6075	100.4123

122.5377	139.1032	176.8660
202.5011	221.6388	223.0822
230.1437	242.6309	259.4852
266.1628	273.1838	275.2702
317.0990	356.7313	408.0363
408.6730	413.7804	417.0164
427.4433	441.2988	443.0568
446.4988	513.9607	514.3704
516.5585	528.6487	536.0339
602.9903	629.5180	631.1999
633.8667	637.0559	703.7378
713.4011	714.1588	717.5792
718.1814	718.4210	719.0024
732.8074	748.6880	757.6006
768.7394	773.0281	774.7305
775.0339	810.5946	841.0882
863.7165	873.5908	877.5911
880.4308	885.0580	936.0997
948.4324	955.2318	956.7641
971.5274	989.0592	990.1539
999.5243	1001.1507	1004.5055
1014.5647	1014.6935	1015.5782
1016.5708	1017.6610	1021.8278
1022.6671	1025.9114	1027.0211
1039.4122	1057.3018	1067.2909
1070.4225	1073.0758	1073.2153
1074.0787	1081.3185	1095.5960
1108.8766	1121.0256	1126.6739
1130.3486	1131.0808	1137.0898
1141.1329	1144.0982	1144.5549
1157.3518	1188.4777	1191.4189
1191.9233	1198.3104	1198.7388
1218.6372	1223.3258	1228.8163
1231.6874	1250.0940	1268.0313
1297.0271	1331.5953	1334.7765
1335.6334	1339.2747	1348.3330
1363.4080	1370.9742	1371.3720
1374.6557	1377.7596	1392.9516
1415.6630	1460.3481	1490.2697
1494.3233	1497.5485	1502.2205
1508.8131	1514.0967	1524.4615
1531.6340	1541.8360	1547.2061
1551.0377	1570.9570	1671.0661
1672.5116	1674.2189	1685.8915
1690.4273	1690.4655	1692.5279
1714.3952	1912.0850	3058.3391
3068.5620	3078.3486	3104.5665
3116.0886	3131.8027	3133.6552
3142.3146	3170.1129	3197.4980
3197.6797	3200.8933	3204.4730
3209.6357	3209.9609	3210.2982
3215.4837	3216.1840	3217.8982
3221.3954	3223.8571	3224.0885
3226.3819	3228.2793	3229.1356
3229.5592	3238.1117	3238.4981
3240.4894	3248.0665	3250.3495

TS23

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.411789	0.565601	-0.532709
2	6	0	1.442212	1.566502	-1.049422
3	6	0	1.510416	-0.372017	-0.845336
4	1	0	1.473691	2.211986	-0.169541
5	1	0	1.056847	2.040396	-1.954406
6	1	0	1.170988	-1.052020	-1.630226
7	6	0	2.541507	0.609540	-1.210872
8	6	0	3.824612	0.608629	-1.545637
9	1	0	1.585697	-0.819597	0.148335
10	15	0	-2.783538	0.700621	-0.033282
11	6	0	-3.272897	0.387766	1.710314
12	6	0	-2.567155	-0.601888	2.403346
13	6	0	-4.309832	1.066368	2.357819

14	6	0	-2.906619	-0.924985	3.713237
15	1	0	-1.742435	-1.111646	1.909703
16	6	0	-4.641812	0.748725	3.673251
17	1	0	-4.856321	1.847355	1.835880
18	6	0	-3.944674	-0.248512	4.350512
19	1	0	-2.354567	-1.697107	4.240049
20	1	0	-5.445973	1.283100	4.169849
21	1	0	-4.204382	-0.492980	5.375949
22	6	0	-3.857321	-0.463803	-0.964800
23	6	0	-5.051360	-0.984451	-0.455137
24	6	0	-3.446484	-0.829005	-2.251209
25	6	0	-5.826387	-1.846477	-1.227064
26	1	0	-5.372705	-0.720790	0.549102
27	6	0	-4.225418	-1.685940	-3.023531
28	1	0	-2.505072	-0.443558	-2.636963
29	6	0	-5.416109	-2.196073	-2.511500
30	1	0	-6.750383	-2.248350	-0.822697
31	1	0	-3.897596	-1.963528	-4.020491
32	1	0	-6.020551	-2.870649	-3.110107
33	6	0	-3.542818	2.337825	-0.378210
34	6	0	-2.773338	3.473338	-0.100904
35	6	0	-4.839494	2.497295	-0.875814
36	6	0	-3.297975	4.746787	-0.297830
37	1	0	-1.755729	3.350709	0.264426
38	6	0	-5.359873	3.773362	-1.081140
39	1	0	-5.442696	1.624447	-1.109396
40	6	0	-4.593073	4.898211	-0.789195
41	1	0	-2.693131	5.620387	-0.075340
42	1	0	-6.365889	3.887444	-1.473222
43	1	0	-5.001470	5.891124	-0.950546
44	1	0	4.309941	1.558045	-1.775048
45	6	0	4.675862	-0.626914	-1.603080
46	6	0	5.849288	-0.570666	-0.618911
47	1	0	5.075298	-0.759077	-2.618994
48	1	0	4.056881	-1.507280	-1.388627
49	6	0	6.751923	-1.807152	-0.707482
50	1	0	6.450871	0.327794	-0.811168
51	1	0	5.464820	-0.471449	0.403726
52	1	0	6.152718	-2.705421	-0.513174
53	1	0	7.135970	-1.897664	-1.731510
54	6	0	7.901328	-1.738620	0.267021
55	6	0	9.075038	-1.056471	-0.063769
56	6	0	7.796821	-2.304434	1.539562
57	6	0	10.118386	-0.943947	0.850209
58	1	0	9.170561	-0.611917	-1.052121
59	6	0	8.837422	-2.195778	2.458070
60	1	0	6.889035	-2.838965	1.809963
61	6	0	10.002546	-1.514584	2.115730
62	1	0	11.024012	-0.412442	0.573633
63	1	0	8.738546	-2.645845	3.441384
64	1	0	10.815747	-1.429913	2.829819

Zero-point correction= 0.532290 (Hartree/Particle)
Thermal correction to Energy= 0.564163
Thermal correction to Enthalpy= 0.565108
Thermal correction to Gibbs Free Energy= 0.459412
Sum of electronic and zero-point Energies= -1666.784054
Sum of electronic and thermal Energies= -1666.752181
Sum of electronic and thermal Enthalpies= -1666.751237
Sum of electronic and thermal Free Energies= -1666.856933
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1667.258558
Frequencies

-212.8888	7.7024	10.4757
19.3086	22.7384	24.7852
28.7112	34.8593	42.7167
42.8989	45.4557	54.1306
56.6802	58.6732	62.1064
67.4624	97.1582	111.3314
124.2558	132.0503	181.1573
189.6738	216.7993	218.9029
242.2061	257.4764	258.9962
265.3973	271.0059	350.9490
366.0421	371.0067	407.4837
408.5385	412.7988	418.0313
435.7289	440.0311	441.3115

444.8071	513.3111	514.7328
515.6439	522.7209	531.9691
551.3275	593.0874	604.4512
628.9320	630.5931	631.5582
634.6406	703.2741	714.4258
715.3270	718.4497	719.3012
720.4459	722.1089	730.1539
745.6735	771.2971	776.0363
777.4612	777.8602	818.7032
845.8386	878.9006	882.8586
883.5102	885.8366	888.5524
910.3471	940.5672	941.4342
951.1428	957.0988	957.5412
959.1965	995.6020	1005.2248
1005.8651	1007.3090	1012.5374
1014.5713	1014.7179	1015.4123
1018.6506	1021.3839	1026.6732
1029.0708	1029.5776	1047.1112
1067.2152	1071.1028	1071.4132
1071.5217	1074.2947	1076.6986
1103.4210	1125.0959	1127.4744
1129.7027	1130.4962	1136.6379
1139.4509	1140.3183	1143.7562
1155.7290	1192.2198	1192.9315
1197.4487	1198.0131	1216.7907
1221.8963	1225.9054	1226.8127
1230.6982	1248.2507	1269.5023
1298.2516	1333.4157	1333.8445
1337.0144	1338.9206	1348.3279
1365.3559	1369.6451	1369.9137
1370.2414	1373.2679	1388.1621
1413.0752	1418.2641	1449.3534
1496.0123	1500.4647	1500.7389
1507.4580	1512.9774	1518.0498
1530.4512	1545.4414	1545.6592
1547.8272	1565.6358	1671.8630
1673.4899	1674.1467	1686.0508
1686.9886	1687.4977	1689.0689
1710.6542	1866.8443	3050.6197
3063.8617	3073.7463	3095.9869
3098.3888	3107.1921	3109.3349
3128.2009	3165.7270	3189.6235
3196.1488	3200.9635	3201.0302
3204.6904	3211.4911	3212.7282
3215.7278	3216.8033	3218.9370
3223.6037	3224.3151	3228.4347
3229.7116	3230.1430	3232.5901
3237.4752	3239.3987	3240.0050
3244.9610	3245.1620	3250.4517

INT34

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.609697	-0.330654	-1.289470
2	6	0	0.600425	-0.955212	0.253239
3	6	0	1.383750	-0.535190	-1.825552
4	1	0	0.478528	-2.042240	0.250159
5	1	0	0.283472	-0.501462	1.195608
6	1	0	1.703216	0.273864	-2.487961
7	6	0	1.832274	-0.454781	-0.401890
8	6	0	2.874149	0.170551	0.156442
9	1	0	1.499866	-1.522063	-2.283628
10	15	0	-2.803477	-0.029067	-0.139425
11	6	0	-2.883641	-1.103943	1.343679
12	6	0	-2.448277	-2.426770	1.202256
13	6	0	-3.355083	-0.666706	2.584428
14	6	0	-2.497434	-3.302927	2.281338
15	1	0	-2.061290	-2.763563	0.242905
16	6	0	-3.395704	-1.543918	3.665904
17	1	0	-3.686651	0.360332	2.708095
18	6	0	-2.969342	-2.860833	3.515996
19	1	0	-2.156906	-4.326572	2.161699
20	1	0	-3.758949	-1.195278	4.627623

21	1	0	-2.998139	-3.540279	4.362019
22	6	0	-4.412233	-0.329896	-0.967681
23	6	0	-5.482129	-0.986888	-0.353598
24	6	0	-4.560684	0.143111	-2.276874
25	6	0	-6.683471	-1.159687	-1.037542
26	1	0	-5.376468	-1.366469	0.658599
27	6	0	-5.763829	-0.021952	-2.954722
28	1	0	-3.727995	0.644488	-2.766250
29	6	0	-6.827290	-0.675822	-2.335037
30	1	0	-7.508079	-1.673862	-0.553517
31	1	0	-5.868977	0.352182	-3.968099
32	1	0	-7.764649	-0.812740	-2.864954
33	6	0	-2.999376	1.662454	0.541494
34	6	0	-1.834228	2.369265	0.860857
35	6	0	-4.245867	2.256846	0.762884
36	6	0	-1.915816	3.646478	1.408212
37	1	0	-0.862851	1.916687	0.671405
38	6	0	-4.323805	3.537388	1.304115
39	1	0	-5.155214	1.718839	0.507367
40	6	0	-3.160392	4.231667	1.629178
41	1	0	-1.007146	4.186797	1.654158
42	1	0	-5.294688	3.994411	1.468955
43	1	0	-3.224706	5.230730	2.049164
44	1	0	2.915273	0.238482	1.244796
45	6	0	4.019746	0.781575	-0.597646
46	6	0	5.373779	0.264144	-0.102891
47	1	0	4.010440	1.878670	-0.499681
48	1	0	3.914022	0.566338	-1.668607
49	6	0	6.561932	0.915578	-0.821126
50	1	0	5.466324	0.447048	0.976395
51	1	0	5.419757	-0.824158	-0.234658
52	1	0	6.478965	0.727945	-1.898865
53	1	0	6.511350	2.003591	-0.684612
54	6	0	7.881868	0.395566	-0.308914
55	6	0	8.501481	0.988695	0.793859
56	6	0	8.481538	-0.726876	-0.883966
57	6	0	9.689408	0.476859	1.308534
58	1	0	8.045607	1.864362	1.250670
59	6	0	9.669157	-1.243875	-0.373507
60	1	0	8.009653	-1.199002	-1.742662
61	6	0	10.277318	-0.642816	0.725311
62	1	0	10.158276	0.954630	2.163574
63	1	0	10.121871	-2.115672	-0.836320
64	1	0	11.204946	-1.042460	1.122938

Zero-point correction= 0.533869 (Hartree/Particle)
Thermal correction to Energy= 0.565639
Thermal correction to Enthalpy= 0.566584
Thermal correction to Gibbs Free Energy= 0.462591
Sum of electronic and zero-point Energies= -1666.791217
Sum of electronic and thermal Energies= -1666.759447
Sum of electronic and thermal Enthalpies= -1666.758502
Sum of electronic and thermal Free Energies= -1666.862495
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1667.286262
Frequencies

4.9646	15.4013	21.5148
28.5335	30.6150	35.4689
39.0462	42.0717	44.1998
52.7535	54.1361	61.4387
65.7690	78.0925	86.5950
106.1717	109.7320	134.1575
136.6964	190.5209	194.2696
215.0255	220.7752	247.9339
255.9214	258.8294	266.1721
271.2603	311.2008	359.0469
402.1158	409.0632	410.0501
414.4358	415.4503	436.0256
443.6465	446.8200	456.6161
476.0735	513.1926	516.3911
521.2558	526.2989	548.1216
603.2590	609.7191	628.2414
629.3002	630.2286	638.6001
686.2372	703.4794	715.1875
716.1047	719.5016	719.8504
720.8718	723.7714	725.6859

744.5993	771.1726	773.3982
777.6653	781.2920	815.7034
843.0404	864.5038	870.6293
882.5365	885.5270	894.2077
894.4063	937.3243	951.8650
955.2039	964.5057	986.0924
988.2799	1003.0913	1004.3667
1010.2015	1013.3900	1014.5224
1014.7960	1015.8319	1016.3444
1020.3594	1021.6441	1028.1890
1028.8701	1035.3795	1047.1763
1068.0991	1070.5820	1072.1977
1072.6313	1073.6458	1081.7604
1095.8685	1116.9888	1125.1473
1126.2277	1126.9191	1141.1482
1143.5017	1145.5873	1146.2175
1164.9914	1191.8275	1192.4707
1192.6594	1199.9116	1224.0851
1225.1404	1225.8347	1227.3390
1234.3739	1252.3355	1271.0894
1300.5711	1333.2017	1333.5697
1337.1036	1338.2784	1347.6700
1368.3552	1370.7401	1371.1499
1371.7928	1376.8812	1388.7830
1413.3066	1446.5163	1466.2310
1495.8285	1496.9709	1498.3598
1506.5196	1513.0289	1522.7045
1530.7665	1544.3078	1546.7836
1548.2107	1571.2132	1670.3921
1672.0125	1672.5954	1687.3809
1690.8057	1692.5229	1693.5505
1711.6752	1785.9485	3029.6313
3060.3616	3070.1846	3090.2388
3093.3017	3098.5071	3103.7848
3124.2465	3160.3207	3166.6496
3175.0967	3192.8783	3198.1603
3206.3074	3207.3950	3208.2697
3214.5907	3216.1340	3216.3341
3217.3719	3220.7433	3221.4521
3221.7060	3223.9220	3231.0272
3233.9904	3235.4355	3244.1224
3244.2606	3244.9504	3245.8446

TS24

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.579737	-0.274716	-1.710913
2	6	0	-0.327148	1.924867	-0.636693
3	6	0	-1.479171	0.429699	-2.143731
4	1	0	0.432976	1.807547	0.133906
5	1	0	-0.002864	2.447991	-1.533397
6	1	0	-2.168046	-0.381641	-2.365444
7	6	0	-1.375231	0.888125	-0.795825
8	6	0	-2.055916	0.481922	0.339298
9	1	0	-1.353430	1.164587	-2.937897
10	1	0	-2.086548	2.601578	0.380293
11	6	0	-0.722952	5.550247	-0.068488
12	6	0	0.191000	4.934221	0.993044
13	6	0	-0.614223	3.724508	1.482655
14	7	0	-1.273066	3.249845	0.254366
15	1	0	-0.210840	6.073102	-0.878031
16	1	0	-1.446754	6.246601	0.372314
17	1	0	1.124546	4.583298	0.541402
18	1	0	0.442024	5.616868	1.806726
19	15	0	2.397984	-0.759606	-0.329232
20	6	0	1.878788	-2.011526	0.916677
21	6	0	0.519252	-2.037217	1.260570
22	6	0	2.754913	-2.911034	1.528988
23	6	0	0.053356	-2.937784	2.214052
24	1	0	-0.172330	-1.343618	0.781275
25	6	0	2.281008	-3.821809	2.471640
26	1	0	3.808334	-2.911236	1.264262
27	6	0	0.932557	-3.834733	2.817934

28	1	0	-1.001904	-2.945997	2.472349
29	1	0	2.968820	-4.523867	2.933274
30	1	0	0.565688	-4.546608	3.551123
31	6	0	2.730467	0.718325	0.728343
32	6	0	2.353085	0.808006	2.070598
33	6	0	3.292918	1.844206	0.108538
34	6	0	2.536937	1.998020	2.779350
35	1	0	1.913380	-0.051266	2.568654
36	6	0	3.486241	3.023787	0.817167
37	1	0	3.576402	1.790282	-0.940597
38	6	0	3.102090	3.106832	2.157687
39	1	0	2.243190	2.049750	3.823971
40	1	0	3.935362	3.882064	0.325405
41	1	0	3.249998	4.029739	2.710990
42	6	0	4.104609	-1.268246	-0.779443
43	6	0	4.276775	-1.934914	-1.995853
44	6	0	5.220560	-1.024420	0.029778
45	6	0	5.540383	-2.366958	-2.391678
46	1	0	3.413184	-2.103544	-2.635536
47	6	0	6.484052	-1.450503	-0.369103
48	1	0	5.097970	-0.496899	0.972735
49	6	0	6.644198	-2.124262	-1.578964
50	1	0	5.663439	-2.882284	-3.339169
51	1	0	7.344884	-1.254422	0.263049
52	1	0	7.630906	-2.453171	-1.890382
53	6	0	-1.499290	4.364510	-0.618039
54	8	0	-2.167321	4.291564	-1.612031
55	1	0	-1.375078	4.012305	2.217139
56	1	0	0.010338	2.934379	1.908686
57	1	0	-1.593932	0.694216	1.310232
58	6	0	-3.059765	-0.633803	0.307659
59	6	0	-3.849915	-0.740064	1.610966
60	1	0	-2.574302	-1.612619	0.115658
61	1	0	-3.754888	-0.487222	-0.531314
62	6	0	-4.834447	-1.917787	1.640975
63	1	0	-3.146357	-0.846594	2.448913
64	1	0	-4.394489	0.198865	1.778030
65	1	0	-5.282437	-1.990923	2.639561
66	1	0	-4.282428	-2.850821	1.470170
67	6	0	-5.930286	-1.785314	0.610667
68	6	0	-5.900427	-2.510047	-0.582246
69	6	0	-6.985981	-0.893249	0.820084
70	6	0	-6.898281	-2.350627	-1.541444
71	1	0	-5.082924	-3.204664	-0.760693
72	6	0	-7.985553	-0.729983	-0.133473
73	1	0	-7.022257	-0.322606	1.745825
74	6	0	-7.944401	-1.460034	-1.319600
75	1	0	-6.857081	-2.923408	-2.463045
76	1	0	-8.798605	-0.033488	0.048908
77	1	0	-8.722804	-1.334446	-2.065742

Zero-point correction= 0.647216 (Hartree/Particle)
Thermal correction to Energy= 0.684982
Thermal correction to Enthalpy= 0.685926
Thermal correction to Gibbs Free Energy= 0.568999
Sum of electronic and zero-point Energies= -1953.134701
Sum of electronic and thermal Energies= -1953.096936
Sum of electronic and thermal Enthalpies= -1953.095991
Sum of electronic and thermal Free Energies= -1953.212919
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1953.732148
Frequencies

-538.8867	5.8306	14.2635
21.2091	23.8348	30.5219
32.1552	34.7583	38.0581
40.3162	44.9398	50.9306
53.4235	58.8412	62.7580
65.7345	75.8204	77.3566
88.7275	102.6875	119.0450
123.9832	152.3255	156.5676
176.0506	183.4286	198.3313
205.5507	214.3840	223.3809
251.5089	254.1086	262.0792
264.9623	277.3731	288.6132
338.1536	341.1634	366.2244
384.4198	405.3633	409.3983

413.7333	416.1538	425.1216
432.7205	450.3420	457.4280
492.1085	506.2120	510.4305
514.1559	530.0907	537.8630
554.3286	582.9564	589.2208
627.6284	628.8305	629.2952
632.2461	636.0328	655.5726
679.3737	697.4063	699.7589
709.4914	713.7143	716.4589
717.7067	719.2243	719.6641
758.4811	766.4289	772.1872
776.6697	777.8856	820.3970
830.2583	841.3364	867.1881
872.2846	875.9636	877.9027
879.1131	886.8768	908.9545
923.5210	939.3546	940.4538
941.8437	949.7007	953.9319
959.7439	985.1204	998.6867
999.1800	999.6380	1005.4489
1012.6742	1014.3018	1014.8256
1015.9470	1016.9870	1018.4336
1021.5240	1026.1115	1028.3441
1042.6945	1060.6423	1068.7958
1070.1922	1070.5693	1079.1779
1082.9095	1089.3337	1095.0649
1108.3698	1118.4151	1123.1801
1125.4088	1128.3846	1135.3536
1137.4684	1141.2235	1154.2918
1156.2633	1169.7054	1173.5485
1186.8940	1188.0746	1191.8673
1196.8206	1215.4336	1217.6490
1218.2307	1221.0337	1223.8138
1225.6245	1229.3177	1238.7985
1251.3047	1272.9525	1282.9922
1312.2018	1317.4535	1328.4070
1329.1064	1329.9773	1336.9129
1362.0754	1362.4151	1362.4466
1367.8980	1370.0283	1373.0939
1374.8576	1386.2845	1397.2132
1426.9980	1462.8659	1483.3561
1491.5628	1492.0410	1493.1572
1495.5735	1505.8343	1511.1412
1515.4556	1520.5302	1523.2533
1526.0632	1542.7640	1543.1310
1543.2750	1547.2245	1569.5991
1617.4872	1665.4005	1667.4061
1671.2115	1684.9328	1687.2927
1689.0258	1689.7223	1710.8795
1912.4284	2944.0277	3045.2662
3048.1144	3065.9034	3068.1308
3093.0281	3097.3358	3098.5447
3099.8272	3113.2596	3116.0074
3149.9038	3161.4233	3172.8218
3175.9763	3185.9158	3186.9848
3194.3338	3198.4491	3200.5159
3201.4164	3203.9325	3209.3737
3214.8162	3215.9515	3218.9453
3219.5964	3222.8465	3224.7709
3225.4727	3228.7625	3233.0661
3234.6835	3235.0901	3239.8182
3243.7645	3246.0801	3277.5653

INT35

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.673792	-0.196865	-0.781545
2	6	0	4.001063	0.099074	0.455319
3	6	0	2.627036	0.819433	-1.454774
4	1	0	4.363848	0.339812	1.457627
5	1	0	3.519725	-0.882836	0.432696
6	1	0	2.369355	1.612615	-2.152322
7	6	0	3.165975	1.175119	-0.175807
8	6	0	3.115921	2.366786	0.496329

9	1	0	2.969938	-0.106163	-1.933491
10	1	0	4.792045	-0.077193	-1.392879
11	6	0	7.349249	-0.839265	0.450513
12	6	0	7.177654	0.658398	0.723885
13	6	0	6.182942	1.112513	-0.348166
14	7	0	5.241567	-0.041507	-0.456818
15	1	0	7.573527	-1.453175	1.325209
16	1	0	8.132148	-1.028657	-0.294143
17	1	0	6.760200	0.824450	1.721248
18	1	0	8.114825	1.212054	0.657898
19	15	0	-1.206167	-1.213997	-0.040655
20	6	0	6.035343	-1.277040	-0.155687
21	8	0	5.599191	-2.355961	-0.396342
22	1	0	6.666350	1.242908	-1.319004
23	1	0	5.591989	1.999856	-0.099997
24	6	0	2.285609	3.517701	0.008117
25	6	0	0.789868	3.301437	0.282160
26	1	0	2.422697	3.637279	-1.077528
27	1	0	2.615888	4.459414	0.465268
28	6	0	-0.117247	4.296551	-0.447149
29	1	0	0.526188	2.282770	-0.037045
30	1	0	0.598386	3.352257	1.362646
31	1	0	0.080563	5.318333	-0.097761
32	1	0	0.132760	4.274168	-1.516788
33	6	0	-1.576975	3.959474	-0.265274
34	6	0	-2.096192	2.794698	-0.840925
35	6	0	-2.425575	4.758657	0.501424
36	6	0	-3.428272	2.440052	-0.659934
37	1	0	-1.433157	2.147027	-1.414764
38	6	0	-3.762061	4.409228	0.685889
39	1	0	-2.034551	5.666502	0.955588
40	6	0	-4.266687	3.249585	0.105173
41	1	0	-3.807097	1.521573	-1.101288
42	1	0	-4.407761	5.043221	1.287169
43	1	0	-5.304425	2.967921	0.257750
44	6	0	-2.233378	-0.225687	1.132368
45	6	0	-3.602811	-0.432895	1.332993
46	6	0	-1.599276	0.812321	1.821860
47	6	0	-4.317021	0.373120	2.215071
48	1	0	-4.117326	-1.220672	0.788031
49	6	0	-2.313434	1.623296	2.699901
50	1	0	-0.542349	0.993928	1.638015
51	6	0	-3.673604	1.404032	2.897572
52	1	0	-5.380553	0.205329	2.359624
53	1	0	-1.811922	2.441142	3.208779
54	1	0	-4.237727	2.046422	3.567579
55	6	0	-2.469769	-1.652754	-1.316697
56	6	0	-3.322097	-2.758735	-1.238829
57	6	0	-2.579932	-0.791800	-2.414639
58	6	0	-4.278614	-2.983751	-2.227696
59	1	0	-3.236942	-3.449872	-0.403651
60	6	0	-3.543953	-1.008057	-3.395055
61	1	0	-1.886395	0.042757	-2.498670
62	6	0	-4.396643	-2.105809	-3.302166
63	1	0	-4.932635	-3.848132	-2.158230
64	1	0	-3.619831	-0.327137	-4.237570
65	1	0	-5.143919	-2.281977	-4.070075
66	6	0	-1.025495	-2.825662	0.843226
67	6	0	-0.121995	-3.747531	0.298336
68	6	0	-1.723208	-3.172745	2.003182
69	6	0	0.062570	-4.994438	0.886035
70	1	0	0.443742	-3.468931	-0.588381
71	6	0	-1.527748	-4.417886	2.600475
72	1	0	-2.418629	-2.467538	2.448445
73	6	0	-0.639965	-5.332176	2.042064
74	1	0	0.763035	-5.700063	0.448989
75	1	0	-2.073610	-4.671688	3.504480
76	1	0	-0.490414	-6.301789	2.507708
77	1	0	3.547943	2.426601	1.493630

Zero-point correction= 0.650688 (Hartree/Particle)
Thermal correction to Energy= 0.688240
Thermal correction to Enthalpy= 0.689185
Thermal correction to Gibbs Free Energy= 0.575399
Sum of electronic and zero-point Energies= -1953.148397

Sum of electronic and thermal Energies= -1953.110844
Sum of electronic and thermal Enthalpies= -1953.109900
Sum of electronic and thermal Free Energies= -1953.223685
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1953.763721
Frequencies

13.2296	20.4682	22.2178
28.3568	35.1332	36.1477
40.9609	44.2634	46.2064
51.2963	55.2550	58.3167
63.0248	71.8366	75.5129
84.5413	94.3761	97.1834
103.0385	112.9689	128.2015
150.7793	166.7283	173.7185
181.4437	198.6477	217.8860
220.0934	233.6653	259.0878
263.2316	265.4355	273.0767
275.3952	290.7535	313.1541
345.1533	374.9162	407.7824
410.8066	413.4628	414.5784
421.8032	433.5937	441.0516
447.7692	452.4049	490.0395
511.0423	512.7162	518.8783
524.3858	532.0969	555.4652
573.6670	597.8046	617.4514
619.6140	628.8315	631.1597
631.3116	633.9529	643.2423
685.2556	702.3148	710.8287
712.2996	714.6061	715.0529
716.8585	717.4959	719.8265
745.5568	764.6788	770.9926
771.8311	775.3911	785.3336
822.2014	839.9758	845.8510
855.8377	872.9354	875.6869
882.4042	888.1312	905.3127
925.9117	933.9942	940.5940
949.0728	953.1713	958.1309
973.3079	988.4466	995.3676
1000.7087	1007.6541	1009.4631
1011.5526	1013.1132	1014.6198
1015.4074	1016.3749	1017.8455
1019.9290	1021.0138	1025.5036
1056.5289	1068.9957	1070.7680
1072.1764	1072.5737	1072.8150
1077.4095	1080.4080	1095.5356
1121.8727	1122.7944	1126.6862
1127.3404	1137.6340	1138.1069
1139.4118	1142.7607	1146.5664
1173.2422	1186.4165	1189.5281
1194.9583	1197.4240	1199.8259
1220.1793	1224.4624	1224.7467
1227.3073	1228.4484	1245.1827
1246.1915	1258.7539	1274.2356
1286.8700	1306.5826	1310.5537
1332.9680	1333.5779	1335.7002
1338.4328	1341.7198	1357.3255
1358.5832	1367.7945	1369.7383
1370.4395	1371.2950	1371.6101
1381.3401	1390.0596	1408.0828
1413.2734	1446.1461	1481.4271
1494.9009	1498.1762	1498.9855
1502.1223	1504.0868	1505.2251
1510.7939	1514.3682	1525.9044
1526.6400	1541.3647	1545.0115
1547.1948	1547.7717	1563.1375
1660.1000	1669.1725	1672.3431
1674.3129	1682.2965	1686.8820
1687.7967	1689.5634	1708.5033
1969.9176	3040.1124	3048.8786
3062.0109	3072.5493	3080.0278
3095.0620	3101.9863	3113.3310
3114.8678	3123.7580	3127.6399
3174.0499	3175.4050	3178.1271
3183.5258	3188.5576	3194.5542
3196.7546	3197.0275	3202.7773
3202.9396	3203.8287	3205.5860

3206.4425	3209.6117	3215.5646
3216.4094	3220.1722	3220.4209
3221.0284	3229.1702	3229.5329
3233.7186	3239.4031	3240.8917
3244.5298	3245.5339	3263.2941

INT36

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.800318	0.146453	-1.644672
2	6	0	-0.245043	1.919960	-1.436983
3	6	0	-1.158795	0.058106	-2.377664
4	1	0	-0.175524	2.480012	-2.372761
5	1	0	0.043496	2.517903	-0.568485
6	1	0	-1.624615	-0.927467	-2.325179
7	6	0	-1.447479	1.055758	-1.320419
8	6	0	-2.285596	0.971415	-0.260257
9	1	0	-1.145343	0.463598	-3.391092
10	1	0	-0.852431	-1.132475	-0.084064
11	6	0	0.609247	-4.086431	-0.050576
12	6	0	-0.761644	-4.389842	0.562503
13	6	0	-1.297828	-3.000584	0.954708
14	7	0	-0.620157	-2.121951	0.011132
15	1	0	0.918460	-4.764656	-0.847111
16	1	0	1.401815	-4.062028	0.707332
17	1	0	-1.415319	-4.832577	-0.194437
18	1	0	-0.717348	-5.069976	1.414646
19	15	0	2.708982	0.526502	-0.143592
20	6	0	3.042261	2.232581	0.425946
21	6	0	2.912461	3.262394	-0.511032
22	6	0	3.409833	2.542287	1.740344
23	6	0	3.167480	4.581789	-0.145687
24	1	0	2.593037	3.023638	-1.523046
25	6	0	3.660324	3.861839	2.104659
26	1	0	3.493388	1.748734	2.479023
27	6	0	3.542260	4.881394	1.161223
28	1	0	3.061238	5.375029	-0.878868
29	1	0	3.942935	4.095923	3.126473
30	1	0	3.733955	5.910676	1.448672
31	6	0	4.363717	-0.221764	-0.385470
32	6	0	5.539426	0.312771	0.149440
33	6	0	4.421584	-1.398193	-1.144191
34	6	0	6.758105	-0.325554	-0.066747
35	1	0	5.506632	1.231965	0.726954
36	6	0	5.641531	-2.038026	-1.346807
37	1	0	3.506334	-1.811877	-1.562008
38	6	0	6.810242	-1.501713	-0.810912
39	1	0	7.668691	0.098017	0.345811
40	1	0	5.678894	-2.950301	-1.934108
41	1	0	7.762606	-1.995643	-0.978025
42	6	0	2.079287	-0.291624	1.380103
43	6	0	0.866426	0.184375	1.900704
44	6	0	2.680711	-1.406489	1.964959
45	6	0	0.283908	-0.426910	3.003971
46	1	0	0.366534	1.026988	1.425238
47	6	0	2.084291	-2.029851	3.063689
48	1	0	3.615771	-1.790564	1.566317
49	6	0	0.893971	-1.538035	3.589857
50	1	0	-0.652306	-0.043640	3.399321
51	1	0	2.562004	-2.894792	3.514685
52	1	0	0.437914	-2.019373	4.449983
53	1	0	-2.381981	-2.918684	0.842549
54	1	0	-1.030102	-2.733343	1.983655
55	6	0	0.459156	-2.668998	-0.575447
56	8	0	1.222558	-2.132054	-1.385831
57	1	0	-2.215965	1.740113	0.510663
58	6	0	-3.355841	-0.068770	-0.074586
59	6	0	-4.773616	0.514260	-0.077039
60	1	0	-3.218703	-0.607554	0.879878
61	1	0	-3.284645	-0.827743	-0.866296
62	6	0	-5.850573	-0.555623	0.146163
63	1	0	-4.859012	1.281288	0.704030
64	1	0	-4.951926	1.024320	-1.031439

65	1	0	-5.776953	-1.307354	-0.650275
66	1	0	-5.648602	-1.075924	1.091675
67	6	0	-7.241346	0.026530	0.174425
68	6	0	-7.824666	0.427100	1.378549
69	6	0	-7.954650	0.229421	-1.009735
70	6	0	-9.087285	1.012553	1.402405
71	1	0	-7.280566	0.274585	2.308071
72	6	0	-9.217170	0.814477	-0.992575
73	1	0	-7.511687	-0.078211	-1.954478
74	6	0	-9.788444	1.207697	0.215300
75	1	0	-9.525447	1.314547	2.349163
76	1	0	-9.756874	0.961124	-1.923446
77	1	0	-10.774535	1.661611	0.231590

Zero-point correction= 0.649132 (Hartree/Particle)
Thermal correction to Energy= 0.687074
Thermal correction to Enthalpy= 0.688019
Thermal correction to Gibbs Free Energy= 0.571751
Sum of electronic and zero-point Energies= -1953.215507
Sum of electronic and thermal Energies= -1953.177564
Sum of electronic and thermal Enthalpies= -1953.176620
Sum of electronic and thermal Free Energies= -1953.292887
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1953.811279
Frequencies

7.5085	14.5156	18.7178
25.8286	29.5916	36.4404
36.8605	41.5736	43.9128
50.2803	53.8810	57.3485
63.7338	67.4335	73.8823
79.6096	96.7779	104.7228
108.6355	116.7777	128.8431
134.8071	147.3300	160.0165
175.3928	196.7863	203.6862
208.1736	222.7709	237.2860
244.1047	254.2767	257.9355
264.1343	283.1555	286.3422
347.3333	361.7555	404.5983
408.7546	412.4342	415.4219
416.1286	425.5386	438.4527
454.6449	465.0716	505.5952
506.0054	513.8171	516.2806
518.6627	530.5153	544.1145
544.8238	601.0062	626.5031
628.7689	631.8317	634.1446
634.3490	644.8327	696.0222
699.7769	711.2452	714.5815
718.2125	718.6695	720.8648
724.6303	731.2280	744.0698
753.3923	765.6856	768.2611
773.0014	775.8958	780.9021
805.8845	833.7364	836.9248
850.9422	870.2573	878.2579
885.0773	894.5970	901.3947
916.8685	927.8858	935.4097
946.2555	951.5740	957.4875
967.5053	970.1859	986.3554
997.9732	1005.7500	1009.9896
1012.6363	1014.4786	1014.8497
1015.9116	1017.5129	1017.7452
1021.9298	1025.3085	1028.8524
1031.2966	1035.1101	1036.6820
1061.7409	1068.9557	1070.8757
1071.6467	1072.6813	1075.7574
1079.5861	1105.3369	1114.7390
1119.0690	1123.8324	1126.1202
1132.2081	1138.8082	1141.1070
1141.9041	1145.9933	1163.4508
1183.5162	1187.5894	1191.1811
1198.9595	1201.4609	1212.8127
1217.6777	1230.4460	1230.6787
1234.5538	1238.1952	1250.1492
1266.1419	1270.7661	1304.5497
1307.6424	1331.0219	1335.4280
1336.0859	1341.9041	1343.1341
1348.8795	1362.1540	1362.8056

1364.7818	1367.8096	1375.9883
1379.1442	1389.1881	1403.7478
1411.2681	1476.8050	1490.4625
1494.0010	1496.2783	1499.2314
1501.0751	1501.1939	1507.2819
1512.9060	1514.5388	1530.5326
1530.8191	1542.9928	1548.6720
1550.4125	1560.6574	1563.8533
1669.4454	1671.1191	1672.6372
1686.3022	1687.0173	1688.3100
1690.8346	1710.4120	1717.0799
1788.4329	2991.9793	3060.8923
3072.7563	3081.4503	3096.0206
3100.5839	3103.8704	3105.9698
3112.2316	3115.2562	3126.3750
3155.6532	3156.6770	3169.6674
3177.3831	3182.9299	3189.4383
3190.9837	3195.7182	3206.0294
3206.5442	3209.7447	3210.2651
3214.3248	3215.6908	3217.6214
3222.3059	3222.9426	3223.4169
3227.1511	3228.9214	3235.7152
3236.2003	3239.2061	3242.5401
3242.9738	3243.6038	3504.4946

TS25

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.014359	0.598097	-1.640281
2	6	0	0.369793	2.556607	-1.348180
3	6	0	-0.533901	1.268782	-3.078394
4	1	0	0.918156	3.176870	-2.056836
5	1	0	0.389395	2.920077	-0.321118
6	1	0	-1.209278	0.522786	-3.487570
7	6	0	-0.830306	1.896427	-1.835233
8	6	0	-1.906934	1.464945	-0.997342
9	1	0	0.113852	1.770826	-3.793327
10	1	0	-1.473927	0.037708	-0.837765
11	6	0	-0.468398	-3.359391	-0.588421
12	6	0	-1.975181	-3.429373	-0.343539
13	6	0	-2.362875	-1.948180	-0.169398
14	7	0	-1.333228	-1.198761	-0.881434
15	1	0	-0.073649	-4.113769	-1.271417
16	1	0	0.106878	-3.410677	0.346427
17	1	0	-2.477087	-3.839734	-1.225033
18	1	0	-2.253577	-4.038597	0.519214
19	15	0	2.526949	0.249035	0.168589
20	6	0	3.093423	1.671169	1.169293
21	6	0	3.349163	2.877305	0.509022
22	6	0	3.305406	1.583169	2.548688
23	6	0	3.821231	3.978859	1.216879
24	1	0	3.169822	2.948905	-0.561488
25	6	0	3.771334	2.688464	3.255419
26	1	0	3.102104	0.650844	3.068932
27	6	0	4.030527	3.885157	2.590877
28	1	0	4.016834	4.911867	0.697859
29	1	0	3.930085	2.615330	4.326876
30	1	0	4.389831	4.746728	3.145234
31	6	0	4.064850	-0.646061	-0.257543
32	6	0	5.314849	-0.305064	0.264770
33	6	0	3.952595	-1.717904	-1.154139
34	6	0	6.445802	-1.030552	-0.105912
35	1	0	5.409953	0.526433	0.957115
36	6	0	5.085738	-2.441728	-1.511611
37	1	0	2.975782	-1.981149	-1.556030
38	6	0	6.332533	-2.097945	-0.991756
39	1	0	7.415652	-0.758170	0.299043
40	1	0	4.995064	-3.271788	-2.205396
41	1	0	7.215422	-2.660659	-1.279292
42	6	0	1.701587	-0.839589	1.391544
43	6	0	0.381623	-0.530477	1.744826
44	6	0	2.327136	-1.945583	1.973404
45	6	0	-0.291037	-1.304318	2.685845

46	1	0	-0.124896	0.309816	1.271352
47	6	0	1.643534	-2.728663	2.902771
48	1	0	3.347833	-2.197456	1.699519
49	6	0	0.337073	-2.407866	3.262117
50	1	0	-1.307948	-1.046753	2.966118
51	1	0	2.135574	-3.587841	3.348159
52	1	0	-0.192226	-3.015590	3.989657
53	1	0	-3.352413	-1.724996	-0.585149
54	1	0	-2.377140	-1.658812	0.891011
55	6	0	-0.276334	-1.956433	-1.145052
56	8	0	0.787039	-1.622016	-1.730163
57	1	0	-1.991502	2.029883	-0.065658
58	6	0	-3.246948	1.136999	-1.641781
59	6	0	-4.350852	1.032232	-0.590516
60	1	0	-3.187773	0.173340	-2.176920
61	1	0	-3.541106	1.880644	-2.399775
62	6	0	-5.668256	0.481691	-1.148802
63	1	0	-4.013249	0.384811	0.231178
64	1	0	-4.529699	2.017977	-0.141363
65	1	0	-6.031530	1.142688	-1.945178
66	1	0	-5.475678	-0.494699	-1.613950
67	6	0	-6.721021	0.332786	-0.078915
68	6	0	-6.693410	-0.765153	0.785975
69	6	0	-7.708579	1.301439	0.109726
70	6	0	-7.626993	-0.895453	1.808914
71	1	0	-5.929420	-1.528144	0.648426
72	6	0	-8.646711	1.176823	1.131886
73	1	0	-7.742125	2.161773	-0.554512
74	6	0	-8.609109	0.077391	1.984775
75	1	0	-7.592842	-1.759087	2.466425
76	1	0	-9.409676	1.938776	1.260338
77	1	0	-9.342066	-0.023776	2.779110

Zero-point correction= 0.644757 (Hartree/Particle)
Thermal correction to Energy= 0.681712
Thermal correction to Enthalpy= 0.682656
Thermal correction to Gibbs Free Energy= 0.571520
Sum of electronic and zero-point Energies= -1953.204371
Sum of electronic and thermal Energies= -1953.167416
Sum of electronic and thermal Enthalpies= -1953.166472
Sum of electronic and thermal Free Energies= -1953.277609
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1953.781762
Frequencies

-1223.1389	13.7060	18.0756
26.0123	32.9603	35.8848
42.2376	45.2698	48.4868
51.2615	54.9056	60.9602
67.0091	73.2356	83.5560
83.6165	96.2469	107.2015
123.8435	133.2075	142.2151
146.2772	161.2940	170.1061
181.6323	196.2727	200.8897
216.3195	223.9211	237.1748
243.1238	255.3419	265.7969
275.2780	282.4147	286.8218
298.2040	344.9619	376.3479
404.2530	407.7319	412.3082
417.1263	417.8116	431.9326
436.9178	445.9636	457.1243
462.3901	511.3144	514.8494
519.5223	530.8581	535.5892
561.7281	571.8298	600.5289
626.8629	627.8369	628.7333
637.4370	660.7716	690.3347
702.5786	714.6894	716.1718
718.7693	719.7124	720.9526
723.1981	725.5005	746.5975
762.4508	769.6247	772.8363
774.8297	777.0704	786.4865
810.4512	843.3359	860.7607
877.3058	882.5275	884.8761
887.4797	888.1432	902.6822
912.7206	930.4095	940.3722
954.4748	955.0336	956.6370
966.6975	971.0864	992.7541

996.2338	1001.0182	1005.5277
1006.4909	1013.5562	1014.5467
1014.7261	1016.5789	1017.4811
1021.6479	1024.2831	1026.5188
1037.9514	1039.3647	1040.4711
1071.1191	1071.8448	1072.2204
1073.6839	1075.7868	1080.8591
1084.9995	1099.5525	1123.3466
1126.9475	1127.3153	1128.9390
1134.8779	1139.0489	1140.6041
1145.8815	1147.5298	1174.2105
1191.1035	1191.9343	1192.4948
1194.9391	1197.5057	1222.4690
1225.7515	1229.6549	1230.7373
1236.1106	1240.8864	1255.2013
1262.0530	1291.0467	1302.0114
1315.4338	1331.5275	1333.3861
1337.1768	1340.4091	1349.4921
1358.3737	1361.4823	1368.6637
1371.3983	1373.8190	1375.5628
1377.0231	1384.5422	1399.8988
1425.4618	1481.4893	1493.4695
1494.6288	1496.4129	1498.3571
1499.1409	1510.1198	1512.0187
1522.0402	1524.6838	1526.5184
1538.3162	1546.0767	1546.6030
1547.3880	1548.9929	1561.4826
1570.0662	1595.7263	1669.5319
1673.2592	1674.3643	1685.2903
1688.3653	1688.9493	1690.0306
1712.5101	1736.3432	3008.5328
3040.7553	3059.0706	3066.9401
3070.7306	3084.6394	3097.7718
3101.7714	3116.0268	3119.4980
3125.4350	3139.1380	3164.8100
3171.3171	3172.2268	3197.1602
3202.4957	3204.2933	3205.2076
3209.2503	3210.0052	3210.5967
3214.1184	3218.3257	3220.5645
3223.5737	3224.1490	3224.3256
3226.7061	3227.1916	3232.3130
3236.8423	3236.9825	3240.4366
3243.2756	3244.8729	3266.1619

INT37

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.716836	-0.079857	-1.432928
2	6	0	0.257528	-1.947525	-1.754848
3	6	0	0.921867	0.038587	-2.921609
4	1	0	-0.284817	-2.349875	-2.610168
5	1	0	0.371495	-2.626246	-0.913059
6	1	0	1.472853	0.973392	-2.942105
7	6	0	1.231334	-0.928721	-1.959576
8	6	0	2.327273	-0.666542	-0.956685
9	1	0	0.335161	-0.213577	-3.802231
10	1	0	2.111339	-1.206594	-0.026077
11	6	0	-1.046516	3.979166	-0.073684
12	6	0	0.276167	4.579440	0.405408
13	6	0	1.191905	3.333577	0.508444
14	7	0	0.616519	2.303568	-0.346382
15	1	0	-1.587751	4.584648	-0.805138
16	1	0	-1.736790	3.757857	0.752246
17	1	0	0.669959	5.268561	-0.348622
18	1	0	0.196100	5.127036	1.348688
19	15	0	-2.443595	-0.475520	0.147675
20	6	0	-2.515911	-2.085261	1.014810
21	6	0	-2.365216	-3.244349	0.244478
22	6	0	-2.735277	-2.199452	2.389614
23	6	0	-2.441312	-4.499470	0.838080
24	1	0	-2.191499	-3.156611	-0.826079
25	6	0	-2.799415	-3.458389	2.984119
26	1	0	-2.852527	-1.305409	2.995562

27	6	0	-2.654873	-4.606993	2.211469
28	1	0	-2.328573	-5.393093	0.231977
29	1	0	-2.964731	-3.539859	4.053980
30	1	0	-2.707202	-5.585907	2.677933
31	6	0	-4.124208	-0.274904	-0.547809
32	6	0	-5.177446	-1.135598	-0.227193
33	6	0	-4.339003	0.797767	-1.424722
34	6	0	-6.438538	-0.929471	-0.782849
35	1	0	-5.017553	-1.966790	0.453551
36	6	0	-5.603928	0.997422	-1.969583
37	1	0	-3.515718	1.471724	-1.656387
38	6	0	-6.652312	0.134718	-1.653835
39	1	0	-7.253093	-1.602454	-0.533232
40	1	0	-5.769330	1.828555	-2.648205
41	1	0	-7.635352	0.291588	-2.087473
42	6	0	-2.346262	0.764480	1.486018
43	6	0	-1.087829	1.053396	2.027327
44	6	0	-3.478448	1.415018	1.983401
45	6	0	-0.971609	1.969600	3.069338
46	1	0	-0.197884	0.586962	1.611174
47	6	0	-3.355000	2.340729	3.017466
48	1	0	-4.455936	1.203734	1.559017
49	6	0	-2.103566	2.616228	3.562366
50	1	0	0.006088	2.185928	3.488508
51	1	0	-4.238211	2.846948	3.394595
52	1	0	-2.008099	3.339211	4.366675
53	1	0	2.223992	3.555905	0.211829
54	1	0	1.239486	2.971465	1.548034
55	6	0	-0.592317	2.651147	-0.666870
56	8	0	-1.421088	1.949009	-1.365763
57	1	0	2.322983	0.404588	-0.720047
58	6	0	3.694403	-1.096232	-1.501071
59	6	0	4.834693	-0.735271	-0.553173
60	1	0	3.861922	-0.610404	-2.471710
61	1	0	3.694923	-2.178330	-1.691193
62	6	0	6.203943	-1.178795	-1.083700
63	1	0	4.845816	0.350449	-0.391399
64	1	0	4.664942	-1.191549	0.431258
65	1	0	6.212098	-2.270698	-1.191912
66	1	0	6.350688	-0.760356	-2.087208
67	6	0	7.331695	-0.741335	-0.182253
68	6	0	7.982434	0.475809	-0.396291
69	6	0	7.713475	-1.516732	0.915392
70	6	0	8.991237	0.907928	0.459866
71	1	0	7.695533	1.088554	-1.247882
72	6	0	8.721161	-1.089668	1.775419
73	1	0	7.216880	-2.468299	1.092511
74	6	0	9.364202	0.124967	1.549361
75	1	0	9.488207	1.855449	0.274678
76	1	0	9.007532	-1.707221	2.621415
77	1	0	10.152554	0.458260	2.217081

Zero-point correction= 0.649590 (Hartree/Particle)
Thermal correction to Energy= 0.687421
Thermal correction to Enthalpy= 0.688365
Thermal correction to Gibbs Free Energy= 0.573540
Sum of electronic and zero-point Energies= -1953.238569
Sum of electronic and thermal Energies= -1953.200737
Sum of electronic and thermal Enthalpies= -1953.199793
Sum of electronic and thermal Free Energies= -1953.314619
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1953.822221
Frequencies

10.9856	16.4007	19.9189
22.2635	29.6435	39.2656
45.8422	50.6992	54.4667
55.2716	61.7743	65.5062
66.1820	69.5827	79.7521
84.1298	99.5510	111.0383
115.0567	124.7596	127.0027
132.9381	140.9624	143.6037
162.8510	179.8867	203.6095
218.4079	224.2714	224.7564
254.4913	258.4766	272.6381
274.1308	278.6702	296.5248
335.1059	350.3801	357.1531

386.7838	408.4153	411.5817
416.3857	417.5203	426.6779
436.4910	450.6933	457.0582
461.4840	512.5183	517.3434
525.4871	534.3211	555.6431
571.0278	595.7880	627.2865
628.5583	629.8720	636.7506
654.7990	694.9594	704.2055
711.8065	716.1251	718.5875
720.1354	722.5822	724.1055
725.0766	744.1501	766.6023
768.5826	769.8683	774.6033
776.2724	795.9044	802.3333
832.4804	843.4260	872.3241
875.4696	876.5451	885.1800
903.1415	905.8525	918.9852
923.5126	924.6612	938.9747
945.4962	950.0529	952.2443
965.6791	969.0002	991.7114
996.6703	998.7959	1001.6807
1013.8327	1014.6271	1015.7833
1016.4001	1017.1890	1020.7065
1022.3690	1023.4473	1034.6030
1045.0857	1045.7110	1065.7952
1070.9281	1071.8091	1073.6298
1080.3280	1087.7684	1088.6275
1090.4428	1094.1945	1119.5916
1126.4662	1126.8819	1130.4797
1135.2612	1142.4680	1143.0790
1145.0858	1162.3337	1182.6896
1190.6346	1192.3547	1195.0258
1196.8025	1223.4326	1223.4787
1225.3711	1232.5870	1233.1702
1250.7052	1252.3896	1264.8187
1272.7472	1300.7552	1326.4940
1333.0916	1334.5929	1338.9036
1340.1946	1340.7169	1348.3479
1354.7868	1369.6503	1370.1009
1371.0011	1377.0866	1380.4811
1384.1831	1415.7825	1427.3548
1432.0224	1470.9897	1494.8010
1497.1443	1498.6398	1499.5279
1514.5948	1516.1953	1521.4820
1523.2998	1527.7785	1538.7849
1539.6629	1540.7156	1544.5936
1545.6497	1548.9288	1570.7235
1573.7006	1672.3976	1674.2560
1675.5374	1685.9491	1686.1917
1688.7889	1688.9462	1689.8566
1714.1031	3028.6137	3054.7672
3065.1445	3074.0062	3076.3785
3076.6924	3087.2232	3091.4531
3098.9951	3106.2756	3126.1439
3136.4597	3136.6104	3145.9439
3148.2809	3184.5551	3200.3459
3200.5705	3207.0118	3207.2706
3207.8867	3210.8092	3211.8606
3212.2359	3216.7381	3218.0602
3220.0950	3223.6326	3224.2040
3225.8769	3229.6531	3229.8946
3235.9886	3236.9814	3238.3558
3239.6464	3243.1584	3281.0735

INT38

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.206363	0.389567	3.100098
2	1	0	-0.942397	0.955264	3.667192
3	1	0	0.820440	0.707916	3.252624
4	6	0	-0.469238	-1.102455	2.911523
5	1	0	0.389233	-1.766831	2.942600
6	6	0	-0.601234	-0.159924	1.790124
7	6	0	-1.307924	0.047808	0.636072

8	46	0	0.946380	-0.085819	0.128492
9	1	0	-1.381090	-1.517911	3.335681
10	6	0	-1.553885	1.420628	0.101541
11	6	0	-1.630656	1.631799	-1.284315
12	6	0	-1.835787	2.905357	-1.801147
13	1	0	-1.521606	0.783365	-1.954725
14	6	0	-1.900410	3.800165	0.430580
15	6	0	-1.970841	3.997245	-0.945549
16	1	0	-1.887021	3.046515	-2.876616
17	1	0	-2.011686	4.641975	1.107582
18	1	0	-2.132282	4.991900	-1.349379
19	15	0	3.196856	-0.217219	-0.502703
20	6	0	3.608042	-1.216971	-1.998034
21	6	0	4.371230	-0.948289	0.717762
22	6	0	4.077774	1.354006	-0.901950
23	6	0	-1.695985	2.524770	0.949140
24	1	0	-1.652244	2.378926	2.022634
25	6	0	-2.005700	-1.108198	-0.006541
26	6	0	-3.278994	-0.943136	-0.566583
27	6	0	-1.442980	-2.392287	-0.005292
28	6	0	-3.966152	-2.025054	-1.109460
29	1	0	-3.735946	0.042023	-0.570115
30	6	0	-2.129589	-3.471789	-0.548687
31	1	0	-0.448412	-2.527901	0.411574
32	6	0	-3.395031	-3.293774	-1.105192
33	1	0	-4.953304	-1.873501	-1.535838
34	1	0	-1.670669	-4.456083	-0.544528
35	1	0	-3.927944	-4.136489	-1.534722
36	1	0	4.053227	-1.964649	0.965056
37	1	0	5.394391	-0.975412	0.326090
38	1	0	4.353615	-0.355796	1.636428
39	1	0	3.087520	-0.803135	-2.865991
40	1	0	4.686066	-1.223955	-2.194500
41	1	0	3.260342	-2.243690	-1.855869
42	1	0	3.566604	1.859138	-1.725722
43	1	0	4.047700	2.016106	-0.032514
44	1	0	5.121505	1.171366	-1.181565

Zero-point correction= 0.367198 (Hartree/Particle)
Thermal correction to Energy= 0.390828
Thermal correction to Enthalpy= 0.391772
Thermal correction to Gibbs Free Energy= 0.310165
Sum of electronic and zero-point Energies= -1205.095978
Sum of electronic and thermal Energies= -1205.072348
Sum of electronic and thermal Enthalpies= -1205.071404
Sum of electronic and thermal Free Energies= -1205.153011
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1205.42671
Frequencies

12.4726	22.7858	28.8139
30.5734	42.4548	59.4692
68.7988	87.2754	106.5397
112.8761	127.0329	134.3746
151.7993	165.2193	177.8907
190.4012	212.3948	222.7904
224.9426	245.9189	252.6922
260.2501	284.8676	304.3926
326.2506	391.7039	396.2307
413.7455	422.2298	467.4219
523.0274	621.3371	630.9627
631.6087	650.5909	684.9982
696.5887	712.9337	715.7673
736.7516	743.3240	772.5681
775.8100	793.0900	798.2655
866.1021	866.8778	867.4938
872.2147	891.5121	900.1779
931.2428	944.1442	946.1501
976.5839	977.1871	989.2931
992.9441	994.1142	1013.4393
1014.3224	1018.1802	1018.8545
1051.1975	1060.8586	1071.4581
1077.8076	1085.7174	1096.3395
1115.1928	1126.0253	1134.6022
1180.5882	1187.2746	1188.0860
1214.1044	1220.4776	1256.0041
1317.7635	1346.5197	1347.4131

1349.5738	1350.5832	1364.5428
1369.4220	1372.1190	1472.7106
1483.5438	1490.4364	1492.0884
1493.8727	1499.6125	1501.3696
1503.4374	1511.5912	1512.8530
1554.5226	1558.7237	1671.5057
1674.7721	1697.6226	1700.7379
1743.6254	3066.6896	3068.7961
3074.4058	3148.1764	3156.6710
3158.4882	3159.2985	3165.9990
3172.8506	3177.4218	3184.3492
3200.7516	3204.8775	3209.4267
3210.5440	3218.9737	3221.3615
3227.3662	3229.3013	3236.9887
3239.2199	3242.6002	3247.0555

TS26

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.034020	-2.319851	-1.900183
2	1	0	0.278002	-1.898361	-2.851063
3	1	0	-0.797472	-3.102148	-1.996489
4	6	0	1.081245	-2.589850	-0.890720
5	1	0	0.817506	-3.392308	-0.199554
6	6	0	0.572248	-1.257296	-0.559398
7	6	0	1.232611	-0.099820	-0.312167
8	46	0	-1.478872	-1.219821	-0.704376
9	1	0	2.114111	-2.670720	-1.238770
10	6	0	0.640314	1.247784	-0.516567
11	6	0	0.887209	2.280558	0.400717
12	6	0	0.350585	3.551729	0.214999
13	1	0	1.513790	2.077790	1.265588
14	6	0	-0.691052	2.809190	-1.823035
15	6	0	-0.439467	3.823104	-0.900555
16	1	0	0.551460	4.332004	0.943174
17	1	0	-1.296152	3.012143	-2.701799
18	1	0	-0.853063	4.815576	-1.050805
19	15	0	-2.662404	-0.076596	1.053578
20	6	0	-1.568384	-0.029089	2.533063
21	6	0	-4.247932	-0.671771	1.786032
22	6	0	-3.013386	1.714671	0.826498
23	6	0	-0.157810	1.537471	-1.633687
24	1	0	-0.339016	0.756393	-2.366268
25	6	0	2.633917	-0.168164	0.190396
26	6	0	3.598600	0.750972	-0.247941
27	6	0	3.034194	-1.164569	1.090643
28	6	0	4.917218	0.665613	0.186031
29	1	0	3.306679	1.534505	-0.941674
30	6	0	4.352984	-1.251332	1.524564
31	1	0	2.291592	-1.865687	1.461083
32	6	0	5.301884	-0.336971	1.073341
33	1	0	5.647932	1.383617	-0.174461
34	1	0	4.638173	-2.030019	2.225941
35	1	0	6.330402	-0.401603	1.414649
36	1	0	-4.141620	-1.717292	2.087640
37	1	0	-4.535976	-0.074364	2.657652
38	1	0	-5.042211	-0.613371	1.036653
39	1	0	-2.077975	2.226842	0.581726
40	1	0	-3.707586	1.858736	-0.005940
41	1	0	-3.440782	2.153761	1.734726
42	1	0	-0.606115	0.398212	2.233365
43	1	0	-2.001645	0.570406	3.341080
44	1	0	-1.391624	-1.047692	2.888973

Zero-point correction= 0.365758 (Hartree/Particle)
Thermal correction to Energy= 0.388526
Thermal correction to Enthalpy= 0.389470
Thermal correction to Gibbs Free Energy= 0.311773
Sum of electronic and zero-point Energies= -1205.062911
Sum of electronic and thermal Energies= -1205.040143
Sum of electronic and thermal Enthalpies= -1205.039199
Sum of electronic and thermal Free Energies= -1205.116896
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1205.388105

Frequencies

-270.8215	14.0504	38.6510
51.1995	59.8866	67.6171
75.9882	79.2127	90.1433
115.2538	118.0725	126.1544
153.2555	159.2988	172.4720
180.4797	193.5371	202.0127
241.0062	247.6971	255.0623
257.7700	288.5234	312.2758
324.0126	402.5547	417.5700
422.4372	435.3162	467.2636
517.0907	596.6395	620.8092
630.8366	645.6007	654.0182
685.4721	718.6544	723.2594
732.3069	747.4884	749.8942
765.0680	795.0836	798.7679
804.3701	850.2159	868.3415
870.9396	873.2519	881.7574
935.5422	948.0737	955.0789
972.0870	974.9606	977.8100
987.5341	992.5134	995.5695
1000.9560	1013.8779	1017.9194
1019.2160	1021.8182	1055.9291
1074.7480	1075.2874	1119.7624
1122.0588	1154.3853	1181.8867
1185.3628	1189.2134	1211.5710
1212.7851	1214.7058	1243.5972
1317.9306	1340.6979	1344.2441
1345.3024	1348.4407	1362.8797
1365.8556	1367.3102	1450.5174
1478.7985	1481.5166	1488.2614
1495.7227	1496.3689	1500.2096
1501.1267	1506.0298	1508.1930
1551.1328	1555.7636	1645.8212
1667.5645	1675.8978	1692.5543
1699.2250	3067.8769	3068.2300
3070.0288	3075.5517	3100.1595
3159.1663	3162.3638	3164.9303
3166.5432	3171.8911	3172.0680
3175.1244	3203.4801	3208.8661
3210.1430	3214.7827	3221.3520
3224.6081	3226.0238	3232.7205
3232.9665	3238.0692	3242.0756

INT39

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.114203	-3.054484	-1.077756
2	1	0	0.050761	-3.036999	-2.155674
3	1	0	-0.595670	-3.981142	-0.752575
4	6	0	1.113253	-2.611945	-0.266948
5	1	0	1.113173	-3.092978	0.718192
6	6	0	0.624977	-1.208940	-0.204420
7	6	0	1.289775	-0.041694	-0.131090
8	46	0	-1.328567	-1.504169	-0.509200
9	1	0	2.104481	-2.753671	-0.720789
10	6	0	0.666383	1.290131	-0.353753
11	6	0	1.054467	2.391703	0.423779
12	6	0	0.470815	3.641481	0.241923
13	1	0	1.818154	2.255928	1.184463
14	6	0	-0.884149	2.745849	-1.533752
15	6	0	-0.508724	3.823604	-0.734179
16	1	0	0.779534	4.476182	0.864205
17	1	0	-1.620650	2.883058	-2.321028
18	1	0	-0.959869	4.799977	-0.882322
19	15	0	-2.857561	0.152529	0.676347
20	6	0	-2.000088	1.307548	1.821024
21	6	0	-3.982346	-0.740645	1.837234
22	6	0	-4.045111	1.295736	-0.149214
23	6	0	-0.299742	1.494322	-1.348734
24	1	0	-0.573984	0.661073	-1.989959
25	6	0	2.756286	-0.057253	0.156001
26	6	0	3.633456	0.761511	-0.569264

27	6	0	3.294782	-0.899986	1.134940
28	6	0	5.003499	0.723684	-0.335002
29	1	0	3.230222	1.429313	-1.325717
30	6	0	4.666035	-0.938150	1.371879
31	1	0	2.624194	-1.518747	1.723763
32	6	0	5.526432	-0.128069	0.636556
33	1	0	5.665613	1.359682	-0.915097
34	1	0	5.061364	-1.598191	2.138286
35	1	0	6.595874	-0.155643	0.821325
36	1	0	-3.384719	-1.367265	2.505064
37	1	0	-4.576492	-0.042531	2.436376
38	1	0	-4.657764	-1.391489	1.274568
39	1	0	-1.544156	2.114171	1.240215
40	1	0	-2.704314	1.733822	2.543468
41	1	0	-1.204214	0.777063	2.350521
42	1	0	-3.483278	1.996803	-0.772261
43	1	0	-4.727304	0.729000	-0.788771
44	1	0	-4.628247	1.860029	0.586408

Zero-point correction= 0.367895 (Hartree/Particle)
Thermal correction to Energy= 0.390663
Thermal correction to Enthalpy= 0.391607
Thermal correction to Gibbs Free Energy= 0.314608
Sum of electronic and zero-point Energies= -1205.068204
Sum of electronic and thermal Energies= -1205.045436
Sum of electronic and thermal Enthalpies= -1205.044492
Sum of electronic and thermal Free Energies= -1205.121491
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1205.394646
Frequencies

19.1374	42.6520	55.1391
62.3759	73.1206	79.8626
89.4517	92.8213	97.7534
115.7797	127.9853	147.2828
166.0228	177.7011	209.1909
217.6263	242.0874	245.8092
250.5008	255.5631	275.5102
283.9109	308.4519	314.8166
366.2204	417.4576	419.8653
426.8357	471.8270	506.2004
543.0850	614.5104	624.9596
630.8912	652.2679	670.8057
676.0152	696.3099	721.5931
725.8776	740.9870	744.6768
767.2648	797.0407	806.3085
813.4211	853.3697	861.6214
870.0816	879.8825	888.9716
932.3519	954.9857	960.0905
978.1013	980.3587	990.1176
994.7261	999.8128	1007.6772
1017.3809	1018.4827	1019.9898
1024.7938	1035.4770	1071.8935
1075.9455	1089.5241	1117.1431
1121.3822	1131.2834	1186.8480
1190.1632	1213.1431	1214.8029
1220.2912	1247.2580	1302.4671
1316.8014	1341.4165	1342.7973
1345.9868	1349.0588	1364.9244
1365.4481	1367.3466	1465.6269
1486.4126	1489.1421	1491.9802
1493.3873	1500.6043	1501.5674
1502.4739	1504.4428	1510.8310
1553.1750	1558.0898	1665.1763
1669.9513	1692.2279	1695.7852
1704.2560	3052.3277	3071.1649
3072.6081	3085.9944	3095.3748
3104.0169	3161.1306	3162.0744
3177.5883	3177.9188	3179.5111
3181.3628	3193.1462	3206.7016
3210.4193	3215.5036	3219.8799
3222.6228	3225.4974	3233.6664
3238.5673	3239.2969	3246.7131

INT40

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	46	0	-2.550303	-0.037512	-0.048932
2	6	0	-0.093328	0.756162	-0.123296
3	6	0	-0.080867	-0.812016	-0.056802
4	1	0	-0.417684	1.299777	0.763695
5	1	0	-0.360568	1.228748	-1.067968
6	1	0	-0.355612	-1.356800	-0.958921
7	6	0	1.142074	-0.016583	-0.059802
8	6	0	2.473910	-0.001062	-0.021265
9	1	0	-0.381609	-1.293887	0.873670
10	6	0	3.243538	-1.273498	0.035324
11	6	0	4.411919	-1.360250	0.802905
12	6	0	2.806769	-2.413282	-0.648904
13	6	0	5.114806	-2.556904	0.894286
14	1	0	4.763105	-0.481900	1.336850
15	6	0	3.511966	-3.609030	-0.560945
16	1	0	1.915378	-2.352268	-1.265188
17	6	0	4.667566	-3.686056	0.212563
18	1	0	6.013909	-2.606449	1.500879
19	1	0	3.162429	-4.481227	-1.105094
20	1	0	5.218820	-4.618894	0.278940
21	6	0	3.213162	1.290792	-0.035867
22	6	0	4.416527	1.410946	-0.742350
23	6	0	2.711937	2.416606	0.626950
24	6	0	5.090043	2.626610	-0.796604
25	1	0	4.819361	0.543662	-1.257603
26	6	0	3.387405	3.631497	0.575999
27	1	0	1.792356	2.329718	1.197002
28	6	0	4.577903	3.741891	-0.138056
29	1	0	6.017546	2.702414	-1.355961
30	1	0	2.985825	4.492545	1.101691
31	1	0	5.106058	4.689539	-0.176770
32	15	0	-4.803080	0.000894	0.032013
33	6	0	-5.581575	0.201430	1.694230
34	6	0	-5.744206	-1.466029	-0.578815
35	6	0	-5.676272	1.342313	-0.888274
36	1	0	-6.826380	-1.321586	-0.479270
37	1	0	-5.500708	-1.644231	-1.629681
38	1	0	-5.446166	-2.350884	-0.009982
39	1	0	-6.675718	0.222302	1.629108
40	1	0	-5.275423	-0.625829	2.340094
41	1	0	-5.230204	1.131310	2.149354
42	1	0	-6.763438	1.279017	-0.762218
43	1	0	-5.327998	2.313910	-0.527767
44	1	0	-5.432780	1.271931	-1.951855

Zero-point correction= 0.367185 (Hartree/Particle)
Thermal correction to Energy= 0.390873
Thermal correction to Enthalpy= 0.391817
Thermal correction to Gibbs Free Energy= 0.308297
Sum of electronic and zero-point Energies= -1205.081365
Sum of electronic and thermal Energies= -1205.057678
Sum of electronic and thermal Enthalpies= -1205.056733
Sum of electronic and thermal Free Energies= -1205.140253
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1205.415767
Frequencies

6.0502	21.8452	24.8089
33.4675	39.5167	50.6751
58.6700	70.7016	97.3882
103.6290	127.2666	132.1874
148.0004	158.9366	193.3682
197.5038	213.9474	219.9681
232.9779	244.5982	258.5466
266.6865	290.4543	302.8324
338.3040	399.0160	408.6705
417.2119	423.1115	461.6085
525.1845	624.8901	631.9880
636.7636	657.2693	688.8470
697.1518	715.2457	717.3968
737.3595	740.9883	742.8515
775.6570	798.3079	803.5326
841.5194	865.6815	872.0730
873.9554	875.7274	901.3488
933.3437	947.8682	951.8773

973.6931	976.1026	993.8170
995.0713	995.9608	1017.4674
1018.2110	1019.1477	1021.3998
1045.0223	1053.8541	1067.8137
1074.5650	1082.1239	1090.0181
1107.2383	1122.8141	1129.3665
1154.1914	1188.5231	1192.4015
1209.0373	1215.7319	1266.6721
1325.7780	1346.3743	1347.5691
1348.1362	1359.2150	1364.7724
1367.8775	1370.4152	1459.5685
1481.9370	1484.1228	1492.6619
1494.0332	1500.0178	1502.1031
1505.2243	1511.6384	1513.5968
1556.0345	1562.7484	1675.4642
1679.2131	1702.9033	1704.6578
1864.0122	3067.1969	3070.1529
3071.4125	3129.0909	3130.3382
3159.0537	3160.9492	3161.6555
3177.5233	3178.4396	3179.3768
3204.7794	3209.9553	3210.2896
3211.8777	3215.2626	3218.6290
3220.6266	3225.7136	3229.5172
3234.7661	3237.7315	3242.3487

TS27

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-2.177039	-0.139283	0.084459
2	6	0	-0.280783	0.902775	0.128162
3	6	0	-0.222814	-1.040331	0.207459
4	1	0	-0.480145	1.438169	1.058278
5	1	0	-0.434610	1.495131	-0.777496
6	1	0	-0.376942	-1.681622	-0.662923
7	6	0	0.845532	-0.035414	0.131823
8	6	0	2.180644	0.008408	0.049069
9	1	0	-0.350705	-1.542772	1.169714
10	6	0	2.990225	-1.240023	0.042151
11	6	0	4.166299	-1.314235	0.800683
12	6	0	2.603738	-2.362370	-0.698520
13	6	0	4.919000	-2.482497	0.836048
14	1	0	4.483706	-0.444829	1.369787
15	6	0	3.359059	-3.531589	-0.666809
16	1	0	1.715523	-2.307940	-1.319315
17	6	0	4.516848	-3.597483	0.103057
18	1	0	5.822591	-2.522132	1.436848
19	1	0	3.046489	-4.390017	-1.253788
20	1	0	5.106996	-4.508372	0.125590
21	6	0	2.900254	1.307987	-0.034408
22	6	0	4.016371	1.439077	-0.871496
23	6	0	2.484611	2.424850	0.699927
24	6	0	4.682524	2.654036	-0.986835
25	1	0	4.356356	0.576225	-1.437442
26	6	0	3.153189	3.640215	0.587881
27	1	0	1.643543	2.330064	1.378805
28	6	0	4.252034	3.760946	-0.258504
29	1	0	5.540472	2.736264	-1.647343
30	1	0	2.820341	4.493113	1.171845
31	1	0	4.774004	4.709012	-0.344339
32	15	0	-4.587549	0.026681	-0.060350
33	6	0	-5.537501	0.496590	1.448973
34	6	0	-5.507753	-1.488102	-0.572387
35	6	0	-5.251038	1.249217	-1.270977
36	1	0	-6.612706	0.554100	1.246481
37	1	0	-5.358902	-0.242195	2.234859
38	1	0	-5.187612	1.466272	1.812802
39	1	0	-6.584582	-1.298048	-0.640359
40	1	0	-5.139975	-1.827690	-1.544181
41	1	0	-5.329654	-2.285569	0.153955
42	1	0	-6.346580	1.245751	-1.286350
43	1	0	-4.898290	2.249967	-1.007512
44	1	0	-4.874926	1.011558	-2.269560

Zero-point correction= 0.365061 (Hartree/Particle)
Thermal correction to Energy= 0.388090
Thermal correction to Enthalpy= 0.389034
Thermal correction to Gibbs Free Energy= 0.308620
Sum of electronic and zero-point Energies= -1205.062992
Sum of electronic and thermal Energies= -1205.039962
Sum of electronic and thermal Enthalpies= -1205.039018
Sum of electronic and thermal Free Energies= -1205.119432
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1205.393339
Frequencies

-187.3528	18.7670	19.9505
26.9725	32.6162	53.5619
65.9080	67.9831	69.7826
101.9294	115.6805	123.1444
136.7507	140.9003	186.5082
205.6635	215.9877	220.7404
243.8398	252.9960	261.2846
296.7870	304.2202	313.3773
352.3706	386.8455	417.8064
422.7012	459.0324	473.5622
530.6122	536.5123	583.5970
626.7476	632.7759	642.4684
664.4696	686.5084	708.4834
718.7506	723.4258	738.0898
742.9862	747.2756	785.5127
799.6366	805.2389	864.2708
865.9076	874.5266	883.3482
935.9393	937.9175	947.6043
950.2539	964.9788	978.6049
979.9535	985.7962	995.1306
997.2257	1002.2304	1012.9800
1016.9762	1022.1719	1023.6952
1028.7549	1077.9047	1078.6860
1122.3312	1129.9574	1131.3434
1192.2384	1193.8038	1208.8435
1220.4540	1220.7011	1254.1515
1324.2477	1346.4898	1348.6679
1351.8119	1366.1692	1370.4775
1371.7984	1373.9151	1412.3540
1433.4389	1484.0847	1490.2300
1492.6940	1500.7837	1500.8848
1506.2813	1509.4694	1511.8509
1559.0767	1565.0313	1674.5730
1677.2683	1702.3784	1704.2615
1811.3337	3067.5488	3071.2829
3073.0687	3093.8347	3098.8867
3159.3372	3162.4347	3164.0529
3174.2425	3180.0188	3182.2959
3185.5507	3190.5838	3207.8940
3217.6217	3218.0663	3225.2282
3225.9090	3232.0899	3233.5926
3239.6554	3241.8126	3249.0674

INT41

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.823912	-1.121733	-0.409464
2	6	0	0.694234	0.430355	-1.149160
3	6	0	0.007110	-1.713015	-1.242213
4	1	0	1.061939	0.543809	-2.173105
5	1	0	0.804378	1.337844	-0.551535
6	1	0	-0.462489	-2.569667	-0.761049
7	6	0	-0.548332	-0.359227	-0.990195
8	6	0	-1.717052	0.050793	-0.436951
9	1	0	0.223463	-1.892538	-2.299995
10	6	0	-2.771607	-0.914441	-0.032441
11	6	0	-4.098365	-0.724089	-0.445009
12	6	0	-2.488799	-2.012052	0.789314
13	6	0	-5.098158	-1.616269	-0.077731
14	1	0	-4.336449	0.137764	-1.062878
15	6	0	-3.488598	-2.909389	1.158112
16	1	0	-1.475710	-2.144093	1.160060
17	6	0	-4.796022	-2.718172	0.722083

18	1	0	-6.117069	-1.454025	-0.417120
19	1	0	-3.245606	-3.753969	1.796479
20	1	0	-5.576799	-3.415649	1.009947
21	6	0	-1.988538	1.488013	-0.184649
22	6	0	-2.679737	1.890064	0.968784
23	6	0	-1.588966	2.486406	-1.086308
24	6	0	-2.935260	3.233188	1.223560
25	1	0	-3.016870	1.131720	1.670105
26	6	0	-1.840542	3.830667	-0.831350
27	1	0	-1.094336	2.194219	-2.008686
28	6	0	-2.512432	4.212612	0.327732
29	1	0	-3.468220	3.516196	2.126698
30	1	0	-1.524198	4.581775	-1.549695
31	1	0	-2.714733	5.260943	0.524601
32	15	0	3.753049	0.122524	0.504266
33	6	0	4.388329	1.357585	-0.703042
34	6	0	5.320380	-0.622266	1.126336
35	6	0	3.277578	1.203612	1.915895
36	1	0	4.840111	0.839690	-1.553440
37	1	0	3.550672	1.954314	-1.075585
38	1	0	5.130595	2.021771	-0.248337
39	1	0	6.018153	0.149078	1.468606
40	1	0	5.102222	-1.298314	1.957593
41	1	0	5.793697	-1.203072	0.329967
42	1	0	4.097934	1.867403	2.208053
43	1	0	2.409299	1.805430	1.632952
44	1	0	2.992965	0.584955	2.771112

Zero-point correction= 0.366779 (Hartree/Particle)
Thermal correction to Energy= 0.389689
Thermal correction to Enthalpy= 0.390634
Thermal correction to Gibbs Free Energy= 0.311532
Sum of electronic and zero-point Energies= -1205.071549
Sum of electronic and thermal Energies= -1205.048639
Sum of electronic and thermal Enthalpies= -1205.047694
Sum of electronic and thermal Free Energies= -1205.126796
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1205.405818
Frequencies

20.9876	26.3975	28.6245
42.8441	53.1216	59.8592
71.9091	75.4721	101.8953
128.5824	131.3589	154.1011
168.2769	181.9510	203.8890
229.0791	234.7445	248.3939
251.9390	255.5752	278.8664
307.6529	312.5814	366.1540
416.8065	419.3222	425.1489
443.3621	485.1766	498.4568
547.9305	601.9275	627.4427
632.4645	635.7562	660.6214
684.6761	702.4000	717.6973
721.1485	726.2685	745.3254
751.9297	764.6220	784.2595
793.3230	811.7366	866.5559
870.9570	873.9289	878.7221
933.0949	941.7524	953.3222
963.0455	978.7683	983.0937
985.8581	992.5884	995.4333
997.2589	1004.2430	1013.0566
1013.6231	1019.5343	1022.4308
1043.6627	1073.4318	1076.9654
1109.8727	1120.3800	1125.8202
1185.5450	1186.6072	1211.6016
1216.0777	1237.3478	1254.5430
1322.0808	1340.7062	1350.6271
1351.8916	1363.0698	1366.0733
1372.5541	1375.4276	1457.8326
1476.1858	1484.7621	1488.4474
1491.3880	1500.3813	1501.6384
1502.4437	1505.4070	1510.8260
1554.5962	1562.2493	1667.1074
1671.1905	1694.1745	1703.5489
1711.6952	3074.6761	3076.4144
3078.3294	3096.6036	3103.6879
3163.7936	3166.2602	3168.7555

3174.6744	3175.4291	3178.2595
3183.5478	3199.0805	3199.5197
3202.8566	3208.8805	3208.9736
3215.4537	3215.7286	3224.0553
3226.5818	3231.7022	3236.4865

TS28

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.709380	1.061691	-1.112817
2	6	0	-0.231529	-1.047808	-0.901761
3	6	0	0.277202	0.976742	-2.081608
4	1	0	-0.802583	-1.355067	-0.031374
5	1	0	-0.640228	-1.362913	-1.858729
6	1	0	0.741180	1.952172	-2.191777
7	6	0	0.536940	0.223147	-0.912370
8	6	0	1.448319	0.502665	0.136071
9	1	0	0.036771	0.455041	-3.007068
10	1	0	1.830643	-1.546780	-0.461213
11	6	0	0.920359	-4.464524	-1.612054
12	6	0	0.208276	-4.417202	-0.256946
13	6	0	0.893755	-3.244860	0.456661
14	7	0	1.132533	-2.293868	-0.645942
15	1	0	0.318942	-4.835200	-2.444194
16	1	0	1.834241	-5.069305	-1.567727
17	1	0	-0.855042	-4.194136	-0.394823
18	1	0	0.288626	-5.346161	0.309238
19	6	0	1.226507	-0.072525	1.472965
20	6	0	-0.063842	-0.191576	2.027835
21	6	0	2.293788	-0.581491	2.245654
22	6	0	-0.286573	-0.841651	3.240574
23	1	0	-0.894997	0.263594	1.490563
24	6	0	2.074619	-1.221055	3.458246
25	1	0	3.306759	-0.474087	1.863684
26	6	0	0.779231	-1.374859	3.960658
27	1	0	-1.297741	-0.910446	3.636369
28	1	0	2.920882	-1.611931	4.016875
29	1	0	0.611194	-1.878408	4.907267
30	6	0	2.542815	1.474201	-0.045293
31	6	0	2.953689	2.311696	1.006599
32	6	0	3.252972	1.576689	-1.257817
33	6	0	4.009519	3.205561	0.855806
34	1	0	2.427066	2.258691	1.955657
35	6	0	4.297532	2.477673	-1.412423
36	1	0	2.978894	0.923981	-2.083195
37	6	0	4.686763	3.302213	-0.356078
38	1	0	4.295501	3.838961	1.691120
39	1	0	4.823699	2.527496	-2.361927
40	1	0	5.505048	4.005010	-0.477449
41	15	0	-3.646925	0.847173	0.214298
42	6	0	-5.347397	1.136103	-0.440154
43	6	0	-3.669912	1.907959	1.722792
44	6	0	-3.864533	-0.816481	0.987088
45	6	0	1.337176	-3.025129	-1.862631
46	8	0	1.739369	-2.511921	-2.870024
47	1	0	1.853809	-3.539765	0.893155
48	1	0	0.294463	-2.771384	1.238947
49	1	0	-3.673514	2.961060	1.428909
50	1	0	-4.545695	1.705104	2.349248
51	1	0	-2.760572	1.726883	2.304306
52	1	0	-5.420845	2.157349	-0.823618
53	1	0	-5.539017	0.450174	-1.269850
54	1	0	-6.108369	0.987795	0.333637
55	1	0	-2.960175	-1.075507	1.548238
56	1	0	-4.723391	-0.840444	1.667002
57	1	0	-4.006926	-1.567652	0.204754

Zero-point correction= 0.481040 (Hartree/Particle)
Thermal correction to Energy= 0.509887
Thermal correction to Enthalpy= 0.510831
Thermal correction to Gibbs Free Energy= 0.419282
Sum of electronic and zero-point Energies= -1491.423432
Sum of electronic and thermal Energies= -1491.394585

Sum of electronic and thermal Enthalpies= -1491.393641
Sum of electronic and thermal Free Energies= -1491.485190
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1491.865737
Frequencies

-522.2897	24.0919	28.9028
37.8849	43.9189	46.4949
53.6497	59.0214	61.9499
71.3440	81.1622	90.2588
98.4514	104.4597	125.6619
144.2736	146.7319	160.5738
169.8843	181.7059	196.0953
215.8413	225.8534	242.0099
247.7571	258.8453	262.4188
266.7005	305.4214	310.6157
318.6803	342.1676	387.3558
409.8528	421.5349	428.2253
437.3891	488.1645	500.8889
537.0645	546.6253	566.2393
609.9001	630.1709	632.6630
633.1706	642.2933	675.0924
686.0306	702.9348	713.5995
718.8351	728.2501	742.5970
745.8208	777.8736	785.3967
804.0198	840.6392	860.1485
865.4607	869.2712	872.7052
874.4690	881.5423	901.0266
919.0468	928.4048	936.0948
943.0592	960.3710	972.0899
975.8314	979.4272	990.3557
992.4060	996.9262	1004.8962
1005.7721	1013.1219	1014.7517
1016.2642	1046.3357	1074.4887
1078.2528	1079.4235	1089.8847
1109.6614	1117.6977	1128.1468
1136.1782	1157.3744	1183.0063
1188.4112	1210.1361	1214.2925
1218.0275	1224.8885	1233.7466
1249.0770	1283.4983	1310.9303
1316.4128	1325.8548	1337.9751
1348.3174	1352.7999	1360.8419
1364.0880	1367.6056	1372.5430
1374.8487	1385.1631	1443.0931
1462.7139	1485.0188	1486.3614
1487.1640	1491.0813	1496.1966
1499.5175	1501.5271	1505.1279
1511.2901	1515.4389	1524.0757
1536.5760	1543.2940	1548.8982
1555.8956	1648.6979	1662.7174
1682.9930	1698.5237	1914.1502
3068.3080	3073.6861	3075.1768
3097.7957	3103.6004	3115.7608
3153.7124	3155.1324	3161.7527
3165.0433	3168.0251	3170.6762
3172.7249	3173.2557	3179.3937
3180.0563	3183.2421	3184.9975
3193.6555	3195.2636	3197.8927
3198.9384	3202.1308	3209.4745
3211.2505	3216.6776	3229.6626
3230.7092	3260.4842	3294.6093

INT42

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.989861	0.220661	-1.012209
2	6	0	0.542382	-1.496518	-0.912555
3	6	0	-0.029495	0.440636	-2.256286
4	1	0	0.509501	-1.889734	0.101987
5	1	0	-0.198655	-2.001056	-1.536256
6	1	0	0.033922	1.480858	-2.552201
7	6	0	0.460749	0.008427	-1.017188
8	6	0	1.091677	0.773746	0.008359
9	1	0	-0.225434	-0.279039	-3.049883
10	1	0	1.911242	-1.638316	-2.468394

11	6	0	2.752666	-3.836705	-0.197852
12	6	0	3.166867	-2.502602	0.440132
13	6	0	3.117132	-1.511553	-0.725437
14	7	0	1.910206	-1.962962	-1.494923
15	1	0	2.148798	-4.484849	0.442395
16	1	0	3.611515	-4.425658	-0.539073
17	1	0	2.470982	-2.195323	1.227461
18	1	0	4.165057	-2.537769	0.877811
19	6	0	1.207868	0.249560	1.369553
20	6	0	0.207969	-0.553884	1.966454
21	6	0	2.370083	0.477260	2.146274
22	6	0	0.397787	-1.161233	3.205591
23	1	0	-0.738035	-0.673288	1.438472
24	6	0	2.546769	-0.111313	3.390468
25	1	0	3.146967	1.123147	1.743087
26	6	0	1.572145	-0.957524	3.927047
27	1	0	-0.394899	-1.777642	3.623470
28	1	0	3.460860	0.082315	3.945871
29	1	0	1.714916	-1.421650	4.897631
30	6	0	1.618015	2.120714	-0.267836
31	6	0	1.548819	3.140246	0.702005
32	6	0	2.261742	2.446419	-1.478470
33	6	0	2.091098	4.400166	0.478091
34	1	0	1.054897	2.927286	1.646061
35	6	0	2.799417	3.706879	-1.705779
36	1	0	2.341663	1.687361	-2.253060
37	6	0	2.720321	4.698148	-0.728652
38	1	0	2.009755	5.160136	1.250506
39	1	0	3.292635	3.914756	-2.651719
40	1	0	3.138578	5.683969	-0.905980
41	15	0	-3.830339	0.014454	0.335461
42	6	0	-4.178749	-1.633710	1.099653
43	6	0	-5.520185	0.436214	-0.282204
44	6	0	-3.779845	1.052780	1.861932
45	6	0	1.951883	-3.469523	-1.426343
46	8	0	1.406210	-4.129518	-2.248302
47	1	0	3.977621	-1.626427	-1.391656
48	1	0	2.976967	-0.468117	-0.436467
49	1	0	-3.733841	2.107775	1.578281
50	1	0	-4.655145	0.887193	2.501106
51	1	0	-2.869868	0.820283	2.423327
52	1	0	-4.356165	-2.372384	0.313195
53	1	0	-3.304183	-1.954808	1.673939
54	1	0	-5.049185	-1.600013	1.765323
55	1	0	-5.771437	-0.210945	-1.127027
56	1	0	-6.280002	0.321958	0.499546
57	1	0	-5.524126	1.469877	-0.638911

Zero-point correction= 0.483285 (Hartree/Particle)
Thermal correction to Energy= 0.512449
Thermal correction to Enthalpy= 0.513393
Thermal correction to Gibbs Free Energy= 0.419334
Sum of electronic and zero-point Energies= -1491.425590
Sum of electronic and thermal Energies= -1491.396427
Sum of electronic and thermal Enthalpies= -1491.395483
Sum of electronic and thermal Free Energies= -1491.489542
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1491.880506
Frequencies

12.4002	15.8312	27.0379
30.2382	37.0921	48.9585
54.9244	61.2276	66.9571
83.0794	93.7212	94.0437
110.1278	123.8876	132.8437
141.7534	170.0003	181.1474
192.5440	207.5538	216.2343
222.3086	225.7575	236.5446
255.0191	256.7824	264.4237
293.4444	308.8672	325.7768
351.5603	375.7063	416.0993
420.0760	434.6770	439.3794
481.7698	502.5772	536.5847
553.8372	573.0262	608.2356
627.4369	628.3718	632.5833
635.0367	652.1619	674.8331
683.6225	710.8797	718.7963

730.4378	731.9918	732.7177
736.9841	777.7736	784.4708
788.7863	801.9114	828.8289
835.3166	864.7324	869.9766
871.9577	878.6269	907.8560
922.4741	927.7972	930.3569
939.8284	954.2648	965.4697
973.6376	975.0645	990.5682
992.2326	997.0015	1004.3870
1006.7518	1010.0637	1011.4309
1013.4799	1049.6655	1059.8112
1075.5140	1077.9144	1098.1174
1120.7609	1123.8068	1126.6357
1181.9922	1187.4972	1189.0803
1210.0800	1213.9292	1216.8587
1235.5164	1257.3158	1282.6718
1292.3659	1308.4916	1317.9691
1326.5727	1337.1777	1344.2815
1348.0608	1359.7772	1362.9839
1366.4876	1369.2271	1370.0404
1379.3296	1385.9167	1424.8976
1465.7409	1476.1984	1484.2393
1491.7930	1492.7871	1497.3395
1500.7177	1502.9848	1504.0363
1505.9509	1512.2646	1513.4167
1533.1897	1541.8211	1549.2963
1564.4161	1641.6677	1656.4752
1677.9113	1692.4821	1989.5316
3064.8874	3067.1822	3070.4857
3110.5310	3112.0609	3127.4558
3149.1724	3155.4021	3155.6451
3160.0397	3162.6084	3168.7967
3170.1589	3173.4625	3173.9070
3174.8697	3185.0850	3191.9506
3193.9956	3194.4024	3195.5898
3205.2315	3209.5874	3211.5400
3220.2421	3225.5709	3235.8881
3241.7811	3271.8446	3458.4449

INT43

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.585626	-0.467741	-1.182397
2	6	0	0.932847	1.408021	-1.727509
3	6	0	-0.059442	-0.454776	-2.591133
4	1	0	1.371936	1.649354	-2.696287
5	1	0	1.089313	2.182880	-0.978799
6	1	0	-0.723365	-1.305292	-2.665482
7	6	0	-0.371844	0.710712	-1.771297
8	6	0	-1.410837	0.944683	-0.876688
9	1	0	0.449304	-0.225261	-3.527150
10	1	0	-0.304195	-0.700263	0.500597
11	6	0	0.144034	-3.812074	1.493814
12	6	0	-1.279730	-3.477185	1.956151
13	6	0	-1.298137	-1.938757	1.995083
14	7	0	-0.285204	-1.587963	1.006000
15	1	0	0.231833	-4.725837	0.904423
16	1	0	0.846261	-3.882194	2.333328
17	1	0	-2.000263	-3.816187	1.205186
18	1	0	-1.545915	-3.924121	2.915419
19	6	0	-1.325246	2.149773	-0.005466
20	6	0	-1.449627	2.041652	1.389614
21	6	0	-1.104905	3.431641	-0.531876
22	6	0	-1.338631	3.152901	2.219898
23	1	0	-1.647039	1.062990	1.824799
24	6	0	-0.983779	4.545582	0.293786
25	1	0	-1.030321	3.542916	-1.610678
26	6	0	-1.097886	4.413094	1.675872
27	1	0	-1.437293	3.034055	3.295405
28	1	0	-0.814452	5.524318	-0.146168
29	1	0	-1.011966	5.282212	2.320718
30	6	0	-2.609214	0.097976	-0.717116
31	6	0	-3.813293	0.683200	-0.264550

32	6	0	-2.649494	-1.291958	-0.956117
33	6	0	-4.968243	-0.060401	-0.069089
34	1	0	-3.833449	1.751210	-0.070874
35	6	0	-3.812683	-2.036097	-0.768742
36	1	0	-1.748718	-1.820852	-1.236821
37	6	0	-4.982808	-1.432129	-0.321505
38	1	0	-5.869678	0.438512	0.275914
39	1	0	-3.793933	-3.104717	-0.968620
40	1	0	-5.887109	-2.013842	-0.173093
41	15	0	3.168471	0.260347	0.454174
42	6	0	4.303852	1.644544	0.040407
43	6	0	4.299093	-0.989103	1.187024
44	6	0	2.287854	0.918125	1.929682
45	1	0	-2.266955	-1.520092	1.707827
46	1	0	-1.018214	-1.549257	2.982290
47	6	0	0.525368	-2.603078	0.652506
48	8	0	1.428250	-2.573044	-0.190620
49	1	0	4.965585	1.343980	-0.776180
50	1	0	3.713304	2.501032	-0.296866
51	1	0	4.906774	1.941892	0.904502
52	1	0	2.982844	1.314817	2.677269
53	1	0	1.594457	1.707494	1.619396
54	1	0	1.696046	0.113454	2.377238
55	1	0	4.855520	-0.588147	2.040332
56	1	0	3.707191	-1.852450	1.503279
57	1	0	5.003557	-1.329702	0.423215

Zero-point correction= 0.481926 (Hartree/Particle)
Thermal correction to Energy= 0.511076
Thermal correction to Enthalpy= 0.512020
Thermal correction to Gibbs Free Energy= 0.419833
Sum of electronic and zero-point Energies= -1491.492941
Sum of electronic and thermal Energies= -1491.463791
Sum of electronic and thermal Enthalpies= -1491.462847
Sum of electronic and thermal Free Energies= -1491.555034
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1491.929351
Frequencies

21.9785	23.6003	29.8537
33.6306	40.4796	47.2640
62.9754	70.8770	74.7603
88.2168	92.6943	113.8976
115.7939	140.8790	150.4410
156.1451	164.5860	178.7823
192.0978	197.5893	204.5445
217.8743	229.3264	248.6934
252.7711	255.0473	257.5818
265.5895	303.8834	314.6428
338.3920	385.6381	390.6409
420.1405	434.0957	439.9200
464.4423	515.7575	528.8373
542.1087	550.3437	588.6943
619.1584	629.1607	632.1337
639.1343	671.0348	678.0382
681.7963	702.5023	714.8932
719.3137	723.2637	734.9834
745.9012	753.3012	780.0414
786.8688	801.9199	815.0753
838.2264	868.6835	872.9697
875.5054	876.3196	880.4692
915.4069	924.9525	927.2112
931.0452	941.7008	948.2160
976.1873	979.3881	985.0884
989.8838	995.4463	995.8801
1004.8976	1006.6767	1012.3902
1013.7788	1018.4855	1023.4152
1046.8544	1074.6793	1080.3668
1096.8072	1110.7109	1121.1106
1128.1982	1132.1224	1183.9530
1185.3399	1201.6941	1213.5647
1223.6584	1232.7089	1247.0089
1263.4524	1270.6852	1304.7912
1308.2234	1335.0576	1340.8943
1348.9110	1350.3908	1359.4999
1363.8667	1370.8012	1371.2225
1373.9278	1399.6804	1481.4813

1485.2653	1487.4624	1489.9009
1491.9354	1495.2471	1497.7402
1499.2428	1499.7680	1501.0777
1508.4353	1521.7879	1523.9232
1547.6696	1553.0696	1555.9710
1586.9944	1656.4484	1664.0798
1691.7164	1698.6990	1782.4122
3069.8269	3076.0592	3076.5929
3080.6450	3092.9348	3110.9309
3136.6241	3153.7926	3158.7888
3160.9307	3163.8149	3168.7517
3170.0356	3170.8632	3177.8539
3179.6943	3180.5239	3188.7078
3193.2416	3202.6720	3208.2267
3215.4070	3218.8839	3224.4357
3226.2921	3226.9503	3236.3723
3258.5443	3294.8848	3481.0524

TS29

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.557813	-0.416596	-1.198706
2	6	0	0.691399	1.346925	-1.859126
3	6	0	-0.277053	-0.679299	-2.485196
4	1	0	1.042478	1.495337	-2.879639
5	1	0	0.802440	2.215440	-1.216351
6	1	0	-0.901891	-1.556619	-2.383586
7	6	0	-0.457319	0.467050	-1.679361
8	6	0	-1.316708	0.521398	-0.494924
9	1	0	0.224873	-0.565390	-3.443205
10	1	0	-0.587522	-0.435228	0.330345
11	6	0	0.601545	-3.497916	1.791273
12	6	0	-0.816789	-3.282499	2.321076
13	6	0	-0.985032	-1.760272	2.184390
14	7	0	-0.138119	-1.396660	1.048393
15	1	0	0.776742	-4.457361	1.301259
16	1	0	1.356886	-3.379572	2.578754
17	1	0	-1.537861	-3.782957	1.665645
18	1	0	-0.973517	-3.641850	3.340495
19	6	0	-1.342454	1.838904	0.228807
20	6	0	-1.255099	1.868073	1.626748
21	6	0	-1.489288	3.067066	-0.434367
22	6	0	-1.296738	3.068052	2.333742
23	1	0	-1.150690	0.928884	2.164651
24	6	0	-1.525003	4.270398	0.264316
25	1	0	-1.582252	3.068931	-1.518375
26	6	0	-1.426395	4.276274	1.654493
27	1	0	-1.225239	3.058289	3.417680
28	1	0	-1.640785	5.205491	-0.276279
29	1	0	-1.457058	5.213171	2.202262
30	6	0	-2.651435	-0.172651	-0.551109
31	6	0	-3.849355	0.548182	-0.415004
32	6	0	-2.760759	-1.569201	-0.683298
33	6	0	-5.087649	-0.084548	-0.438920
34	1	0	-3.806293	1.625758	-0.289675
35	6	0	-3.999978	-2.203367	-0.712365
36	1	0	-1.860478	-2.175076	-0.716839
37	6	0	-5.173939	-1.465521	-0.594719
38	1	0	-5.992391	0.508697	-0.339131
39	1	0	-4.043944	-3.284217	-0.815450
40	1	0	-6.140344	-1.959708	-0.615188
41	15	0	3.223598	0.472754	0.192564
42	6	0	4.236160	1.926616	-0.287550
43	6	0	4.465863	-0.756789	0.746780
44	6	0	2.446638	1.014865	1.764190
45	1	0	-2.019959	-1.457220	1.993620
46	1	0	-0.644284	-1.243667	3.094611
47	6	0	0.756127	-2.348206	0.798887
48	8	0	1.644716	-2.357659	-0.091686
49	1	0	5.069503	-0.377940	1.577589
50	1	0	3.929445	-1.660842	1.047564
51	1	0	5.120268	-1.017314	-0.089512
52	1	0	3.192374	1.369378	2.483631

53	1	0	1.723019	1.810291	1.558874
54	1	0	1.892944	0.170398	2.186484
55	1	0	4.833217	1.682354	-1.169971
56	1	0	3.573532	2.758437	-0.541664
57	1	0	4.902076	2.232913	0.525577

Zero-point correction= 0.476809 (Hartree/Particle)
Thermal correction to Energy= 0.505344
Thermal correction to Enthalpy= 0.506288
Thermal correction to Gibbs Free Energy= 0.416452
Sum of electronic and zero-point Energies= -1491.477864
Sum of electronic and thermal Energies= -1491.449329
Sum of electronic and thermal Enthalpies= -1491.448385
Sum of electronic and thermal Free Energies= -1491.538220
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1491.908298
Frequencies

-1361.8267	22.6951	29.9105
33.7370	40.0514	46.9345
58.0193	64.0929	74.3541
81.2351	102.8366	107.1246
117.7022	132.0028	155.4053
161.0049	169.3666	179.3190
197.5921	201.2754	205.4215
214.8543	232.1241	244.8040
247.5246	249.8030	256.6788
259.5925	293.4757	298.1810
299.7619	318.7583	356.7008
389.1282	418.9088	433.4054
445.4202	488.7294	520.8547
547.0499	557.0636	565.5685
606.2428	628.6764	632.3374
643.4326	657.8137	684.5139
705.7023	712.4039	722.1277
726.1772	740.8864	749.5740
752.9201	760.5715	787.1661
791.7294	808.1603	813.7388
868.5767	870.6229	872.2667
873.4190	878.0397	890.4303
918.3258	919.5568	937.4448
943.7113	949.9389	957.7487
979.7013	983.6865	985.7255
989.1325	995.3251	998.7357
1007.6641	1010.5508	1013.2535
1018.5464	1019.2247	1024.3772
1028.7715	1073.0538	1078.2220
1087.9890	1099.5628	1119.8947
1128.3340	1133.1679	1183.8418
1185.6956	1192.5534	1213.4454
1220.8248	1231.0788	1241.5899
1268.3671	1284.5002	1313.2884
1314.1545	1323.5218	1342.8317
1346.8467	1350.5959	1357.0465
1360.2353	1363.2868	1368.1730
1372.1884	1405.5502	1438.9059
1474.0003	1477.8648	1484.6394
1491.6619	1493.5259	1495.4803
1499.8635	1501.9238	1506.8355
1509.6228	1515.6031	1521.9802
1543.3875	1550.8054	1554.5770
1561.6050	1596.6113	1665.2875
1669.4530	1695.4047	1700.5857
1727.6644	3043.1599	3069.1289
3075.6262	3078.3795	3086.9478
3097.5089	3135.7607	3153.3030
3157.4434	3163.0362	3166.5455
3166.9046	3168.1123	3170.7828
3182.3574	3182.8078	3185.0398
3195.1995	3198.4763	3203.3242
3209.1389	3211.9296	3219.6474
3221.4159	3229.4462	3230.6957
3239.2682	3245.6637	3293.3976

INT44

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	46	0	-0.852945	-0.902176	-0.796469
2	6	0	0.846327	-2.139639	-0.592356
3	6	0	0.957426	-0.206100	-2.023317
4	1	0	0.747363	-2.842945	-1.418461
5	1	0	1.072911	-2.597634	0.368356
6	1	0	1.121119	0.855333	-2.175011
7	6	0	1.364926	-0.829029	-0.851827
8	6	0	2.043315	-0.073521	0.287636
9	1	0	0.676467	-0.796279	-2.892706
10	1	0	1.597130	-0.458607	1.215213
11	6	0	-3.888179	2.280368	-0.850852
12	6	0	-4.007784	3.071747	0.450925
13	6	0	-3.548514	2.036000	1.504000
14	7	0	-2.680072	1.087613	0.812021
15	1	0	-3.560110	2.859221	-1.717003
16	1	0	-4.826651	1.779933	-1.123807
17	1	0	-3.312693	3.918536	0.435585
18	1	0	-5.008215	3.467925	0.644588
19	6	0	3.527492	-0.403050	0.344092
20	6	0	4.182772	-0.347678	1.577102
21	6	0	4.269718	-0.711813	-0.796980
22	6	0	5.546682	-0.599971	1.671837
23	1	0	3.613222	-0.095237	2.468385
24	6	0	5.637368	-0.965312	-0.705129
25	1	0	3.777414	-0.755270	-1.764681
26	6	0	6.279219	-0.911810	0.527894
27	1	0	6.038471	-0.553721	2.638730
28	1	0	6.200106	-1.206752	-1.601682
29	1	0	7.343785	-1.111770	0.598810
30	6	0	1.756291	1.422085	0.246764
31	6	0	2.686133	2.353954	-0.213902
32	6	0	0.483704	1.860392	0.626044
33	6	0	2.344705	3.703629	-0.299778
34	1	0	3.680577	2.028038	-0.505209
35	6	0	0.140833	3.203465	0.530279
36	1	0	-0.270569	1.154819	0.973904
37	6	0	1.072706	4.131832	0.068393
38	1	0	3.077297	4.419934	-0.659555
39	1	0	-0.861735	3.510827	0.814787
40	1	0	0.809335	5.182709	-0.004742
41	15	0	-2.316990	-2.132143	0.534776
42	6	0	-2.172749	-3.959840	0.381843
43	6	0	-4.100510	-1.842276	0.248972
44	6	0	-2.101555	-1.844086	2.328327
45	1	0	-3.022784	2.506716	2.343545
46	1	0	-4.418179	1.512113	1.935455
47	6	0	-2.863656	1.211541	-0.473228
48	8	0	-2.319623	0.510091	-1.398033
49	1	0	-4.704935	-2.510256	0.870981
50	1	0	-4.310918	-0.801073	0.501158
51	1	0	-4.333893	-2.006341	-0.805778
52	1	0	-2.824199	-2.421678	2.913975
53	1	0	-1.086648	-2.127649	2.622293
54	1	0	-2.239477	-0.772219	2.490878
55	1	0	-2.874253	-4.472315	1.048376
56	1	0	-2.379086	-4.255719	-0.650524
57	1	0	-1.153062	-4.267752	0.629733

Zero-point correction= 0.482402 (Hartree/Particle)
Thermal correction to Energy= 0.511390
Thermal correction to Enthalpy= 0.512334
Thermal correction to Gibbs Free Energy= 0.421010
Sum of electronic and zero-point Energies= -1491.510438
Sum of electronic and thermal Energies= -1491.481451
Sum of electronic and thermal Enthalpies= -1491.480507
Sum of electronic and thermal Free Energies= -1491.571831
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1491.945653
Frequencies
23.7807 26.8762 32.2044
43.0721 45.5031 62.1068
66.3638 77.3299 81.0253
84.9336 92.4448 108.1741
125.2457 127.1401 140.9872

160.5950	164.9617	178.6416
188.0314	191.0283	209.8357
215.7360	238.1684	250.7433
251.0967	260.5389	263.4892
269.5705	287.3059	294.5908
324.9526	332.3857	358.0443
414.8980	415.8626	423.2068
476.1219	497.3575	537.2197
557.6974	580.6882	591.8141
630.3743	630.9989	653.7574
655.3882	686.9913	705.8268
719.4553	722.1566	729.2668
756.3151	762.2410	765.2013
770.0537	782.7046	808.7972
819.9318	838.2768	854.6533
875.8146	880.0021	883.0767
887.8007	900.1281	904.5946
925.1480	926.7537	931.9790
945.0730	956.5172	961.9061
980.8794	984.5740	992.2954
997.7929	1000.6349	1005.1478
1010.4291	1018.1050	1021.9872
1023.1266	1030.5171	1034.8753
1061.4001	1075.8677	1078.2290
1093.0967	1114.8184	1126.3464
1130.8869	1182.3933	1184.0336
1187.2126	1218.2295	1220.3603
1227.2084	1228.7139	1233.6762
1255.2343	1281.2915	1304.3199
1310.9785	1339.4858	1342.7439
1344.3423	1347.7350	1354.8287
1361.6263	1369.9898	1371.3196
1374.6992	1394.4227	1432.6025
1475.1790	1480.3001	1487.7231
1491.7693	1495.1708	1499.6322
1506.6777	1507.3877	1514.3306
1518.5143	1523.8152	1530.4668
1549.1326	1558.3659	1562.2127
1592.1051	1682.3956	1685.1068
1686.9268	1704.0482	1708.5245
3012.2457	3063.0213	3071.9176
3073.3148	3075.8219	3082.7189
3086.6848	3096.0940	3142.9686
3148.0519	3160.7601	3163.3430
3164.6835	3176.7866	3177.7934
3191.5914	3191.9321	3197.2780
3207.4024	3207.4318	3209.7849
3212.0603	3216.7823	3219.1720
3225.8375	3228.7959	3231.3290
3237.2979	3239.2462	3286.8238

INT45

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.744686	-3.146250	-0.423585
2	1	0	-1.460648	-3.826867	0.034241
3	1	0	0.262731	-3.543945	-0.505425
4	6	0	-1.235689	-2.250885	-1.565861
5	1	0	-0.543080	-2.065325	-2.381658
6	6	0	-0.939102	-1.697397	-0.236180
7	6	0	-1.287278	-0.735370	0.663480
8	46	0	0.939022	-0.489508	-0.020221
9	1	0	-2.277085	-2.334948	-1.873445
10	6	0	-2.090581	0.456658	0.235868
11	6	0	-3.475141	0.291115	0.029202
12	6	0	-4.252649	1.399678	-0.325461
13	6	0	-2.311933	2.830087	-0.246595
14	6	0	-3.675853	2.655983	-0.462380
15	1	0	-5.319862	1.266668	-0.486226
16	1	0	-1.856854	3.809240	-0.352390
17	1	0	-4.298430	3.501224	-0.740352
18	6	0	-1.234841	-0.987287	2.154270
19	15	0	3.058776	0.520726	-0.041749

20	6	0	4.324393	-0.061500	1.167830
21	6	0	4.045533	0.476641	-1.600321
22	1	0	-2.256512	-1.123026	2.535175
23	1	0	-0.645787	-1.879635	2.381877
24	1	0	-0.800848	-0.131071	2.679504
25	6	0	-1.535816	1.728978	0.104361
26	1	0	-0.466257	1.837273	0.272375
27	7	0	-4.078755	-0.952353	0.245231
28	1	0	-4.958257	-1.074824	-0.239890
29	1	0	-3.459415	-1.740778	0.103062
30	6	0	3.071305	2.333153	0.304914
31	1	0	2.628267	2.518393	1.287241
32	1	0	4.088027	2.741325	0.284434
33	1	0	2.461453	2.847228	-0.443274
34	1	0	3.469200	0.935293	-2.408214
35	1	0	4.996691	1.009043	-1.487976
36	1	0	4.246823	-0.562006	-1.876223
37	1	0	3.929308	0.041606	2.181928
38	1	0	4.531825	-1.120708	0.993749
39	1	0	5.257383	0.507180	1.084020

Zero-point correction= 0.330541 (Hartree/Particle)
Thermal correction to Energy= 0.352499
Thermal correction to Enthalpy= 0.353443
Thermal correction to Gibbs Free Energy= 0.276657
Sum of electronic and zero-point Energies= -1068.799809
Sum of electronic and thermal Energies= -1068.777851
Sum of electronic and thermal Enthalpies= -1068.776907
Sum of electronic and thermal Free Energies= -1068.853693
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1069.106012
Frequencies

11.7170	24.5251	27.4113
37.0575	74.8748	77.1174
103.3573	115.6329	118.8934
125.2436	133.7578	172.0836
180.6479	183.8357	208.5039
209.5181	214.9188	222.2507
235.0762	254.5227	257.9076
281.7773	320.1275	327.0979
339.1386	363.9374	436.4389
473.5942	525.8070	559.5600
593.5165	602.4783	653.4668
675.7931	684.8827	736.6918
742.3059	765.5504	778.1362
780.5364	807.9490	822.3369
865.3738	869.9649	872.1588
878.4636	902.5494	960.1046
976.6547	979.0988	994.8769
995.3694	997.1144	1028.7040
1055.2015	1064.7406	1072.1127
1086.2078	1096.4859	1099.3181
1118.5926	1172.3412	1177.7980
1189.4707	1202.7618	1292.3303
1326.6381	1339.8657	1346.6065
1348.5589	1364.2896	1371.4804
1426.4760	1481.2251	1483.3851
1492.0700	1493.0132	1499.3880
1501.0791	1501.1653	1504.0769
1513.4808	1517.6945	1521.2423
1561.0168	1669.7219	1681.9302
1708.5846	1776.3346	3056.0328
3067.8774	3070.0919	3071.5268
3129.8819	3140.5219	3148.7799
3159.4071	3160.3764	3161.0088
3168.7263	3177.4884	3177.9783
3178.8712	3197.2084	3199.6738
3224.7067	3227.9116	3236.1895
3246.3102	3574.9485	3677.9428

TS30

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.217681	-2.752866	0.691929

2	1	0	-1.425585	-2.619572	1.750777
3	1	0	-0.502255	-3.558384	0.488231
4	6	0	-2.409240	-2.649672	-0.243597
5	1	0	-2.296072	-3.255726	-1.144306
6	6	0	-1.749245	-1.339927	-0.265033
7	6	0	-2.245539	-0.096790	-0.418132
8	46	0	0.345238	-1.432410	-0.008458
9	1	0	-3.412989	-2.726643	0.180007
10	6	0	-1.525596	1.185537	-0.155916
11	6	0	-0.962517	1.509234	1.100043
12	6	0	-0.392827	2.777247	1.291066
13	6	0	-0.931307	3.417535	-0.965296
14	6	0	-0.382911	3.725627	0.277268
15	1	0	0.039312	3.009932	2.261998
16	1	0	-0.922677	4.143643	-1.771404
17	1	0	0.058140	4.701256	0.458420
18	6	0	-3.654616	0.068123	-0.954271
19	15	0	2.358230	-0.106845	-0.267159
20	6	0	2.170299	1.385118	-1.327532
21	6	0	3.979557	-0.760927	-0.859643
22	6	0	2.847477	0.669039	1.330948
23	1	0	-3.659215	0.584768	-1.920355
24	1	0	-4.142424	-0.898992	-1.093304
25	1	0	-4.260153	0.674744	-0.270268
26	6	0	-1.493731	2.160595	-1.159907
27	1	0	-1.923589	1.917937	-2.127804
28	7	0	-0.926795	0.593562	2.152014
29	1	0	-1.073103	1.006154	3.064952
30	1	0	-1.502325	-0.225312	1.998492
31	1	0	4.294532	-1.594293	-0.225731
32	1	0	3.869295	-1.135879	-1.880807
33	1	0	4.753669	0.014298	-0.844008
34	1	0	3.160135	-0.106748	2.035310
35	1	0	3.661175	1.390970	1.200037
36	1	0	1.969305	1.171415	1.746882
37	1	0	1.333645	1.980574	-0.950876
38	1	0	3.082126	1.992953	-1.322486
39	1	0	1.939470	1.084278	-2.352971

Zero-point correction= 0.328889 (Hartree/Particle)
Thermal correction to Energy= 0.350122
Thermal correction to Enthalpy= 0.351066
Thermal correction to Gibbs Free Energy= 0.277965
Sum of electronic and zero-point Energies= -1068.765678
Sum of electronic and thermal Energies= -1068.744444
Sum of electronic and thermal Enthalpies= -1068.743500
Sum of electronic and thermal Free Energies= -1068.816601
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1069.059581
Frequencies

294.1368	20.1175	44.0014
55.0689	74.7707	76.9697
84.8515	91.6049	115.6255
130.4041	146.2926	151.9033
159.7261	163.2244	181.3381
187.3406	206.3077	237.8248
248.4228	261.3801	290.8738
306.6228	316.9703	334.3900
357.1750	364.8854	436.7538
454.3175	502.3980	533.0973
565.3320	590.7247	628.7039
643.0778	682.1247	725.9813
740.1504	744.1007	764.2558
775.1995	780.7858	809.3554
838.9705	858.9584	864.1105
868.4850	879.6938	955.5920
960.9544	978.2796	980.4710
990.0610	991.4722	1005.1468
1016.8076	1050.8405	1069.1992
1080.5116	1103.8486	1109.6839
1166.5746	1181.1277	1184.0754
1210.2536	1217.5756	1299.9846
1304.5968	1341.2318	1342.8212
1346.3041	1362.5132	1368.1987
1434.5417	1452.3301	1482.7148
1484.5944	1487.9866	1496.4240

1498.0072	1501.7997	1505.7970
1510.8620	1518.8976	1521.5247
1557.4161	1657.6428	1682.5374
1696.1837	1708.1128	3066.8207
3069.7710	3069.9650	3073.1887
3074.0032	3103.5893	3126.0691
3159.4456	3159.6924	3164.9525
3167.7483	3173.5560	3174.8081
3177.0215	3181.8949	3190.1352
3204.9889	3211.9183	3220.4285
3236.3197	3570.8378	3678.0854

INT46

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.225982	-1.130989	0.225287
2	1	0	3.548436	-1.181681	1.267504
3	1	0	4.041285	-0.820059	-0.432795
4	6	0	2.432851	-2.361112	-0.238539
5	1	0	2.685404	-2.650254	-1.266546
6	6	0	1.120635	-1.662077	-0.165583
7	6	0	-0.123720	-2.147724	-0.259456
8	46	0	1.716880	0.234180	0.069865
9	1	0	2.528559	-3.252923	0.397532
10	6	0	-1.389234	-1.368522	-0.118309
11	6	0	-1.716665	-0.660547	1.060243
12	6	0	-2.989109	-0.079560	1.180732
13	6	0	-3.614780	-0.870890	-1.005537
14	6	0	-3.931317	-0.187626	0.166748
15	1	0	-3.232880	0.455030	2.096474
16	1	0	-4.337939	-0.956320	-1.809726
17	1	0	-4.909694	0.266252	0.293074
18	6	0	-0.331274	-3.626323	-0.540085
19	15	0	0.055507	2.151196	-0.259497
20	6	0	-1.325527	1.963066	-1.457187
21	6	0	0.878746	3.666535	-0.927925
22	6	0	-0.800419	2.851514	1.211380
23	1	0	-0.781530	-3.783666	-1.527403
24	1	0	0.613097	-4.175101	-0.516212
25	1	0	-1.013840	-4.069440	0.193981
26	6	0	-2.357511	-1.453488	-1.125637
27	1	0	-2.109223	-2.001320	-2.030759
28	7	0	-0.800081	-0.494675	2.099667
29	1	0	-1.208695	-0.542182	3.024954
30	1	0	0.028740	-1.072266	2.006925
31	1	0	1.678489	3.987085	-0.253889
32	1	0	1.323484	3.442156	-1.901598
33	1	0	0.163286	4.487564	-1.044715
34	1	0	-0.053205	3.229976	1.914848
35	1	0	-1.476847	3.665641	0.930353
36	1	0	-1.358113	2.053138	1.704800
37	1	0	-2.054725	1.250600	-1.064927
38	1	0	-1.817385	2.925390	-1.636579
39	1	0	-0.937146	1.571360	-2.401094

Zero-point correction= 0.331046 (Hartree/Particle)
Thermal correction to Energy= 0.352174
Thermal correction to Enthalpy= 0.353119
Thermal correction to Gibbs Free Energy= 0.281453
Sum of electronic and zero-point Energies= -1068.775223
Sum of electronic and thermal Energies= -1068.754095
Sum of electronic and thermal Enthalpies= -1068.753151
Sum of electronic and thermal Free Energies= -1068.824817
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1069.073557
Frequencies

32.9617	57.7704	72.5739
81.8039	86.0587	96.0073
108.9563	115.4858	129.3069
142.4415	148.1936	168.7077
170.3461	182.5445	198.6213
233.4088	245.8465	264.7310
272.1691	274.6618	305.2979
315.8461	335.1492	356.1930

376.0777	402.6208	439.2762
512.5600	538.6198	555.1440
571.3188	599.9675	648.6731
660.1622	673.3282	678.6827
734.9644	749.7961	771.8617
780.5878	789.1056	818.9986
824.3413	860.3256	869.0809
872.5001	887.8771	970.0957
982.0081	982.5668	986.3280
995.2426	997.2203	1009.1974
1048.5113	1058.2123	1073.2335
1097.1869	1100.7114	1105.4994
1145.3142	1185.5523	1192.3965
1248.7938	1294.1908	1300.2960
1319.3913	1344.0384	1345.2166
1351.2571	1366.2778	1370.5937
1431.7374	1461.8975	1479.8800
1486.2872	1489.8833	1490.1519
1499.2820	1503.4437	1507.8416
1513.1339	1517.6798	1523.0787
1560.9291	1656.1759	1682.9331
1699.9748	1740.3345	3040.1619
3068.6128	3073.2341	3078.2765
3083.9581	3096.0679	3099.0680
3132.9250	3157.8223	3163.0902
3166.7104	3166.9439	3171.8485
3174.1698	3191.3529	3210.9834
3212.8931	3217.6626	3228.9479
3244.2529	3548.3704	3659.9603

INT47

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.983828	0.207233	0.068952
2	6	0	-0.236106	1.511972	-0.196216
3	6	0	-0.586090	0.044951	0.249786
4	1	0	0.215740	1.654464	-1.178693
5	1	0	0.108604	2.208781	0.565561
6	1	0	-0.481866	-0.204408	1.304183
7	6	0	-1.607650	1.011414	-0.124012
8	6	0	-2.902615	1.289354	-0.243440
9	1	0	-0.379529	-0.780311	-0.432715
10	6	0	-3.945813	0.262715	0.024782
11	6	0	-5.041922	0.585310	0.833310
12	6	0	-3.883427	-1.030217	-0.539891
13	6	0	-6.043022	-0.332769	1.121274
14	1	0	-5.096680	1.583181	1.259809
15	6	0	-4.897853	-1.952006	-0.246206
16	6	0	-5.961758	-1.612071	0.575203
17	1	0	-6.873592	-0.055203	1.761235
18	1	0	-4.837678	-2.948169	-0.677662
19	1	0	-6.732864	-2.347881	0.782621
20	6	0	-3.357842	2.674728	-0.632137
21	15	0	4.170609	-0.327229	0.092953
22	6	0	4.620283	-2.114112	0.219196
23	6	0	5.219763	0.356474	1.450684
24	6	0	5.194900	0.151240	-1.367182
25	7	0	-2.829647	-1.422220	-1.368951
26	1	0	-3.088640	-2.138537	-2.035895
27	1	0	-2.357115	-0.645972	-1.817173
28	1	0	-2.500774	3.306205	-0.877808
29	1	0	-4.032654	2.636160	-1.493788
30	1	0	-3.909094	3.155325	0.183812
31	1	0	6.261591	0.026821	1.362513
32	1	0	5.183784	1.448844	1.422369
33	1	0	4.820588	0.032050	2.415443
34	1	0	5.706619	-2.261538	0.210616
35	1	0	4.208806	-2.526423	1.144421
36	1	0	4.175859	-2.659553	-0.617658
37	1	0	6.239525	-0.159893	-1.249783
38	1	0	4.781281	-0.310629	-2.267738
39	1	0	5.155320	1.236023	-1.498021

Zero-point correction= 0.330733 (Hartree/Particle)
Thermal correction to Energy= 0.352671
Thermal correction to Enthalpy= 0.353615
Thermal correction to Gibbs Free Energy= 0.275017
Sum of electronic and zero-point Energies= -1068.787494
Sum of electronic and thermal Energies= -1068.765556
Sum of electronic and thermal Enthalpies= -1068.764612
Sum of electronic and thermal Free Energies= -1068.843210
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1069.096454
Frequencies

8.0377	13.4052	24.6456
35.7633	42.4502	65.1238
93.0407	108.6077	126.0067
128.0486	148.2049	157.8327
186.0209	197.0248	204.7454
213.1656	217.8794	222.1346
248.6111	256.0570	262.7314
292.9127	331.9055	336.9817
374.9878	399.2244	441.9152
472.6832	524.0060	566.1029
590.5392	601.0360	673.3159
684.9792	690.3378	730.5913
738.8390	741.2232	764.8611
782.1076	801.4557	804.2145
859.7020	861.3572	863.8892
884.5458	902.2190	958.2953
963.6588	971.8422	974.6354
991.4712	996.6357	1046.0687
1049.4763	1063.9057	1067.4937
1079.7103	1102.7901	1110.5359
1126.4239	1152.5079	1182.1224
1192.3946	1211.2835	1305.2890
1332.8629	1342.4546	1346.1799
1349.1363	1368.7373	1372.2001
1435.5531	1463.9317	1482.2791
1485.5633	1491.6341	1493.3953
1498.8235	1500.6865	1510.5506
1513.5490	1517.9901	1524.1642
1564.1506	1667.5279	1688.2747
1711.6186	1883.8910	3063.3792
3065.5507	3066.8271	3077.4902
3131.0296	3136.4559	3139.2522
3156.1954	3156.5557	3159.3641
3172.9700	3174.3785	3175.9150
3179.5525	3200.2670	3210.5441
3214.5758	3220.8300	3224.0204
3241.1346	3569.0057	3672.6732

TS31

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.662562	0.179151	0.014484
2	6	0	-0.022015	1.583375	0.229193
3	6	0	0.449851	-0.294099	0.093118
4	1	0	-0.335840	1.971129	1.201329
5	1	0	-0.302601	2.207685	-0.622192
6	1	0	0.478285	-0.844337	-0.850393
7	6	0	1.279472	0.908323	0.169455
8	6	0	2.568117	1.243476	0.077578
9	1	0	0.409407	-0.924635	0.984096
10	6	0	3.630880	0.209721	-0.049506
11	6	0	4.566529	0.299255	-1.085837
12	6	0	3.750386	-0.850549	0.874554
13	6	0	5.583445	-0.633474	-1.245647
14	1	0	4.478459	1.119614	-1.793336
15	6	0	4.778752	-1.788835	0.709805
16	6	0	5.682814	-1.684823	-0.336593
17	1	0	6.286564	-0.543108	-2.066728
18	1	0	4.858489	-2.607210	1.421200
19	1	0	6.469244	-2.426388	-0.439918
20	6	0	2.991572	2.690921	0.066412
21	15	0	-3.989827	-0.438283	-0.163675
22	6	0	-4.356853	-2.244794	-0.084575

23	6	0	-4.910568	0.020805	-1.694741
24	6	0	-5.149011	0.194473	1.124568
25	7	0	2.855018	-0.998806	1.937325
26	1	0	3.261752	-1.445762	2.749455
27	1	0	2.374508	-0.139827	2.180574
28	1	0	2.130989	3.348527	0.216985
29	1	0	3.729936	2.889183	0.851106
30	1	0	3.461348	2.962283	-0.886197
31	1	0	-5.949186	-0.326497	-1.659700
32	1	0	-4.898551	1.107387	-1.815385
33	1	0	-4.412403	-0.419554	-2.562636
34	1	0	-5.432303	-2.439154	-0.162551
35	1	0	-3.838768	-2.757162	-0.899519
36	1	0	-3.984350	-2.650572	0.859644
37	1	0	-6.170309	-0.166138	0.958869
38	1	0	-4.806967	-0.131380	2.110470
39	1	0	-5.147450	1.287680	1.111380

Zero-point correction= 0.328321 (Hartree/Particle)
Thermal correction to Energy= 0.349639
Thermal correction to Enthalpy= 0.350583
Thermal correction to Gibbs Free Energy= 0.274764
Sum of electronic and zero-point Energies= -1068.770869
Sum of electronic and thermal Energies= -1068.749551
Sum of electronic and thermal Enthalpies= -1068.748607
Sum of electronic and thermal Free Energies= -1068.824426
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1069.061109
Frequencies

-207.6711	16.2686	18.0872
24.3148	42.8959	52.6301
68.8888	98.3723	122.3042
124.8074	139.6562	148.9982
166.1206	187.4945	207.6638
214.5543	233.2039	233.5875
251.2497	255.6408	297.7466
309.7582	329.4093	359.0173
397.9796	406.4400	453.3645
478.4772	522.1194	528.1573
570.0800	589.9234	599.6782
605.3704	681.4111	688.7817
693.0554	736.8374	739.6054
753.0113	768.2903	770.3345
803.9079	846.1911	863.7992
868.0230	872.9311	903.0242
938.9879	950.6548	959.5969
976.2351	979.7638	984.8252
987.0172	998.8857	1065.7518
1069.4090	1101.5056	1112.2869
1130.6520	1165.9928	1192.0057
1199.7705	1218.3099	1307.8607
1338.7170	1345.3751	1348.3129
1354.4670	1372.1658	1375.1251
1420.8099	1430.5792	1444.2835
1483.4936	1492.9276	1493.5670
1500.3883	1501.0487	1507.7632
1514.4496	1518.2862	1524.3151
1570.1525	1669.1655	1688.6896
1714.3496	1837.4656	3068.2192
3068.5888	3070.6291	3074.4606
3097.6931	3103.7357	3129.6808
3159.1091	3159.5680	3161.2401
3168.1926	3174.0174	3175.1466
3188.8718	3189.9988	3197.2544
3198.1156	3205.5167	3223.7661
3238.9259	3564.2793	3670.2950

INT48

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.621706	1.030170	0.013117
2	6	0	0.145754	2.471596	-0.267064
3	6	0	-0.072192	0.306156	-0.902864
4	1	0	0.394350	2.971817	-1.208340

5	1	0	0.067756	3.166477	0.572118
6	1	0	-0.303953	-0.703987	-0.559726
7	6	0	-0.896371	1.416873	-0.378006
8	6	0	-2.113165	1.344396	0.206543
9	1	0	0.164855	0.347386	-1.969321
10	6	0	-2.900165	0.086368	0.225472
11	6	0	-3.484991	-0.353744	1.419919
12	6	0	-3.138240	-0.672576	-0.944210
13	6	0	-4.244301	-1.515853	1.494339
14	1	0	-3.323605	0.237397	2.318066
15	6	0	-3.899418	-1.845598	-0.864866
16	6	0	-4.445334	-2.267555	0.339418
17	1	0	-4.671904	-1.830869	2.440738
18	1	0	-4.066650	-2.421871	-1.772118
19	1	0	-5.035494	-3.178616	0.370827
20	6	0	-2.664397	2.519451	0.978016
21	15	0	3.064357	-0.976467	0.185605
22	6	0	2.083404	-2.511875	-0.071309
23	6	0	3.965989	-1.376109	1.743169
24	6	0	4.398325	-1.190368	-1.067304
25	7	0	-2.607343	-0.281619	-2.179046
26	1	0	-3.181623	-0.561957	-2.965044
27	1	0	-2.392615	0.710572	-2.208369
28	1	0	-2.244018	3.458277	0.605190
29	1	0	-3.754664	2.569528	0.892364
30	1	0	-2.426495	2.463492	2.049554
31	1	0	4.483188	-2.338405	1.668914
32	1	0	4.698859	-0.593239	1.957250
33	1	0	3.256283	-1.414267	2.573965
34	1	0	2.716260	-3.404518	-0.033438
35	1	0	1.309146	-2.583206	0.697698
36	1	0	1.586278	-2.461658	-1.044258
37	1	0	4.885611	-2.166304	-0.972031
38	1	0	3.968994	-1.099195	-2.068649
39	1	0	5.147635	-0.403290	-0.947065

Zero-point correction= 0.330041 (Hartree/Particle)
Thermal correction to Energy= 0.351193
Thermal correction to Enthalpy= 0.352137
Thermal correction to Gibbs Free Energy= 0.278161
Sum of electronic and zero-point Energies= -1068.780217
Sum of electronic and thermal Energies= -1068.759065
Sum of electronic and thermal Enthalpies= -1068.758121
Sum of electronic and thermal Free Energies= -1068.832097
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1069.087006
Frequencies

18.6607	22.3048	35.4920
55.6644	75.2842	80.1408
110.9538	116.2386	142.7454
156.7037	162.5898	185.0213
186.5465	209.0749	216.2069
227.6033	247.8815	252.5076
259.2971	269.5012	311.0458
322.1053	372.6886	399.3185
420.4990	449.1232	482.1199
498.8980	528.9607	566.6845
586.5713	594.5157	621.2694
679.0854	683.8301	703.3686
720.3167	738.4994	739.9115
747.1326	770.6925	780.8140
805.1770	849.7098	865.3964
871.9682	875.8257	899.6851
949.9551	957.6091	978.5791
981.1685	983.4086	994.8654
1002.8755	1025.0392	1059.0899
1064.7661	1079.0124	1093.9099
1111.9582	1170.9857	1186.6819
1188.6591	1245.3387	1302.8005
1336.5099	1347.6742	1351.2350
1354.7888	1369.4244	1373.8306
1434.4555	1449.4340	1466.5632
1487.0579	1490.7285	1493.6922
1503.7983	1505.1998	1512.8665
1513.4955	1516.6008	1526.2850
1559.0095	1661.5165	1683.9389

1705.7101	1737.8985	3050.1805
3075.6591	3079.0304	3082.3174
3085.6792	3108.8375	3119.4345
3157.8571	3165.4897	3167.7869
3169.8374	3171.2542	3175.5598
3176.0354	3181.7213	3188.0304
3188.2280	3197.8267	3218.7143
3234.7050	3545.4216	3657.7027

TS32

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.530210	-0.923468	-0.067335
2	6	0	-0.102879	-2.502769	-0.448631
3	6	0	0.512940	-0.380862	-1.350316
4	1	0	-0.496302	-2.805919	-1.420411
5	1	0	-0.076342	-3.288296	0.301699
6	1	0	-0.000405	-0.611916	-2.279762
7	6	0	0.896275	-1.482523	-0.437181
8	6	0	1.974335	-1.314783	0.425059
9	1	0	0.425947	0.636357	-0.979163
10	6	0	2.804818	-0.132784	0.341016
11	6	0	2.980065	0.554142	-0.886936
12	6	0	3.533130	0.389460	1.433358
13	6	0	3.739731	1.710321	-1.005237
14	6	0	4.310375	1.531876	1.318301
15	1	0	3.448580	-0.102794	2.397285
16	6	0	4.409555	2.215390	0.103447
17	1	0	3.827213	2.198135	-1.974374
18	1	0	4.836835	1.907196	2.191111
19	1	0	5.009801	3.114623	0.018295
20	6	0	2.173274	-2.280779	1.561566
21	15	0	-2.945528	0.954803	0.217598
22	1	0	1.555114	-2.038575	2.439883
23	1	0	1.904017	-3.297652	1.256623
24	1	0	3.217643	-2.305472	1.889637
25	7	0	2.309098	-0.016708	-2.013142
26	1	0	2.413395	0.531121	-2.864847
27	1	0	2.611403	-0.982648	-2.164949
28	6	0	-4.631691	0.909799	-0.532409
29	6	0	-3.360170	1.457847	1.943765
30	6	0	-2.321662	2.556361	-0.454247
31	1	0	-1.367277	2.800718	0.021368
32	1	0	-2.149115	2.455426	-1.529708
33	1	0	-3.029269	3.374276	-0.279688
34	1	0	-5.189753	0.066246	-0.116487
35	1	0	-5.186392	1.835530	-0.343371
36	1	0	-4.545752	0.755815	-1.611544
37	1	0	-2.436605	1.667255	2.490138
38	1	0	-4.001064	2.346064	1.964101
39	1	0	-3.871374	0.634759	2.450277

Zero-point correction= 0.330536 (Hartree/Particle)
Thermal correction to Energy= 0.350880
Thermal correction to Enthalpy= 0.351824
Thermal correction to Gibbs Free Energy= 0.279480
Sum of electronic and zero-point Energies= -1068.748003
Sum of electronic and thermal Energies= -1068.727659
Sum of electronic and thermal Enthalpies= -1068.726714
Sum of electronic and thermal Free Energies= -1068.799059
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1069.046961
Frequencies

-492.8186	17.6155	21.5129
31.2196	52.8496	73.0965
108.6870	131.7154	136.4148
160.9322	164.8302	170.0725
173.7906	200.6480	203.9559
225.0619	232.1363	250.4462
255.5530	303.6023	315.4477
333.6756	354.0218	379.6850
420.8965	435.8383	478.0916
484.5897	544.1063	581.3392
590.4105	601.5623	681.1604

683.2639	695.3344	720.6692
739.6277	745.2446	751.7666
760.8716	807.6589	814.7960
830.4127	863.9247	870.1772
871.6024	910.1393	931.9133
940.9481	973.0881	978.9231
984.1087	988.3449	991.0649
1031.5757	1044.1926	1063.4375
1078.7820	1093.8205	1115.1624
1133.2114	1174.7914	1185.0364
1197.2598	1256.1474	1314.3986
1340.5981	1345.4886	1347.3760
1370.6417	1381.3327	1394.7426
1439.1039	1472.6245	1483.1486
1489.9987	1492.0859	1494.7309
1498.5803	1500.9675	1514.4667
1519.2873	1523.0567	1529.3254
1546.2447	1596.7614	1631.1159
1647.2008	1707.5995	3034.5502
3067.3559	3069.2982	3078.7945
3105.6871	3124.4088	3143.7112
3158.4600	3159.4260	3167.0934
3168.1847	3170.0547	3172.8421
3181.4199	3190.8304	3204.9943
3223.5915	3227.2071	3235.1250
3274.1044	3436.5603	3571.7157

INT49

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.485005	-0.753845	0.015124
2	6	0	0.017986	-2.511050	0.180264
3	6	0	1.280417	-1.176429	-1.470349
4	1	0	-0.350785	-3.110907	-0.647574
5	1	0	-0.198636	-2.872940	1.179756
6	1	0	0.951446	-1.934882	-2.183709
7	6	0	1.015510	-1.570152	-0.033251
8	6	0	1.787838	-0.889889	0.943034
9	1	0	0.849164	-0.204595	-1.722782
10	6	0	2.731530	0.093542	0.542692
11	6	0	3.245573	0.114158	-0.777904
12	6	0	3.289473	1.110447	1.372786
13	6	0	4.178623	1.006900	-1.272547
14	6	0	4.216620	2.016931	0.896818
15	1	0	2.954085	1.187302	2.401021
16	6	0	4.674977	1.993292	-0.430516
17	1	0	4.518539	0.929877	-2.304418
18	1	0	4.594937	2.778497	1.573051
19	1	0	5.395830	2.717181	-0.790424
20	6	0	1.420137	-1.101122	2.382307
21	15	0	-3.079958	0.864839	-0.106622
22	1	0	0.421225	-0.691745	2.605407
23	1	0	1.378548	-2.171770	2.620753
24	1	0	2.141247	-0.650457	3.068378
25	7	0	2.778310	-1.006495	-1.605498
26	1	0	3.064869	-0.878985	-2.579614
27	1	0	3.198256	-1.878880	-1.246537
28	6	0	-4.663826	0.463283	-0.972371
29	6	0	-3.756729	1.506763	1.488352
30	6	0	-2.685567	2.471240	-0.934996
31	1	0	-1.828835	2.934303	-0.437714
32	1	0	-2.409253	2.283626	-1.976481
33	1	0	-3.535067	3.164068	-0.909208
34	1	0	-5.124844	-0.407318	-0.497867
35	1	0	-5.368773	1.302781	-0.948015
36	1	0	-4.451290	0.202946	-2.013034
37	1	0	-2.942831	1.936227	2.079013
38	1	0	-4.527102	2.269639	1.326551
39	1	0	-4.184663	0.678318	2.059628

Zero-point correction= 0.333669 (Hartree/Particle)
Thermal correction to Energy= 0.354422
Thermal correction to Enthalpy= 0.355367

Thermal correction to Gibbs Free Energy= 0.280761
Sum of electronic and zero-point Energies= -1068.768028
Sum of electronic and thermal Energies= -1068.747275
Sum of electronic and thermal Enthalpies= -1068.746331
Sum of electronic and thermal Free Energies= -1068.820936
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1069.087612
Frequencies

11.7932	16.5792	27.1352
40.6090	56.0738	78.4013
123.4074	132.0189	132.7569
165.1247	168.4652	178.1304
184.9518	193.2751	210.6798
211.5698	252.7710	262.2482
273.7017	320.4514	322.5622
332.5583	367.1645	401.6606
432.6050	460.0464	487.1035
528.7378	568.6176	584.0376
651.6433	677.3864	680.6279
697.0841	723.8487	728.1226
736.3971	737.6771	745.9561
795.3436	797.7205	852.6754
857.4666	859.1025	863.3550
914.2450	930.4106	956.4067
970.3069	972.5971	985.8272
996.1365	1002.5788	1040.8906
1061.8828	1071.6421	1080.9302
1133.1603	1169.4617	1188.3779
1205.1400	1234.5903	1254.9884
1305.3667	1341.9447	1344.9687
1354.0021	1366.6359	1385.2966
1398.4664	1421.5026	1431.1933
1447.8015	1471.5495	1484.0756
1490.9287	1492.9439	1496.3064
1499.0739	1502.2897	1510.6156
1512.3365	1529.7844	1539.0628
1560.4522	1591.4654	1619.6981
1627.9140	1707.8149	3025.0644
3062.3045	3064.2232	3069.4319
3086.5615	3129.8227	3153.3833
3154.8198	3159.0836	3159.9051
3170.2111	3172.0265	3172.6602
3176.2961	3178.9201	3196.3563
3213.6647	3237.1750	3259.0697
3260.5157	3338.4117	3491.1799

TS33

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.906417	-0.068393	-0.875174
2	6	0	-0.621970	-2.206393	-0.381566
3	6	0	0.829144	-0.994555	-1.736029
4	1	0	-1.007086	-2.757613	-1.236039
5	1	0	-1.022147	-2.501551	0.586046
6	1	0	1.666692	-0.329198	-1.924083
7	6	0	0.681815	-1.614788	-0.461196
8	6	0	1.450627	-1.198909	0.709895
9	1	0	0.361932	-1.459946	-2.602217
10	1	0	0.689262	-0.001489	0.988055
11	6	0	2.580895	-0.274270	0.399279
12	6	0	2.135872	1.073714	0.249713
13	6	0	3.938743	-0.559194	0.321505
14	6	0	3.068833	2.085442	0.001379
15	6	0	4.864924	0.456153	0.074949
16	1	0	4.278155	-1.584384	0.453805
17	6	0	4.422839	1.768414	-0.086470
18	1	0	2.735782	3.113872	-0.114883
19	1	0	5.923320	0.224999	0.005389
20	1	0	5.142568	2.559320	-0.279756
21	6	0	1.674080	-2.234818	1.797057
22	15	0	-2.879751	0.470460	0.345822
23	6	0	-3.642354	2.128575	0.116861
24	6	0	-2.465759	0.476913	2.136443
25	6	0	-4.343223	-0.639973	0.289223

26	1	0	1.999495	-1.753314	2.724370
27	1	0	0.757271	-2.792341	2.020358
28	1	0	2.441582	-2.976206	1.529884
29	7	0	0.762058	1.206765	0.430734
30	1	0	0.500611	2.102563	0.833910
31	1	0	-1.633635	1.165726	2.307256
32	1	0	-3.321653	0.769527	2.753366
33	1	0	-2.130476	-0.522588	2.428224
34	1	0	-4.027184	-1.659490	0.526553
35	1	0	-5.112355	-0.324522	1.001873
36	1	0	-4.765301	-0.641305	-0.719275
37	1	0	-4.036002	2.216870	-0.899237
38	1	0	-4.453572	2.297514	0.832418
39	1	0	-2.877022	2.897480	0.253250

Zero-point correction= 0.325114 (Hartree/Particle)
Thermal correction to Energy= 0.345521
Thermal correction to Enthalpy= 0.346465
Thermal correction to Gibbs Free Energy= 0.275737
Sum of electronic and zero-point Energies= -1068.730553
Sum of electronic and thermal Energies= -1068.710146
Sum of electronic and thermal Enthalpies= -1068.709202
Sum of electronic and thermal Free Energies= -1068.779930
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1069.02709
Frequencies

-1604.7964	24.4351	42.1164
44.6961	75.4723	104.5899
105.3683	116.0175	135.7315
161.6706	166.1291	172.5100
179.2888	181.9288	204.0997
219.7115	220.7886	248.2768
252.9806	269.6242	301.2467
319.4784	341.2843	349.3708
369.3548	475.2354	493.9401
506.4783	543.8290	578.9149
596.0080	614.0078	663.5786
688.2329	696.2080	731.2487
750.1253	753.7225	757.0990
771.3505	777.8849	792.9629
805.7597	854.2602	866.9528
871.7627	878.7847	888.1501
940.9563	948.7421	956.1733
979.3388	980.2463	983.0304
994.5141	997.1499	1035.0630
1060.9504	1074.2162	1079.8381
1124.3829	1170.6370	1181.8378
1185.3334	1278.2794	1305.9249
1324.4948	1345.9413	1348.6236
1351.8983	1367.1858	1373.8484
1413.3783	1440.2827	1479.2214
1482.1930	1484.4919	1489.2130
1497.5797	1501.2026	1508.8780
1511.1578	1516.0416	1520.7874
1533.1645	1533.7098	1549.3393
1651.7191	1697.7909	1806.0554
3037.9093	3075.3645	3077.9468
3079.9080	3103.8261	3141.1059
3158.3790	3164.4383	3166.3773
3168.4715	3169.7024	3174.2162
3175.9111	3181.2009	3187.8498
3191.6204	3208.1754	3224.2090
3249.9448	3262.2029	3542.4060

INT50

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.829977	0.360047	-0.752783
2	6	0	0.577738	2.544965	-0.237362
3	6	0	-0.894437	1.330767	-1.676565
4	1	0	0.941172	3.162785	-1.053401
5	1	0	0.912463	2.828144	0.757318
6	1	0	-1.735069	0.668768	-1.852195
7	6	0	-0.644811	1.837520	-0.390715

8	6	0	-1.406952	1.264016	0.813713
9	1	0	-0.449547	1.817888	-2.541856
10	1	0	-0.629118	0.930503	1.520255
11	6	0	-2.262776	0.045980	0.463165
12	6	0	-1.689769	-1.167816	-0.055405
13	6	0	-3.646153	0.106728	0.647890
14	6	0	-2.593206	-2.215786	-0.365363
15	6	0	-4.503833	-0.948876	0.356998
16	1	0	-4.081762	1.020567	1.037914
17	6	0	-3.956924	-2.121816	-0.156565
18	1	0	-2.175982	-3.133880	-0.774597
19	1	0	-5.571243	-0.851080	0.522758
20	1	0	-4.594790	-2.966180	-0.404205
21	6	0	-2.163368	2.412117	1.492762
22	15	0	2.692716	-0.559039	0.391301
23	6	0	3.122833	-2.252826	-0.172681
24	6	0	2.170768	-0.858935	2.122918
25	6	0	4.338110	0.239664	0.578387
26	1	0	-2.664986	2.072472	2.402837
27	1	0	-1.460231	3.205806	1.762033
28	1	0	-2.912564	2.844136	0.821891
29	7	0	-0.339230	-1.360745	-0.231098
30	1	0	-0.192102	-2.254962	-0.692543
31	1	0	1.212009	-1.384591	2.077901
32	1	0	2.908417	-1.450864	2.674511
33	1	0	2.019972	0.098595	2.629868
34	1	0	4.207397	1.229224	1.024340
35	1	0	4.999775	-0.358125	1.213678
36	1	0	4.800699	0.366315	-0.403940
37	1	0	3.524219	-2.220650	-1.188852
38	1	0	3.856069	-2.720678	0.492263
39	1	0	2.206823	-2.849797	-0.176829

Zero-point correction= 0.331868 (Hartree/Particle)
Thermal correction to Energy= 0.351767
Thermal correction to Enthalpy= 0.352711
Thermal correction to Gibbs Free Energy= 0.283882
Sum of electronic and zero-point Energies= -1068.787855
Sum of electronic and thermal Energies= -1068.767956
Sum of electronic and thermal Enthalpies= -1068.767012
Sum of electronic and thermal Free Energies= -1068.835841
M06-2x/6-311++G(d,p)-LANL2DZ // M06-2x /6-31G(d)-LANL2DZ energy= -1069.084277
Frequencies

26.8023	45.2532	50.7134
92.1456	104.2388	115.2551
131.6567	150.6425	159.7948
175.8585	220.9700	221.3342
234.7001	239.9392	255.9814
258.4517	262.5982	280.6886
295.6655	313.9461	317.6667
339.1754	352.0816	358.6219
415.5967	465.0120	495.2516
539.3030	574.5703	595.7716
633.9562	659.3393	681.9245
692.3697	723.8380	735.3095
747.7993	755.9898	770.1641
782.2004	807.3554	817.0705
823.7050	867.1872	874.9653
875.1295	876.9564	887.8118
955.3273	970.6967	983.4101
985.5232	989.2293	989.6934
1000.2225	1032.2317	1046.5495
1081.1743	1091.0730	1114.8957
1154.2215	1195.6341	1219.5331
1236.1946	1286.9039	1322.3493
1340.3933	1346.5491	1351.7113
1364.1507	1368.8475	1377.9672
1391.1287	1408.1241	1429.4185
1482.3594	1492.3270	1495.8197
1497.5246	1500.8984	1504.7810
1515.6770	1525.2727	1530.2761
1536.7753	1548.8153	1557.9599
1641.9583	1696.0439	3026.7949
3070.0569	3077.8920	3079.7740
3086.9553	3152.5901	3163.5781

3166.7135	3168.9537	3169.1317
3173.4253	3176.8900	3177.6561
3183.9326	3187.8190	3188.0435
3211.9500	3227.4798	3244.2905
3256.8892	3278.4175	3541.6473